Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 03:57 AM JST

PDB ID	:	6K33
EMDB ID	:	EMD-9908
Title	:	Structure of PSI-isiA supercomplex from Thermosynechococcus vulcanus
Authors	:	Akita, F.; Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.
Deposited on	:	2019-05-16
Resolution	:	2.74 Å(reported)
Based on initial model	:	1JB0

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

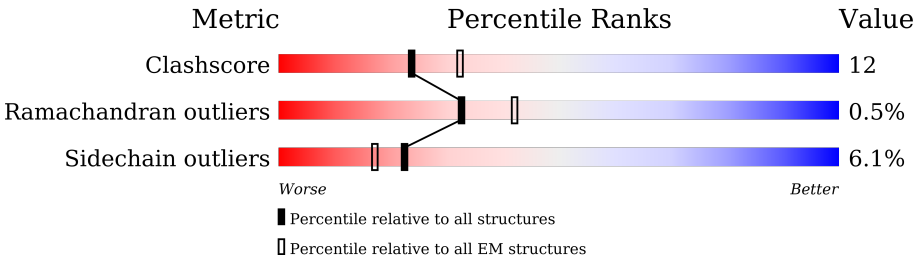
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



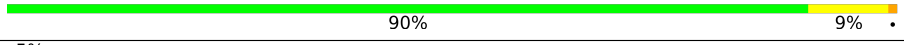
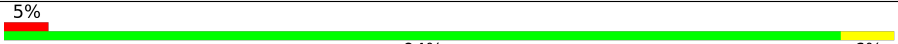
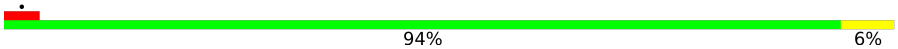
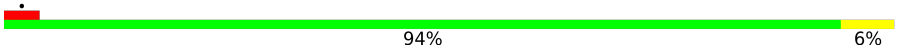
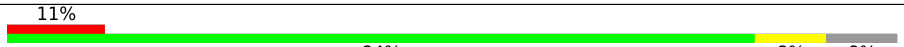
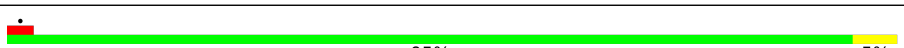
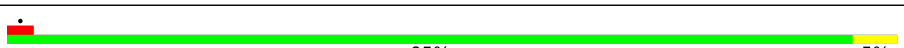
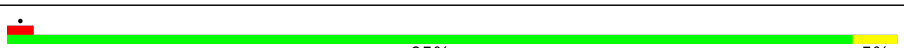
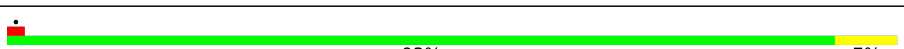
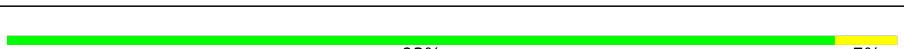
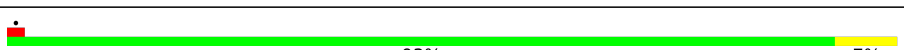
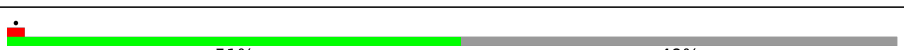
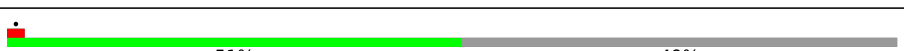
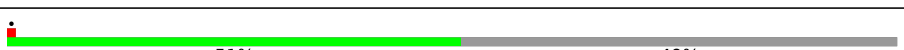
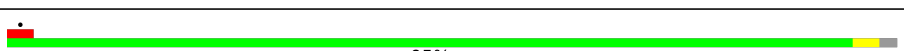
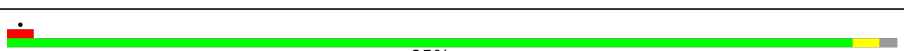
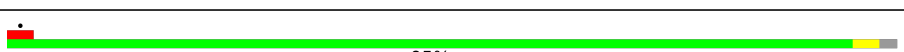
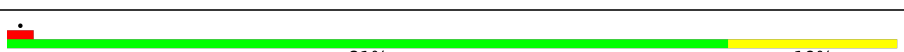
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	aA	755	94% 5%
1	bA	755	94% 5%
1	cA	755	94% 5%
2	aB	740	96%
2	bB	740	96%
2	cB	740	96%
3	aC	80	90% 9%
3	bC	80	90% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	cC	80	
4	aD	138	
4	bD	138	
4	cD	138	
5	aE	75	
5	bE	75	
5	cE	75	
6	aF	164	
6	bF	164	
6	cF	164	
7	aI	38	
7	bI	38	
7	cI	38	
8	aJ	41	
8	bJ	41	
8	cJ	41	
9	aK	85	
9	bK	85	
9	cK	85	
10	aL	154	
10	bL	154	
10	cL	154	
11	aM	31	
11	bM	31	
11	cM	31	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	aX	35	80% 17%
12	bX	35	80% 17%
12	cX	35	80% 17%
13	a1	358	48% 84% 7% 8%
13	a2	358	52% 84% 7% 9%
13	a3	358	37% 85% 8% 7%
13	a4	358	41% 86% 7% 6%
13	a5	358	48% 85% 7% 7%
13	a6	358	54% 84% 8% 8%
13	b1	358	49% 84% 7% 8%
13	b2	358	53% 84% 7% 9%
13	b3	358	38% 85% 8% 7%
13	b4	358	39% 86% 8% 6%
13	b5	358	48% 85% 7% 7%
13	b6	358	53% 84% 8% 8%
13	c1	358	50% 85% 7% 8%
13	c2	358	52% 84% 7% 9%
13	c3	358	39% 85% 8% 7%
13	c4	358	40% 86% 8% 6%
13	c5	358	48% 85% 7% 7%
13	c6	358	54% 84% 7% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL0	aA	801	X	-	-	-
14	CL0	bA	801	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL0	cA	801	X	-	-	-
15	CLA	a1	401	X	-	-	-
15	CLA	a1	402	X	-	-	-
15	CLA	a1	403	X	-	-	-
15	CLA	a1	404	X	-	-	-
15	CLA	a1	405	X	-	-	-
15	CLA	a1	406	X	-	-	-
15	CLA	a1	407	X	-	-	-
15	CLA	a1	408	X	-	-	-
15	CLA	a1	409	X	-	-	-
15	CLA	a1	410	X	-	-	-
15	CLA	a1	411	X	-	-	-
15	CLA	a1	412	X	-	-	-
15	CLA	a1	413	X	-	-	-
15	CLA	a1	415	X	-	-	-
15	CLA	a1	416	X	-	-	-
15	CLA	a1	422	X	-	-	-
15	CLA	a2	402	X	-	-	-
15	CLA	a2	403	X	-	-	-
15	CLA	a2	404	X	-	-	-
15	CLA	a2	405	X	-	-	-
15	CLA	a2	406	X	-	-	-
15	CLA	a2	407	X	-	-	-
15	CLA	a2	408	X	-	-	-
15	CLA	a2	409	X	-	-	-
15	CLA	a2	410	X	-	-	-
15	CLA	a2	411	X	-	-	-
15	CLA	a2	412	X	-	-	-
15	CLA	a2	413	X	-	-	-
15	CLA	a2	414	X	-	-	-
15	CLA	a2	415	X	-	-	-
15	CLA	a2	417	X	-	-	-
15	CLA	a2	418	X	-	-	-
15	CLA	a2	422	X	-	-	-
15	CLA	a3	402	X	-	-	-
15	CLA	a3	403	X	-	-	-
15	CLA	a3	404	X	-	-	-
15	CLA	a3	405	X	-	-	-
15	CLA	a3	406	X	-	-	-
15	CLA	a3	407	X	-	-	-
15	CLA	a3	408	X	-	-	-
15	CLA	a3	409	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a3	410	X	-	-	-
15	CLA	a3	411	X	-	-	-
15	CLA	a3	412	X	-	-	-
15	CLA	a3	413	X	-	-	-
15	CLA	a3	414	X	-	-	-
15	CLA	a3	416	X	-	-	-
15	CLA	a3	417	X	-	-	-
15	CLA	a3	421	X	-	-	-
15	CLA	a4	402	X	-	-	-
15	CLA	a4	403	X	-	-	-
15	CLA	a4	404	X	-	-	-
15	CLA	a4	405	X	-	-	-
15	CLA	a4	406	X	-	-	-
15	CLA	a4	407	X	-	-	-
15	CLA	a4	408	X	-	-	-
15	CLA	a4	409	X	-	-	-
15	CLA	a4	410	X	-	-	-
15	CLA	a4	411	X	-	-	-
15	CLA	a4	412	X	-	-	-
15	CLA	a4	413	X	-	-	-
15	CLA	a4	414	X	-	-	-
15	CLA	a4	416	X	-	-	-
15	CLA	a4	417	X	-	-	-
15	CLA	a4	421	X	-	-	-
15	CLA	a5	402	X	-	-	-
15	CLA	a5	403	X	-	-	-
15	CLA	a5	404	X	-	-	-
15	CLA	a5	405	X	-	-	-
15	CLA	a5	406	X	-	-	-
15	CLA	a5	407	X	-	-	-
15	CLA	a5	408	X	-	-	-
15	CLA	a5	409	X	-	-	-
15	CLA	a5	410	X	-	-	-
15	CLA	a5	411	X	-	-	-
15	CLA	a5	412	X	-	-	-
15	CLA	a5	413	X	-	-	-
15	CLA	a5	414	X	-	-	-
15	CLA	a5	416	X	-	-	-
15	CLA	a5	417	X	-	-	-
15	CLA	a5	420	X	-	-	-
15	CLA	a6	403	X	-	-	-
15	CLA	a6	404	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a6	405	X	-	-	-
15	CLA	a6	406	X	-	-	-
15	CLA	a6	407	X	-	-	-
15	CLA	a6	408	X	-	-	-
15	CLA	a6	409	X	-	-	-
15	CLA	a6	410	X	-	-	-
15	CLA	a6	411	X	-	-	-
15	CLA	a6	412	X	-	-	-
15	CLA	a6	413	X	-	-	-
15	CLA	a6	414	X	-	-	-
15	CLA	a6	415	X	-	-	-
15	CLA	a6	417	X	-	-	-
15	CLA	a6	418	X	-	-	-
15	CLA	a6	422	X	-	-	-
15	CLA	aA	802	X	-	-	-
15	CLA	aA	803	X	-	-	-
15	CLA	aA	804	X	-	-	-
15	CLA	aA	805	X	-	-	-
15	CLA	aA	806	X	-	-	-
15	CLA	aA	807	X	-	-	-
15	CLA	aA	809	X	-	-	-
15	CLA	aA	810	X	-	-	-
15	CLA	aA	811	X	-	-	-
15	CLA	aA	812	X	-	-	-
15	CLA	aA	813	X	-	-	-
15	CLA	aA	814	X	-	-	-
15	CLA	aA	815	X	-	-	-
15	CLA	aA	818	X	-	-	-
15	CLA	aA	819	X	-	-	-
15	CLA	aA	820	X	-	-	-
15	CLA	aA	821	X	-	-	-
15	CLA	aA	822	X	-	-	-
15	CLA	aA	823	X	-	-	-
15	CLA	aA	824	X	-	-	-
15	CLA	aA	825	X	-	-	-
15	CLA	aA	826	X	-	-	-
15	CLA	aA	827	X	-	-	-
15	CLA	aA	828	X	-	-	-
15	CLA	aA	829	X	-	-	-
15	CLA	aA	830	X	-	-	-
15	CLA	aA	831	X	-	-	-
15	CLA	aA	832	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	aA	833	X	-	-	-
15	CLA	aA	834	X	-	-	-
15	CLA	aA	835	X	-	-	-
15	CLA	aA	836	X	-	-	-
15	CLA	aA	838	X	-	-	-
15	CLA	aA	839	X	-	-	-
15	CLA	aA	840	X	-	-	-
15	CLA	aA	841	X	-	-	-
15	CLA	aA	842	X	-	-	-
15	CLA	aA	843	X	-	-	-
15	CLA	aA	844	X	-	-	-
15	CLA	aA	845	X	-	-	-
15	CLA	aB	801	X	-	-	-
15	CLA	aB	802	X	-	-	-
15	CLA	aB	803	X	-	-	-
15	CLA	aB	804	X	-	-	-
15	CLA	aB	805	X	-	-	-
15	CLA	aB	806	X	-	-	-
15	CLA	aB	807	X	-	-	-
15	CLA	aB	809	X	-	-	-
15	CLA	aB	810	X	-	-	-
15	CLA	aB	811	X	-	-	-
15	CLA	aB	812	X	-	-	-
15	CLA	aB	813	X	-	-	-
15	CLA	aB	814	X	-	-	-
15	CLA	aB	815	X	-	-	-
15	CLA	aB	816	X	-	-	-
15	CLA	aB	817	X	-	-	-
15	CLA	aB	818	X	-	-	-
15	CLA	aB	819	X	-	-	-
15	CLA	aB	820	X	-	-	-
15	CLA	aB	821	X	-	-	-
15	CLA	aB	822	X	-	-	-
15	CLA	aB	823	X	-	-	-
15	CLA	aB	824	X	-	-	-
15	CLA	aB	825	X	-	-	-
15	CLA	aB	826	X	-	-	-
15	CLA	aB	827	X	-	-	-
15	CLA	aB	828	X	-	-	-
15	CLA	aB	829	X	-	-	-
15	CLA	aB	830	X	-	-	-
15	CLA	aB	831	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	aB	832	X	-	-	-
15	CLA	aB	833	X	-	-	-
15	CLA	aB	834	X	-	-	-
15	CLA	aB	835	X	-	-	-
15	CLA	aB	836	X	-	-	-
15	CLA	aB	837	X	-	-	-
15	CLA	aB	838	X	-	-	-
15	CLA	aB	839	X	-	-	-
15	CLA	aB	840	X	-	-	-
15	CLA	aB	841	X	-	-	-
15	CLA	aJ	201	X	-	-	-
15	CLA	aJ	202	X	-	-	-
15	CLA	aJ	203	X	-	-	-
15	CLA	aK	102	X	-	-	-
15	CLA	aL	201	X	-	-	-
15	CLA	aL	202	X	-	-	-
15	CLA	aL	203	X	-	-	-
15	CLA	aX	102	X	-	-	-
15	CLA	b1	402	X	-	-	-
15	CLA	b1	403	X	-	-	-
15	CLA	b1	404	X	-	-	-
15	CLA	b1	405	X	-	-	-
15	CLA	b1	406	X	-	-	-
15	CLA	b1	407	X	-	-	-
15	CLA	b1	408	X	-	-	-
15	CLA	b1	409	X	-	-	-
15	CLA	b1	410	X	-	-	-
15	CLA	b1	411	X	-	-	-
15	CLA	b1	412	X	-	-	-
15	CLA	b1	413	X	-	-	-
15	CLA	b1	414	X	-	-	-
15	CLA	b1	416	X	-	-	-
15	CLA	b1	417	X	-	-	-
15	CLA	b2	402	X	-	-	-
15	CLA	b2	403	X	-	-	-
15	CLA	b2	404	X	-	-	-
15	CLA	b2	405	X	-	-	-
15	CLA	b2	406	X	-	-	-
15	CLA	b2	407	X	-	-	-
15	CLA	b2	408	X	-	-	-
15	CLA	b2	409	X	-	-	-
15	CLA	b2	410	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b2	411	X	-	-	-
15	CLA	b2	412	X	-	-	-
15	CLA	b2	413	X	-	-	-
15	CLA	b2	414	X	-	-	-
15	CLA	b2	415	X	-	-	-
15	CLA	b2	417	X	-	-	-
15	CLA	b2	418	X	-	-	-
15	CLA	b2	422	X	-	-	-
15	CLA	b3	402	X	-	-	-
15	CLA	b3	403	X	-	-	-
15	CLA	b3	404	X	-	-	-
15	CLA	b3	405	X	-	-	-
15	CLA	b3	406	X	-	-	-
15	CLA	b3	407	X	-	-	-
15	CLA	b3	408	X	-	-	-
15	CLA	b3	409	X	-	-	-
15	CLA	b3	410	X	-	-	-
15	CLA	b3	411	X	-	-	-
15	CLA	b3	412	X	-	-	-
15	CLA	b3	413	X	-	-	-
15	CLA	b3	414	X	-	-	-
15	CLA	b3	416	X	-	-	-
15	CLA	b3	417	X	-	-	-
15	CLA	b3	421	X	-	-	-
15	CLA	b4	402	X	-	-	-
15	CLA	b4	403	X	-	-	-
15	CLA	b4	404	X	-	-	-
15	CLA	b4	405	X	-	-	-
15	CLA	b4	406	X	-	-	-
15	CLA	b4	407	X	-	-	-
15	CLA	b4	408	X	-	-	-
15	CLA	b4	409	X	-	-	-
15	CLA	b4	410	X	-	-	-
15	CLA	b4	411	X	-	-	-
15	CLA	b4	412	X	-	-	-
15	CLA	b4	413	X	-	-	-
15	CLA	b4	414	X	-	-	-
15	CLA	b4	416	X	-	-	-
15	CLA	b4	417	X	-	-	-
15	CLA	b4	421	X	-	-	-
15	CLA	b5	402	X	-	-	-
15	CLA	b5	403	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b5	404	X	-	-	-
15	CLA	b5	405	X	-	-	-
15	CLA	b5	406	X	-	-	-
15	CLA	b5	407	X	-	-	-
15	CLA	b5	408	X	-	-	-
15	CLA	b5	409	X	-	-	-
15	CLA	b5	410	X	-	-	-
15	CLA	b5	411	X	-	-	-
15	CLA	b5	412	X	-	-	-
15	CLA	b5	413	X	-	-	-
15	CLA	b5	414	X	-	-	-
15	CLA	b5	416	X	-	-	-
15	CLA	b5	417	X	-	-	-
15	CLA	b5	420	X	-	-	-
15	CLA	b6	403	X	-	-	-
15	CLA	b6	404	X	-	-	-
15	CLA	b6	405	X	-	-	-
15	CLA	b6	406	X	-	-	-
15	CLA	b6	407	X	-	-	-
15	CLA	b6	408	X	-	-	-
15	CLA	b6	409	X	-	-	-
15	CLA	b6	410	X	-	-	-
15	CLA	b6	411	X	-	-	-
15	CLA	b6	412	X	-	-	-
15	CLA	b6	413	X	-	-	-
15	CLA	b6	414	X	-	-	-
15	CLA	b6	415	X	-	-	-
15	CLA	b6	417	X	-	-	-
15	CLA	b6	418	X	-	-	-
15	CLA	b6	422	X	-	-	-
15	CLA	bA	802	X	-	-	-
15	CLA	bA	803	X	-	-	-
15	CLA	bA	804	X	-	-	-
15	CLA	bA	805	X	-	-	-
15	CLA	bA	806	X	-	-	-
15	CLA	bA	807	X	-	-	-
15	CLA	bA	809	X	-	-	-
15	CLA	bA	810	X	-	-	-
15	CLA	bA	811	X	-	-	-
15	CLA	bA	812	X	-	-	-
15	CLA	bA	813	X	-	-	-
15	CLA	bA	814	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	bA	815	X	-	-	-
15	CLA	bA	818	X	-	-	-
15	CLA	bA	819	X	-	-	-
15	CLA	bA	820	X	-	-	-
15	CLA	bA	821	X	-	-	-
15	CLA	bA	822	X	-	-	-
15	CLA	bA	823	X	-	-	-
15	CLA	bA	824	X	-	-	-
15	CLA	bA	825	X	-	-	-
15	CLA	bA	826	X	-	-	-
15	CLA	bA	827	X	-	-	-
15	CLA	bA	828	X	-	-	-
15	CLA	bA	829	X	-	-	-
15	CLA	bA	830	X	-	-	-
15	CLA	bA	831	X	-	-	-
15	CLA	bA	832	X	-	-	-
15	CLA	bA	833	X	-	-	-
15	CLA	bA	834	X	-	-	-
15	CLA	bA	835	X	-	-	-
15	CLA	bA	836	X	-	-	-
15	CLA	bA	838	X	-	-	-
15	CLA	bA	839	X	-	-	-
15	CLA	bA	840	X	-	-	-
15	CLA	bA	841	X	-	-	-
15	CLA	bA	842	X	-	-	-
15	CLA	bA	843	X	-	-	-
15	CLA	bA	844	X	-	-	-
15	CLA	bA	845	X	-	-	-
15	CLA	bB	801	X	-	-	-
15	CLA	bB	802	X	-	-	-
15	CLA	bB	803	X	-	-	-
15	CLA	bB	804	X	-	-	-
15	CLA	bB	805	X	-	-	-
15	CLA	bB	806	X	-	-	-
15	CLA	bB	807	X	-	-	-
15	CLA	bB	809	X	-	-	-
15	CLA	bB	810	X	-	-	-
15	CLA	bB	811	X	-	-	-
15	CLA	bB	812	X	-	-	-
15	CLA	bB	813	X	-	-	-
15	CLA	bB	814	X	-	-	-
15	CLA	bB	815	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	bB	816	X	-	-	-
15	CLA	bB	817	X	-	-	-
15	CLA	bB	818	X	-	-	-
15	CLA	bB	819	X	-	-	-
15	CLA	bB	820	X	-	-	-
15	CLA	bB	821	X	-	-	-
15	CLA	bB	822	X	-	-	-
15	CLA	bB	823	X	-	-	-
15	CLA	bB	824	X	-	-	-
15	CLA	bB	825	X	-	-	-
15	CLA	bB	826	X	-	-	-
15	CLA	bB	827	X	-	-	-
15	CLA	bB	828	X	-	-	-
15	CLA	bB	829	X	-	-	-
15	CLA	bB	830	X	-	-	-
15	CLA	bB	831	X	-	-	-
15	CLA	bB	832	X	-	-	-
15	CLA	bB	833	X	-	-	-
15	CLA	bB	834	X	-	-	-
15	CLA	bB	835	X	-	-	-
15	CLA	bB	836	X	-	-	-
15	CLA	bB	837	X	-	-	-
15	CLA	bB	838	X	-	-	-
15	CLA	bB	839	X	-	-	-
15	CLA	bB	840	X	-	-	-
15	CLA	bB	841	X	-	-	-
15	CLA	bF	201	X	-	-	-
15	CLA	bJ	101	X	-	-	-
15	CLA	bJ	102	X	-	-	-
15	CLA	bK	101	X	-	-	-
15	CLA	bL	202	X	-	-	-
15	CLA	bL	203	X	-	-	-
15	CLA	bL	204	X	-	-	-
15	CLA	bX	102	X	-	-	-
15	CLA	c1	402	X	-	-	-
15	CLA	c1	403	X	-	-	-
15	CLA	c1	404	X	-	-	-
15	CLA	c1	405	X	-	-	-
15	CLA	c1	406	X	-	-	-
15	CLA	c1	407	X	-	-	-
15	CLA	c1	408	X	-	-	-
15	CLA	c1	409	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	c1	410	X	-	-	-
15	CLA	c1	411	X	-	-	-
15	CLA	c1	412	X	-	-	-
15	CLA	c1	413	X	-	-	-
15	CLA	c1	414	X	-	-	-
15	CLA	c1	416	X	-	-	-
15	CLA	c1	417	X	-	-	-
15	CLA	c2	402	X	-	-	-
15	CLA	c2	403	X	-	-	-
15	CLA	c2	404	X	-	-	-
15	CLA	c2	405	X	-	-	-
15	CLA	c2	406	X	-	-	-
15	CLA	c2	407	X	-	-	-
15	CLA	c2	408	X	-	-	-
15	CLA	c2	409	X	-	-	-
15	CLA	c2	410	X	-	-	-
15	CLA	c2	411	X	-	-	-
15	CLA	c2	412	X	-	-	-
15	CLA	c2	413	X	-	-	-
15	CLA	c2	414	X	-	-	-
15	CLA	c2	415	X	-	-	-
15	CLA	c2	417	X	-	-	-
15	CLA	c2	418	X	-	-	-
15	CLA	c2	422	X	-	-	-
15	CLA	c3	402	X	-	-	-
15	CLA	c3	403	X	-	-	-
15	CLA	c3	404	X	-	-	-
15	CLA	c3	405	X	-	-	-
15	CLA	c3	406	X	-	-	-
15	CLA	c3	407	X	-	-	-
15	CLA	c3	408	X	-	-	-
15	CLA	c3	410	X	-	-	-
15	CLA	c3	411	X	-	-	-
15	CLA	c3	412	X	-	-	-
15	CLA	c3	413	X	-	-	-
15	CLA	c3	414	X	-	-	-
15	CLA	c3	416	X	-	-	-
15	CLA	c3	417	X	-	-	-
15	CLA	c3	421	X	-	-	-
15	CLA	c4	402	X	-	-	-
15	CLA	c4	403	X	-	-	-
15	CLA	c4	404	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	c4	405	X	-	-	-
15	CLA	c4	406	X	-	-	-
15	CLA	c4	407	X	-	-	-
15	CLA	c4	408	X	-	-	-
15	CLA	c4	409	X	-	-	-
15	CLA	c4	410	X	-	-	-
15	CLA	c4	411	X	-	-	-
15	CLA	c4	412	X	-	-	-
15	CLA	c4	413	X	-	-	-
15	CLA	c4	414	X	-	-	-
15	CLA	c4	416	X	-	-	-
15	CLA	c4	417	X	-	-	-
15	CLA	c4	421	X	-	-	-
15	CLA	c5	402	X	-	-	-
15	CLA	c5	403	X	-	-	-
15	CLA	c5	404	X	-	-	-
15	CLA	c5	405	X	-	-	-
15	CLA	c5	406	X	-	-	-
15	CLA	c5	407	X	-	-	-
15	CLA	c5	408	X	-	-	-
15	CLA	c5	409	X	-	-	-
15	CLA	c5	410	X	-	-	-
15	CLA	c5	411	X	-	-	-
15	CLA	c5	412	X	-	-	-
15	CLA	c5	413	X	-	-	-
15	CLA	c5	414	X	-	-	-
15	CLA	c5	416	X	-	-	-
15	CLA	c5	417	X	-	-	-
15	CLA	c5	420	X	-	-	-
15	CLA	c6	403	X	-	-	-
15	CLA	c6	404	X	-	-	-
15	CLA	c6	405	X	-	-	-
15	CLA	c6	406	X	-	-	-
15	CLA	c6	407	X	-	-	-
15	CLA	c6	408	X	-	-	-
15	CLA	c6	409	X	-	-	-
15	CLA	c6	410	X	-	-	-
15	CLA	c6	411	X	-	-	-
15	CLA	c6	412	X	-	-	-
15	CLA	c6	413	X	-	-	-
15	CLA	c6	414	X	-	-	-
15	CLA	c6	415	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	c6	417	X	-	-	-
15	CLA	c6	418	X	-	-	-
15	CLA	cA	802	X	-	-	-
15	CLA	cA	803	X	-	-	-
15	CLA	cA	804	X	-	-	-
15	CLA	cA	805	X	-	-	-
15	CLA	cA	806	X	-	-	-
15	CLA	cA	807	X	-	-	-
15	CLA	cA	809	X	-	-	-
15	CLA	cA	810	X	-	-	-
15	CLA	cA	811	X	-	-	-
15	CLA	cA	812	X	-	-	-
15	CLA	cA	813	X	-	-	-
15	CLA	cA	814	X	-	-	-
15	CLA	cA	815	X	-	-	-
15	CLA	cA	818	X	-	-	-
15	CLA	cA	819	X	-	-	-
15	CLA	cA	820	X	-	-	-
15	CLA	cA	821	X	-	-	-
15	CLA	cA	822	X	-	-	-
15	CLA	cA	823	X	-	-	-
15	CLA	cA	824	X	-	-	-
15	CLA	cA	825	X	-	-	-
15	CLA	cA	826	X	-	-	-
15	CLA	cA	827	X	-	-	-
15	CLA	cA	828	X	-	-	-
15	CLA	cA	829	X	-	-	-
15	CLA	cA	830	X	-	-	-
15	CLA	cA	831	X	-	-	-
15	CLA	cA	832	X	-	-	-
15	CLA	cA	833	X	-	-	-
15	CLA	cA	834	X	-	-	-
15	CLA	cA	835	X	-	-	-
15	CLA	cA	836	X	-	-	-
15	CLA	cA	838	X	-	-	-
15	CLA	cA	839	X	-	-	-
15	CLA	cA	840	X	-	-	-
15	CLA	cA	841	X	-	-	-
15	CLA	cA	842	X	-	-	-
15	CLA	cA	843	X	-	-	-
15	CLA	cA	844	X	-	-	-
15	CLA	cB	801	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	cB	802	X	-	-	-
15	CLA	cB	803	X	-	-	-
15	CLA	cB	804	X	-	-	-
15	CLA	cB	805	X	-	-	-
15	CLA	cB	806	X	-	-	-
15	CLA	cB	807	X	-	-	-
15	CLA	cB	809	X	-	-	-
15	CLA	cB	810	X	-	-	-
15	CLA	cB	811	X	-	-	-
15	CLA	cB	812	X	-	-	-
15	CLA	cB	813	X	-	-	-
15	CLA	cB	814	X	-	-	-
15	CLA	cB	815	X	-	-	-
15	CLA	cB	816	X	-	-	-
15	CLA	cB	817	X	-	-	-
15	CLA	cB	818	X	-	-	-
15	CLA	cB	819	X	-	-	-
15	CLA	cB	820	X	-	-	-
15	CLA	cB	821	X	-	-	-
15	CLA	cB	822	X	-	-	-
15	CLA	cB	823	X	-	-	-
15	CLA	cB	824	X	-	-	-
15	CLA	cB	825	X	-	-	-
15	CLA	cB	826	X	-	-	-
15	CLA	cB	827	X	-	-	-
15	CLA	cB	828	X	-	-	-
15	CLA	cB	829	X	-	-	-
15	CLA	cB	830	X	-	-	-
15	CLA	cB	831	X	-	-	-
15	CLA	cB	832	X	-	-	-
15	CLA	cB	833	X	-	-	-
15	CLA	cB	834	X	-	-	-
15	CLA	cB	835	X	-	-	-
15	CLA	cB	836	X	-	-	-
15	CLA	cB	837	X	-	-	-
15	CLA	cB	838	X	-	-	-
15	CLA	cB	839	X	-	-	-
15	CLA	cB	840	X	-	-	-
15	CLA	cB	841	X	-	-	-
15	CLA	cF	201	X	-	-	-
15	CLA	cF	203	X	-	-	-
15	CLA	cJ	101	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	cJ	102	X	-	-	-
15	CLA	cK	102	X	-	-	-
15	CLA	cL	201	X	-	-	-
15	CLA	cL	202	X	-	-	-
15	CLA	cL	203	X	-	-	-
15	CLA	cX	102	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 137634 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	bA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	cA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	bB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	cB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	cD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	69	Total	C	N	O	0	0
			539	342	93	104		
5	bE	69	Total	C	N	O	0	0
			539	342	93	104		
5	cE	69	Total	C	N	O	0	0
			539	342	93	104		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	bF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	cF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	bI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	cI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		
8	bJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	aK	43	Total	C	N	O	0	0
			208	122	43	43		
9	bK	43	Total	C	N	O	0	0
			208	122	43	43		
9	cK	43	Total	C	N	O	0	0
			208	122	43	43		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	bL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	cL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

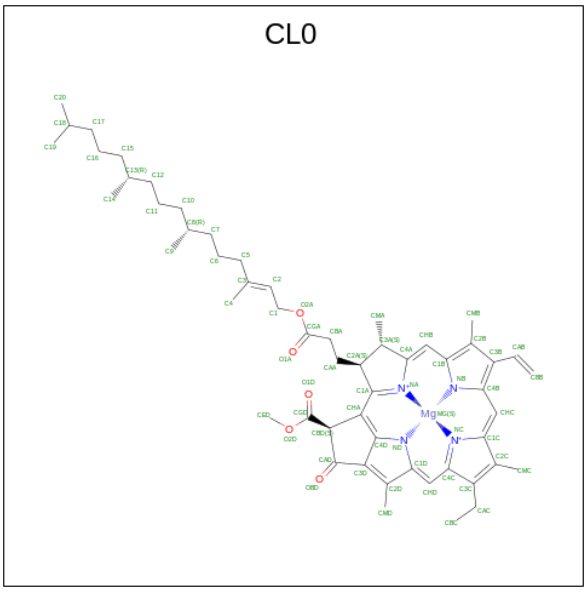
- Molecule 12 is a protein called Photosystem I reaction center subunit psaX.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total	C	N	O	0	0
			233	164	34	35		
12	bX	29	Total	C	N	O	0	0
			233	164	34	35		
12	cX	29	Total	C	N	O	0	0
			233	164	34	35		

- Molecule 13 is a protein called Iron stress in-duced protein A.

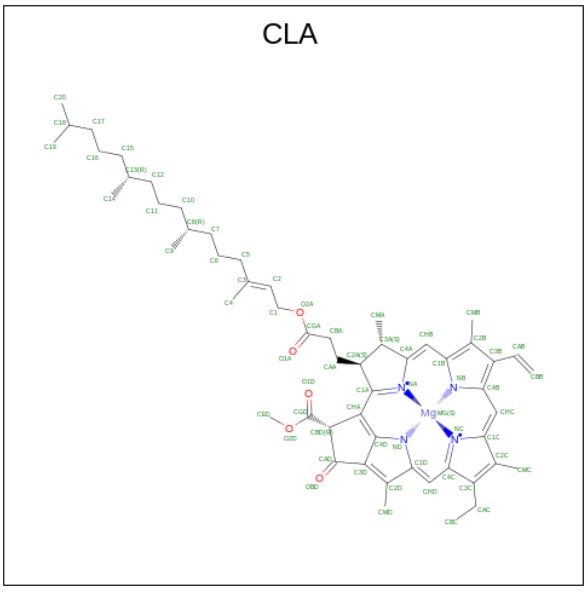
Mol	Chain	Residues	Atoms					AltConf	Trace
13	a1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	a2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	a3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	a5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	b3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	b5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	c3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	c5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		

- Molecule 14 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	aJ	1	Total	C	Mg	N	O	0
			127	101	3	12	11	
15	aJ	1	Total	C	Mg	N	O	0
			127	101	3	12	11	
15	aJ	1	Total	C	Mg	N	O	0
			127	101	3	12	11	
15	aK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	aL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	aL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	aX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a1	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	a6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bA	1	Total	C	Mg	N	O	0
			2557	2119	44	176	218	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
15	bJ	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
15	bK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	bL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	bL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	bX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	b6	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cA	1	Total	C	Mg	N	O	0
			2506	2078	43	172	213	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cB	1	Total	C	Mg	N	O	0
			2414	1994	42	168	210	
15	cF	1	Total	C	Mg	N	O	0
			96	76	2	8	10	
15	cF	1	Total	C	Mg	N	O	0
			96	76	2	8	10	
15	cJ	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
15	cJ	1	Total	C	Mg	N	O	0
			82	66	2	8	6	
15	cK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	cL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
15	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c1	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c2	1	Total	C	Mg	N	O	0
			960	782	18	72	88	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c3	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

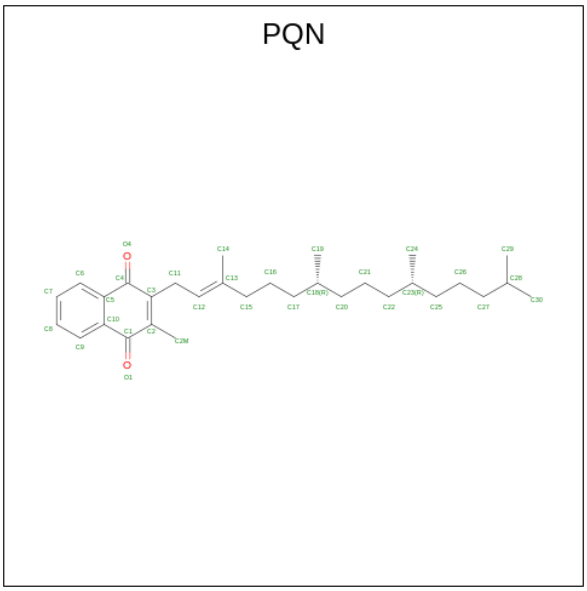
Mol	Chain	Residues	Atoms					AltConf
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c4	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	

Continued on next page...

Continued from previous page...

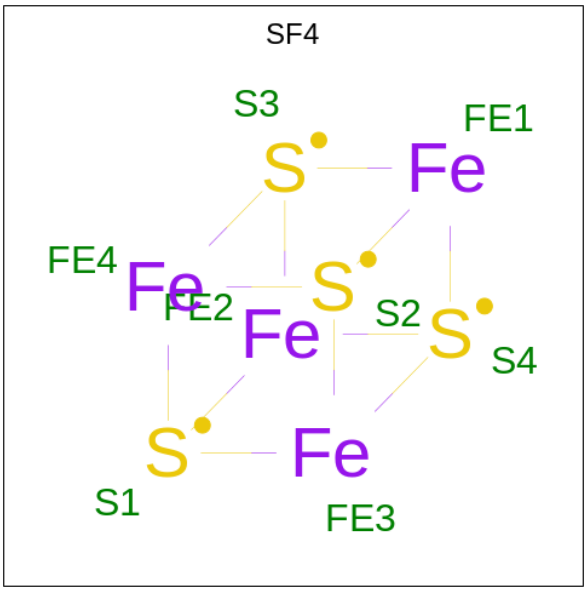
Mol	Chain	Residues	Atoms					AltConf
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c5	1	Total	C	Mg	N	O	0
			895	727	17	68	83	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	
15	c6	1	Total	C	Mg	N	O	0
			830	672	16	64	78	

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



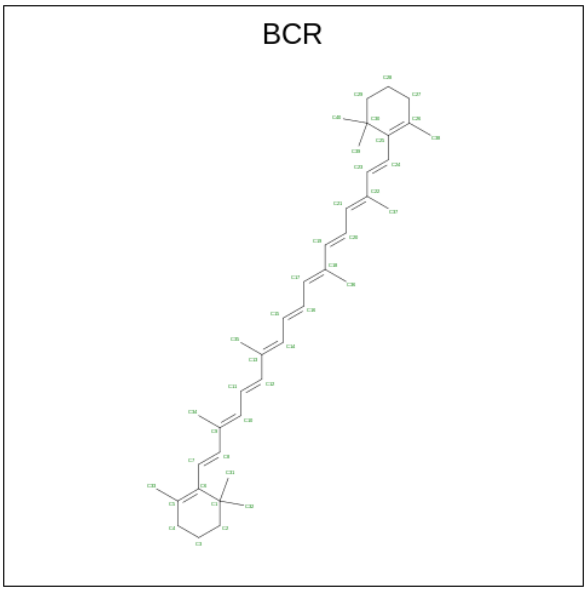
Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	C	O	0
			33	31	2	
16	aB	1	Total	C	O	0
			33	31	2	
16	bA	1	Total	C	O	0
			33	31	2	
16	bB	1	Total	C	O	0
			33	31	2	
16	cA	1	Total	C	O	0
			33	31	2	
16	cB	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total Fe S 8 4 4	0
17	aC	1	Total Fe S 16 8 8	0
17	aC	1	Total Fe S 16 8 8	0
17	bA	1	Total Fe S 8 4 4	0
17	bC	1	Total Fe S 16 8 8	0
17	bC	1	Total Fe S 16 8 8	0
17	cA	1	Total Fe S 8 4 4	0
17	cC	1	Total Fe S 16 8 8	0
17	cC	1	Total Fe S 16 8 8	0

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
18	aA	1	Total C 200 200	0
18	aA	1	Total C 200 200	0
18	aA	1	Total C 200 200	0
18	aA	1	Total C 200 200	0
18	aA	1	Total C 200 200	0
18	aB	1	Total C 225 225	0
18	aB	1	Total C 225 225	0
18	aB	1	Total C 225 225	0
18	aB	1	Total C 225 225	0
18	aB	1	Total C 225 225	0
18	aB	1	Total C 225 225	0
18	aF	1	Total C 120 120	0
18	aF	1	Total C 120 120	0
18	aF	1	Total C 120 120	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	aI	1	Total C 120 120	0
18	aI	1	Total C 120 120	0
18	aI	1	Total C 120 120	0
18	aJ	1	Total C 80 80	0
18	aJ	1	Total C 80 80	0
18	aK	1	Total C 40 40	0
18	aL	1	Total C 40 40	0
18	aM	1	Total C 40 40	0
18	a1	1	Total C 200 200	0
18	a1	1	Total C 200 200	0
18	a1	1	Total C 200 200	0
18	a1	1	Total C 200 200	0
18	a1	1	Total C 200 200	0
18	a2	1	Total C 160 160	0
18	a2	1	Total C 160 160	0
18	a2	1	Total C 160 160	0
18	a2	1	Total C 160 160	0
18	a3	1	Total C 160 160	0
18	a3	1	Total C 160 160	0
18	a3	1	Total C 160 160	0
18	a3	1	Total C 160 160	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	a4	1	Total C 160 160	0
18	a4	1	Total C 160 160	0
18	a4	1	Total C 160 160	0
18	a4	1	Total C 160 160	0
18	a5	1	Total C 120 120	0
18	a5	1	Total C 120 120	0
18	a5	1	Total C 120 120	0
18	a6	1	Total C 200 200	0
18	a6	1	Total C 200 200	0
18	a6	1	Total C 200 200	0
18	a6	1	Total C 200 200	0
18	a6	1	Total C 200 200	0
18	bA	1	Total C 240 240	0
18	bA	1	Total C 240 240	0
18	bA	1	Total C 240 240	0
18	bA	1	Total C 240 240	0
18	bA	1	Total C 240 240	0
18	bA	1	Total C 240 240	0
18	bB	1	Total C 265 265	0
18	bB	1	Total C 265 265	0
18	bB	1	Total C 265 265	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	bB	1	Total C 265 265	0
18	bB	1	Total C 265 265	0
18	bB	1	Total C 265 265	0
18	bB	1	Total C 265 265	0
18	bF	1	Total C 40 40	0
18	bI	1	Total C 80 80	0
18	bI	1	Total C 80 80	0
18	bJ	1	Total C 120 120	0
18	bJ	1	Total C 120 120	0
18	bJ	1	Total C 120 120	0
18	bL	1	Total C 120 120	0
18	bL	1	Total C 120 120	0
18	bL	1	Total C 120 120	0
18	bM	1	Total C 40 40	0
18	b1	1	Total C 160 160	0
18	b1	1	Total C 160 160	0
18	b1	1	Total C 160 160	0
18	b1	1	Total C 160 160	0
18	b2	1	Total C 160 160	0
18	b2	1	Total C 160 160	0
18	b2	1	Total C 160 160	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	b2	1	Total C 160 160	0
18	b3	1	Total C 160 160	0
18	b3	1	Total C 160 160	0
18	b3	1	Total C 160 160	0
18	b3	1	Total C 160 160	0
18	b4	1	Total C 160 160	0
18	b4	1	Total C 160 160	0
18	b4	1	Total C 160 160	0
18	b4	1	Total C 160 160	0
18	b5	1	Total C 120 120	0
18	b5	1	Total C 120 120	0
18	b5	1	Total C 120 120	0
18	b6	1	Total C 200 200	0
18	b6	1	Total C 200 200	0
18	b6	1	Total C 200 200	0
18	b6	1	Total C 200 200	0
18	b6	1	Total C 200 200	0
18	cA	1	Total C 200 200	0
18	cA	1	Total C 200 200	0
18	cA	1	Total C 200 200	0
18	cA	1	Total C 200 200	0

Continued on next page...

Continued from previous page...

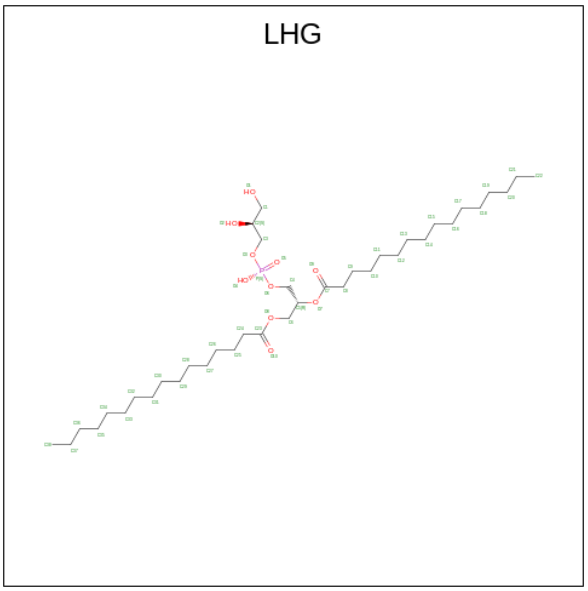
Mol	Chain	Residues	Atoms	AltConf
18	cA	1	Total C 200 200	0
18	cB	1	Total C 225 225	0
18	cB	1	Total C 225 225	0
18	cB	1	Total C 225 225	0
18	cB	1	Total C 225 225	0
18	cB	1	Total C 225 225	0
18	cB	1	Total C 225 225	0
18	cF	1	Total C 120 120	0
18	cF	1	Total C 120 120	0
18	cF	1	Total C 120 120	0
18	cI	1	Total C 80 80	0
18	cI	1	Total C 80 80	0
18	cJ	1	Total C 80 80	0
18	cJ	1	Total C 80 80	0
18	cK	1	Total C 40 40	0
18	cL	1	Total C 40 40	0
18	cM	1	Total C 40 40	0
18	c1	1	Total C 160 160	0
18	c1	1	Total C 160 160	0
18	c1	1	Total C 160 160	0
18	c1	1	Total C 160 160	0

Continued on next page...

Continued from previous page...

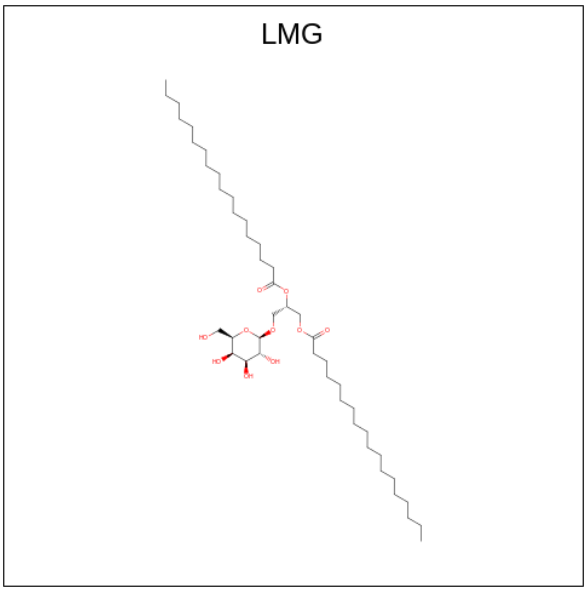
Mol	Chain	Residues	Atoms	AltConf
18	c2	1	Total C 160 160	0
18	c2	1	Total C 160 160	0
18	c2	1	Total C 160 160	0
18	c2	1	Total C 160 160	0
18	c3	1	Total C 160 160	0
18	c3	1	Total C 160 160	0
18	c3	1	Total C 160 160	0
18	c3	1	Total C 160 160	0
18	c4	1	Total C 160 160	0
18	c4	1	Total C 160 160	0
18	c4	1	Total C 160 160	0
18	c4	1	Total C 160 160	0
18	c5	1	Total C 120 120	0
18	c5	1	Total C 120 120	0
18	c5	1	Total C 120 120	0
18	c6	1	Total C 160 160	0
18	c6	1	Total C 160 160	0
18	c6	1	Total C 160 160	0
18	c6	1	Total C 160 160	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
19	aA	1	Total	C	O	P	0
			76	54	20	2	
19	aA	1	Total	C	O	P	0
			76	54	20	2	
19	aX	1	Total	C	O	P	0
			23	12	10	1	
19	bA	1	Total	C	O	P	0
			76	54	20	2	
19	bA	1	Total	C	O	P	0
			76	54	20	2	
19	bX	1	Total	C	O	P	0
			23	12	10	1	
19	cA	1	Total	C	O	P	0
			76	54	20	2	
19	cA	1	Total	C	O	P	0
			76	54	20	2	
19	cX	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
20	aB	1	Total C O 55 45 10	0
20	bB	1	Total C O 55 45 10	0
20	cB	1	Total C O 55 45 10	0

- Molecule 21 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
21	aL	2	Total Ca 2 2	0
21	bL	1	Total Ca 1 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	aA	3	Total O 3 3	0
22	aB	3	Total O 3 3	0
22	aL	1	Total O 1 1	0
22	bA	3	Total O 3 3	0

Continued on next page...

Continued from previous page...

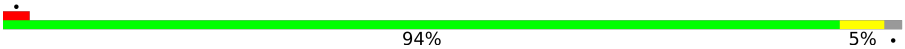
Mol	Chain	Residues	Atoms	AltConf
22	bB	3	Total O 3 3	0
22	bL	1	Total O 1 1	0
22	cA	2	Total O 2 2	0
22	cB	3	Total O 3 3	0
22	cF	1	Total O 1 1	0
22	cL	1	Total O 1 1	0

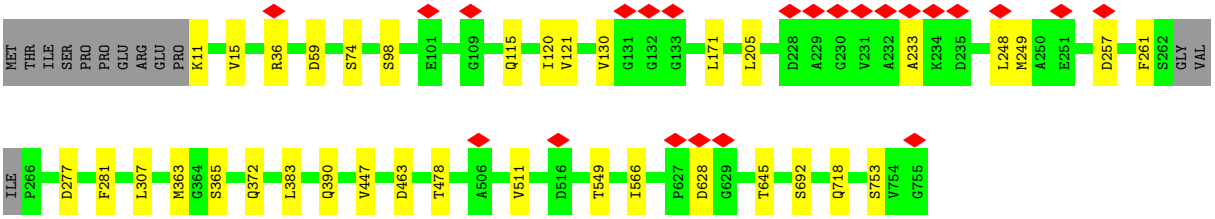
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

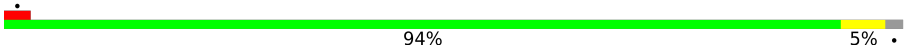
Chain aA:

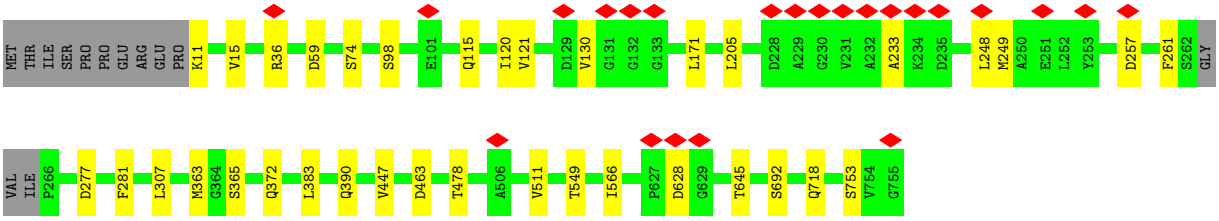




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

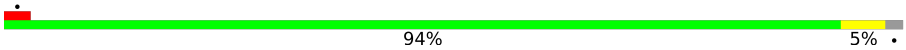
Chain bA:

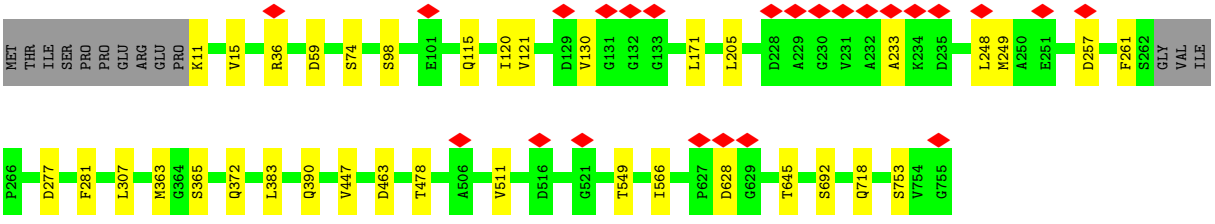




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

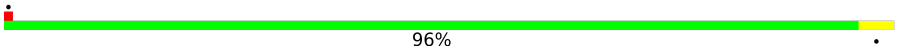
Chain cA:

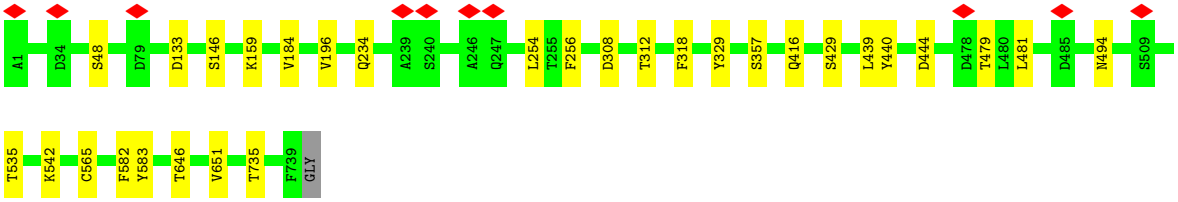




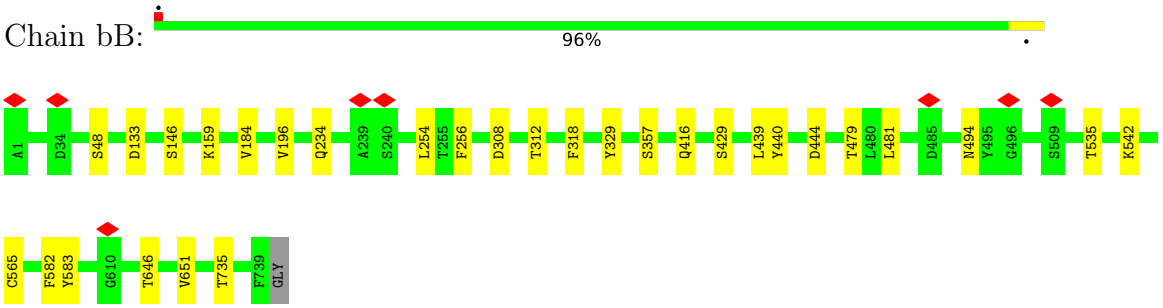
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB:

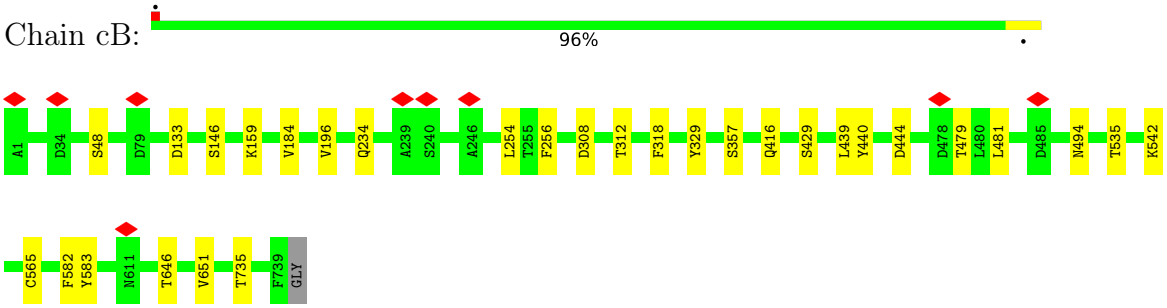




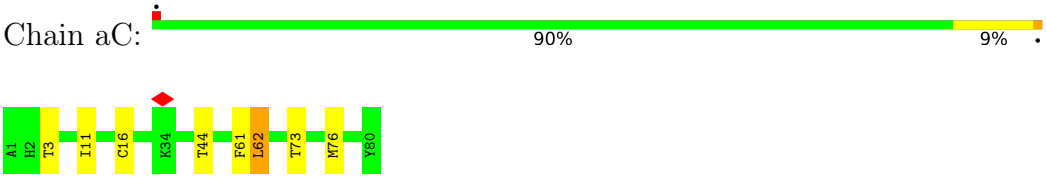
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



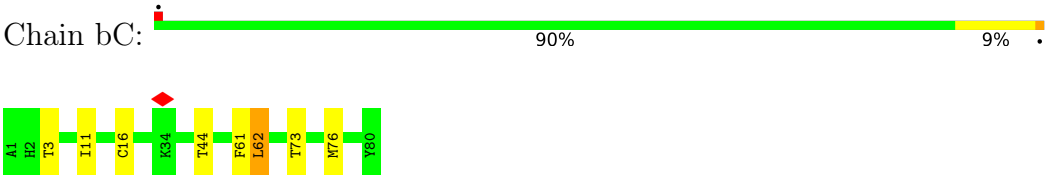
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



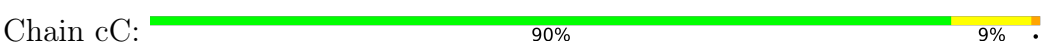
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 3: Photosystem I iron-sulfur center

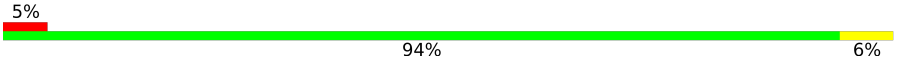


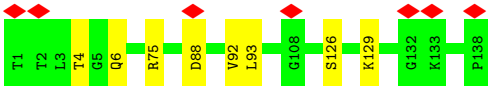
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II

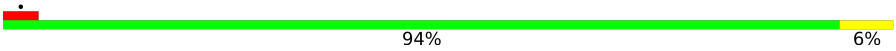
Chain aD:

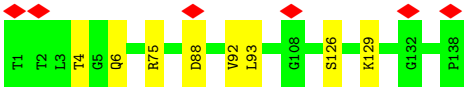




• Molecule 4: Photosystem I reaction center subunit II

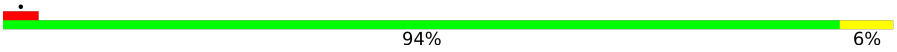
Chain bD:

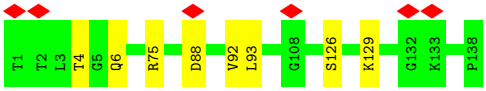




• Molecule 4: Photosystem I reaction center subunit II

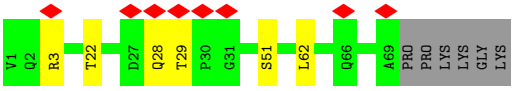
Chain cD:





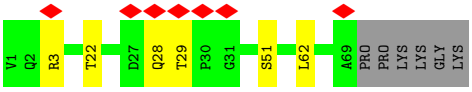
• Molecule 5: Photosystem I reaction center subunit IV

Chain aE:



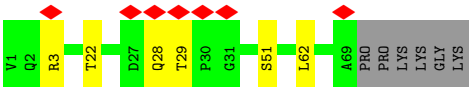
• Molecule 5: Photosystem I reaction center subunit IV

Chain bE:



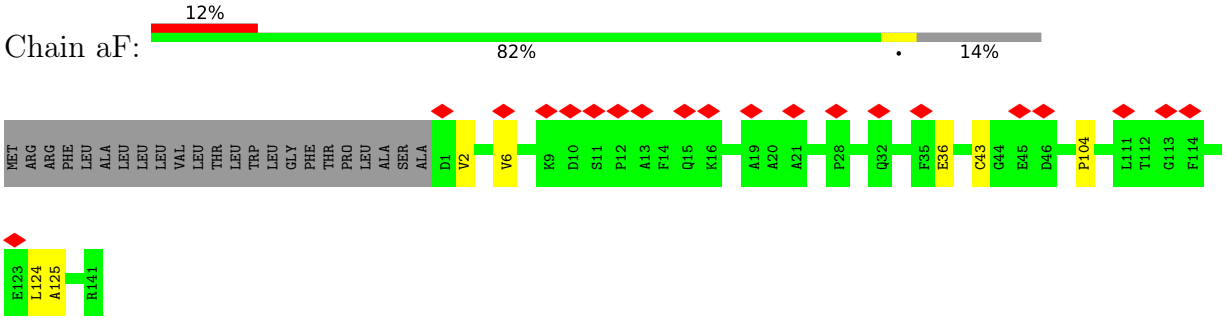
• Molecule 5: Photosystem I reaction center subunit IV

Chain cE:



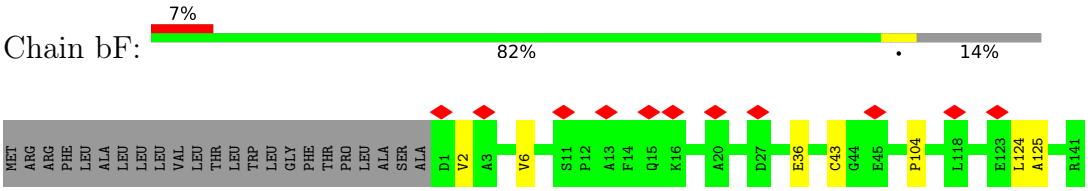
• Molecule 6: Photosystem I reaction center subunit III

Chain aF:



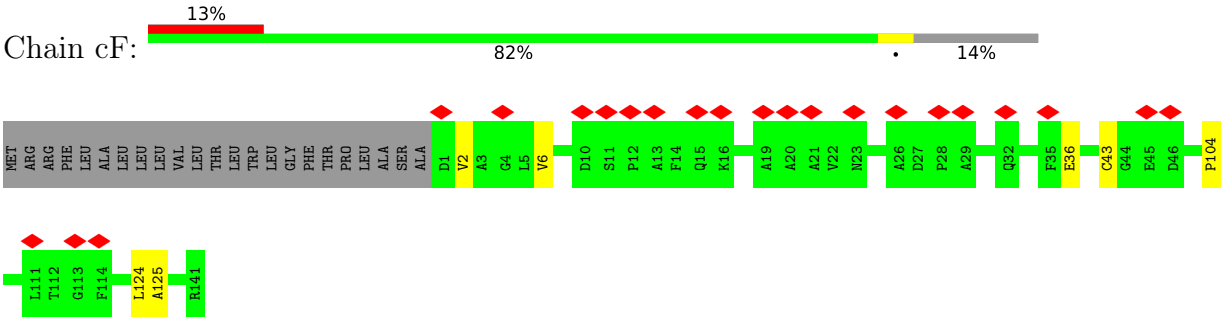
• Molecule 6: Photosystem I reaction center subunit III

Chain bF:



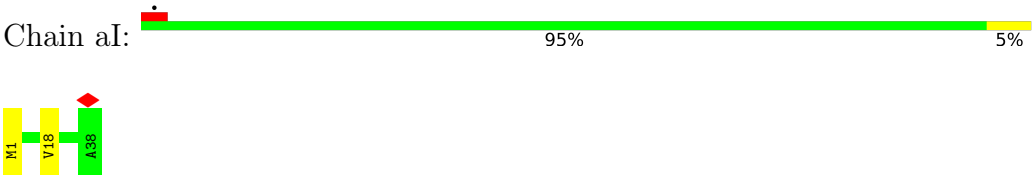
• Molecule 6: Photosystem I reaction center subunit III

Chain cF:



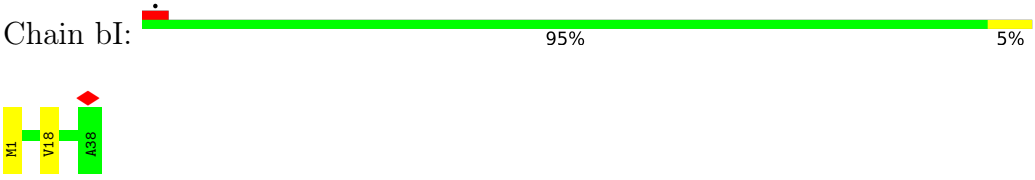
• Molecule 7: Photosystem I reaction center subunit VIII

Chain aI:



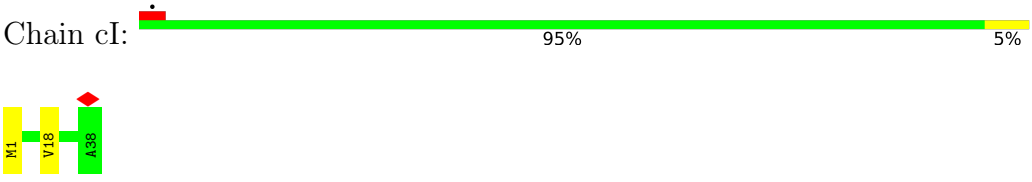
• Molecule 7: Photosystem I reaction center subunit VIII

Chain bI:



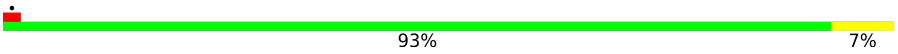
• Molecule 7: Photosystem I reaction center subunit VIII

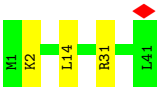
Chain cI:



• Molecule 8: Photosystem I reaction center subunit IX

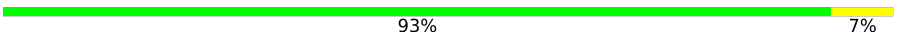
Chain aJ:

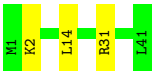




• Molecule 8: Photosystem I reaction center subunit IX

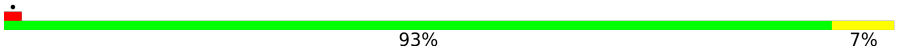
Chain bJ:

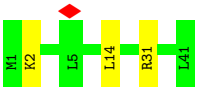




• Molecule 8: Photosystem I reaction center subunit IX

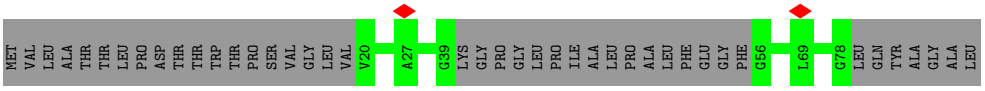
Chain cJ:





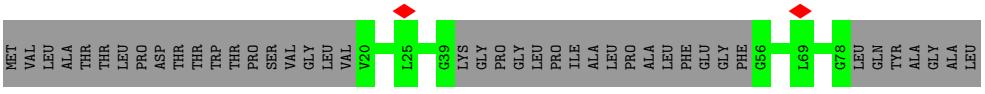
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain aK:



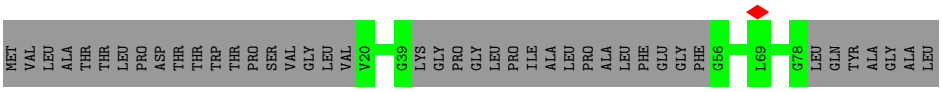
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain bK:



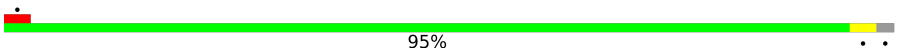
• Molecule 9: Photosystem I reaction center subunit PsaK

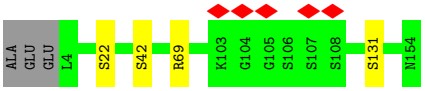
Chain cK:



• Molecule 10: Photosystem I reaction center subunit XI

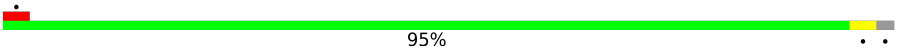
Chain aL:

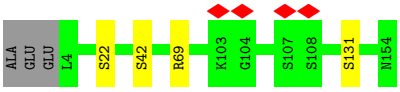




• Molecule 10: Photosystem I reaction center subunit XI

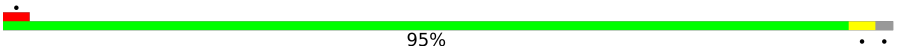
Chain bL:

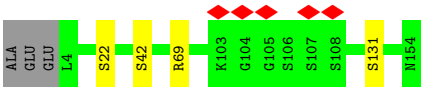




• Molecule 10: Photosystem I reaction center subunit XI

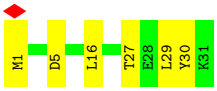
Chain cL:





• Molecule 11: Photosystem I reaction center subunit XII

Chain aM:



• Molecule 11: Photosystem I reaction center subunit XII

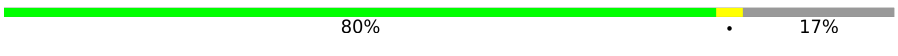
Chain bM:

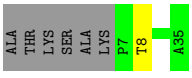
• Molecule 11: Photosystem I reaction center subunit XII

Chain cM:

• Molecule 12: Photosystem I reaction center subunit psaX

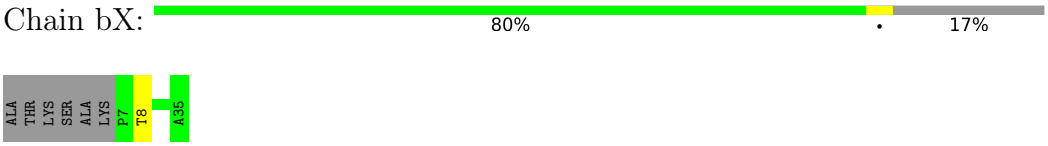
Chain aX:





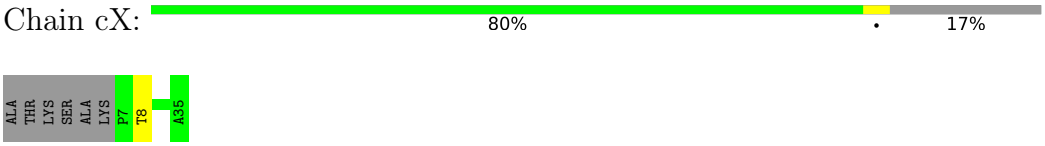
• Molecule 12: Photosystem I reaction center subunit psaX

Chain bX:



• Molecule 12: Photosystem I reaction center subunit psaX

Chain cX:

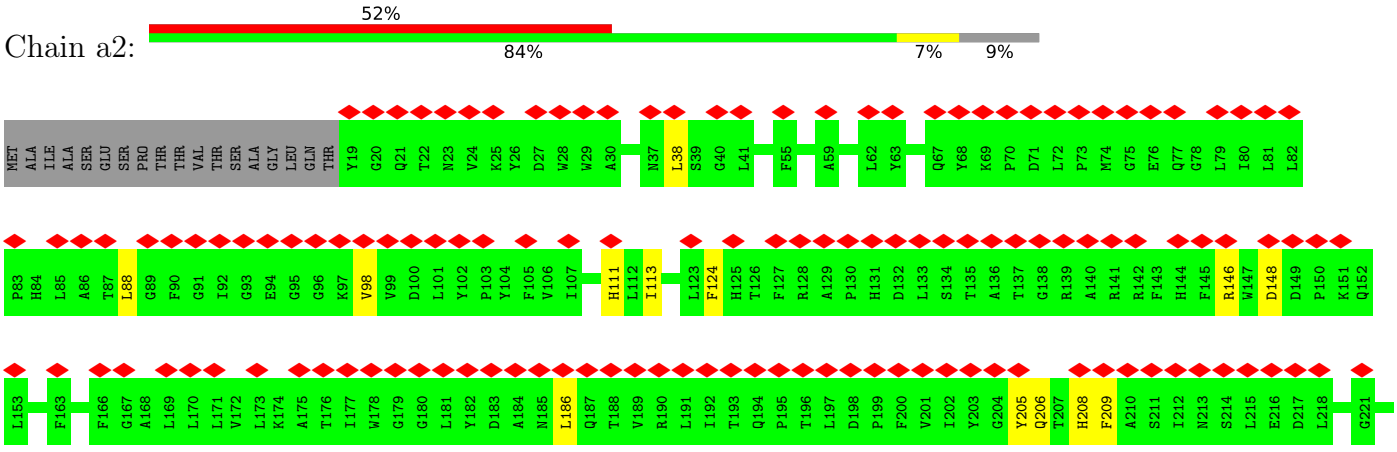


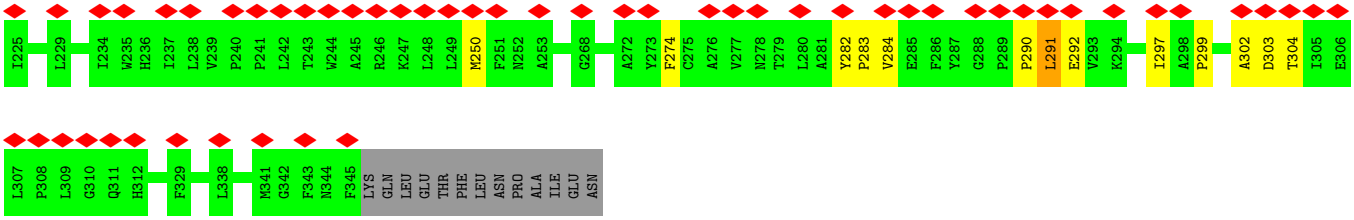
• Molecule 13: Iron stress in-duced protein A

Chain a1:

• Molecule 13: Iron stress in-duced protein A

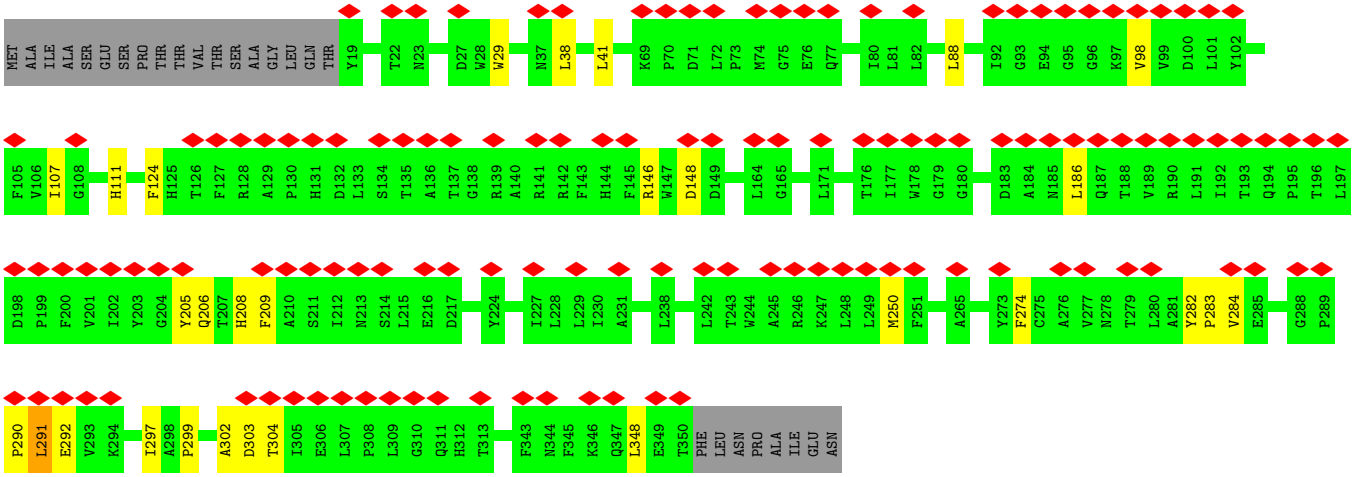
Chain a2:





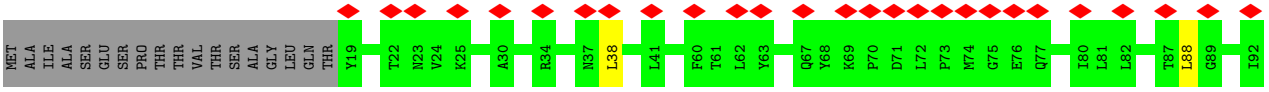
• Molecule 13: Iron stress in-duced protein A

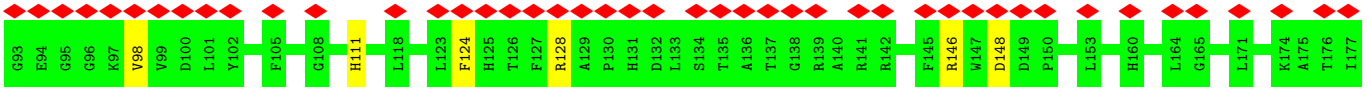
Chain a3:



• Molecule 13: Iron stress in-duced protein A

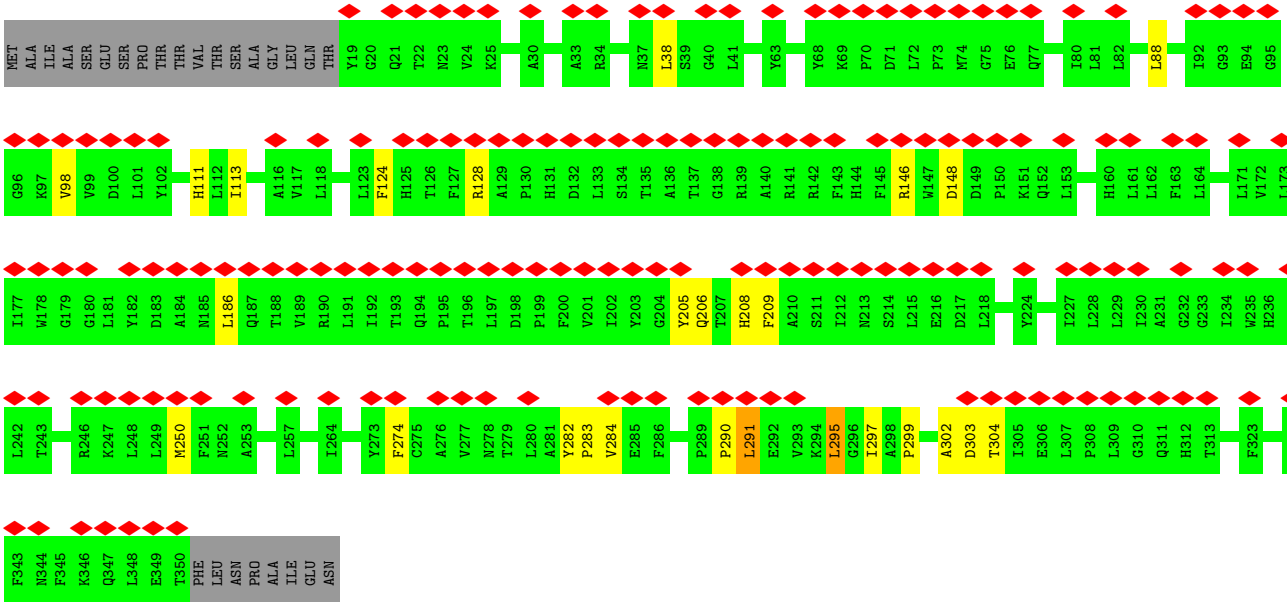
Chain a4:





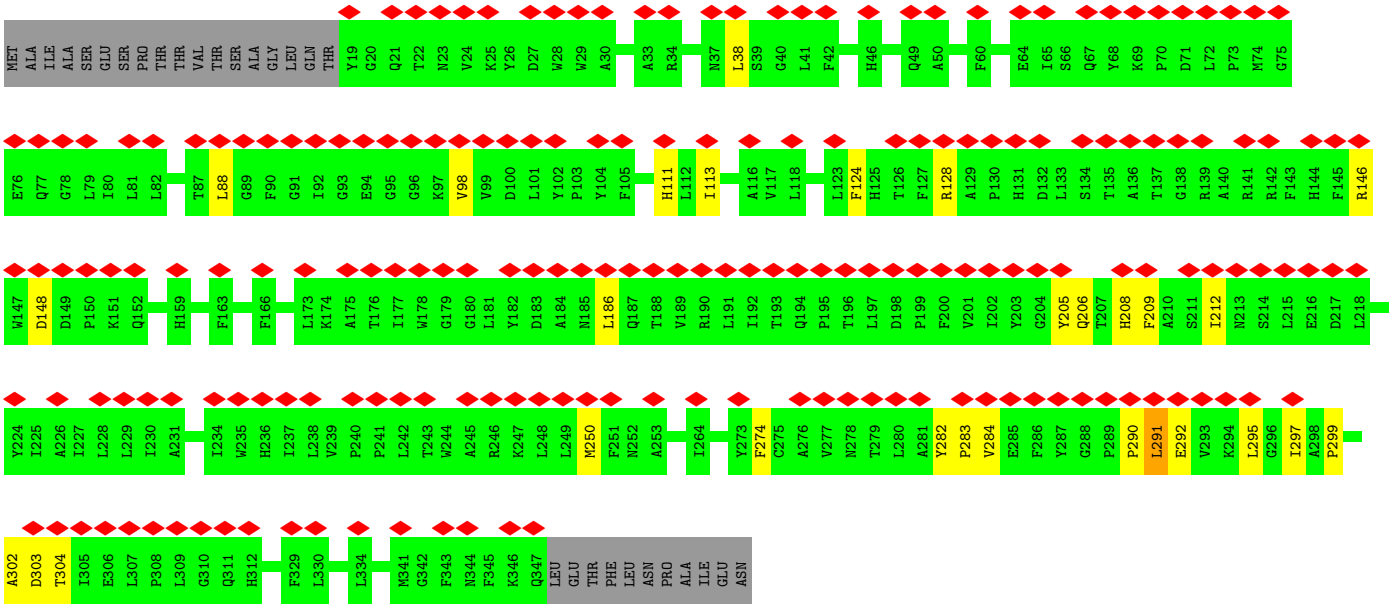
• Molecule 13: Iron stress in-duced protein A

Chain a5:



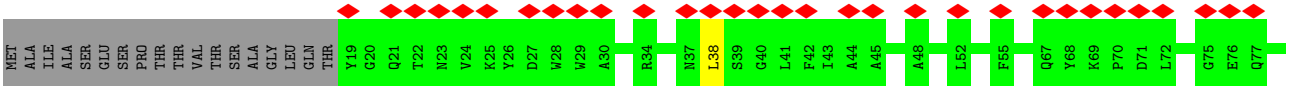
• Molecule 13: Iron stress in-duced protein A

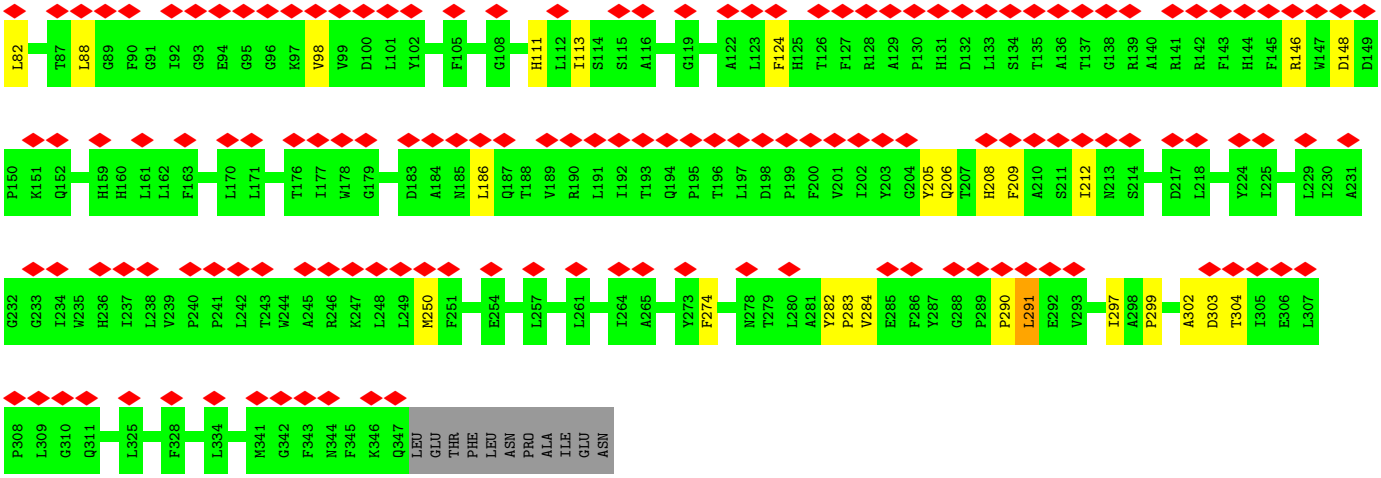
Chain a6:



• Molecule 13: Iron stress in-duced protein A

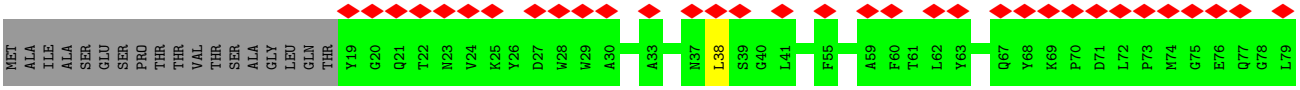
Chain b1:

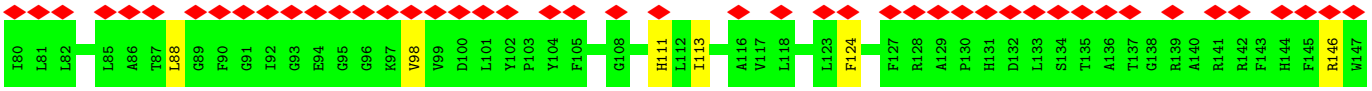


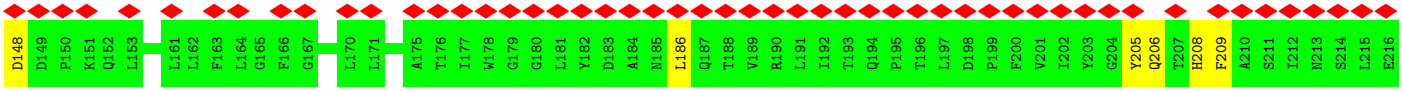


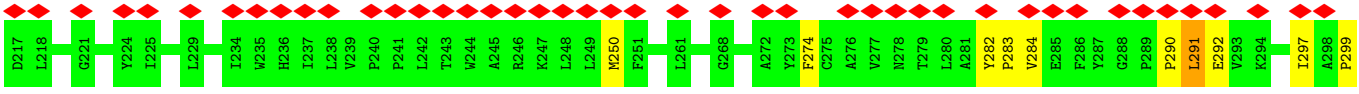
• Molecule 13: Iron stress in-duced protein A

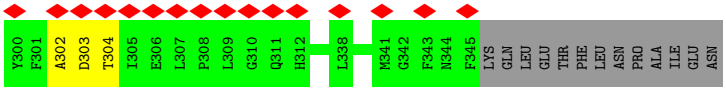
Chain b2:





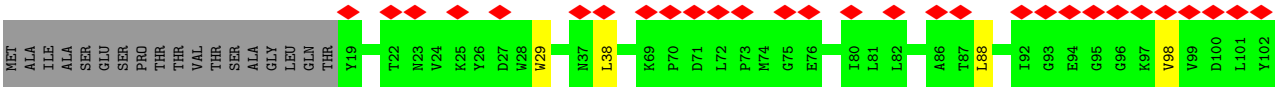


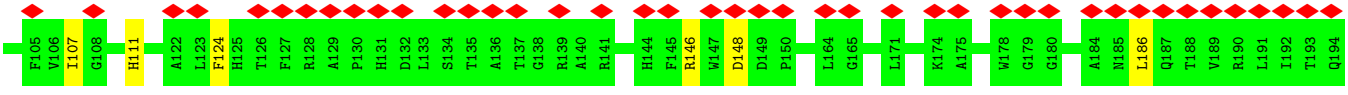


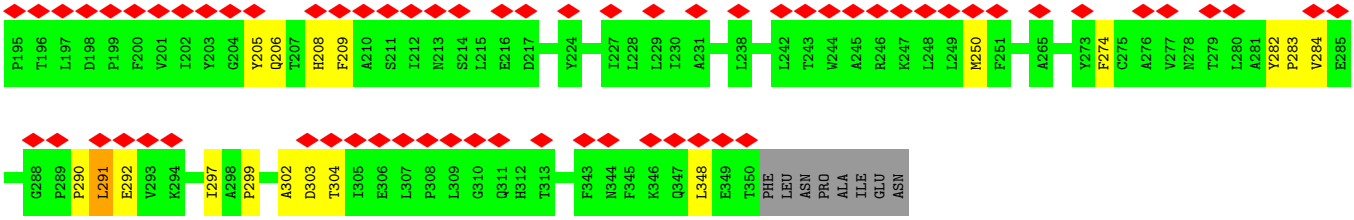


• Molecule 13: Iron stress in-duced protein A

Chain b3:

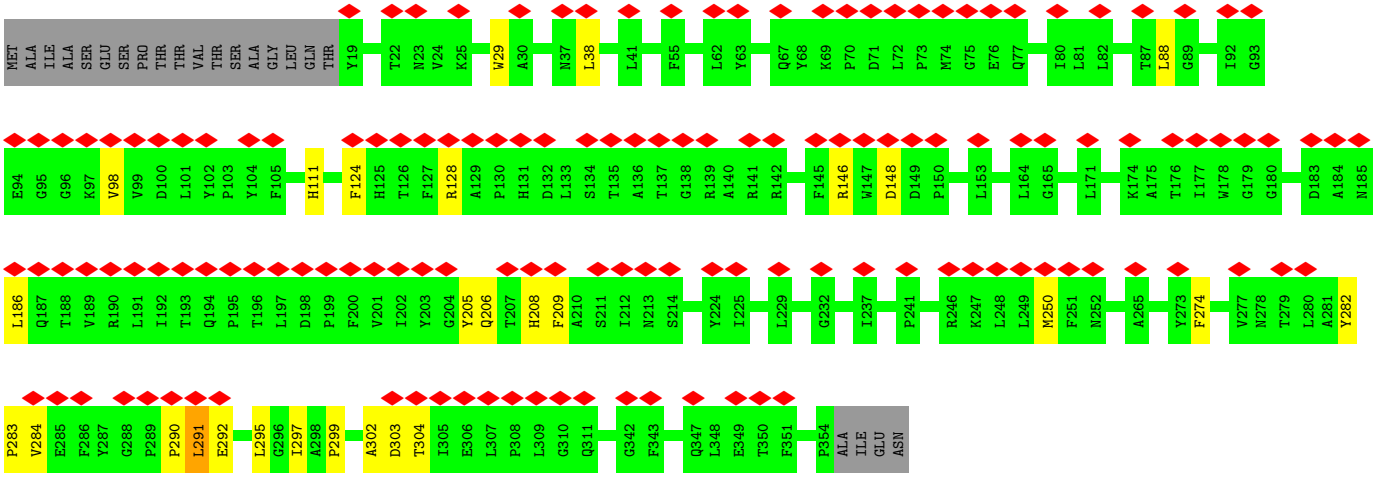






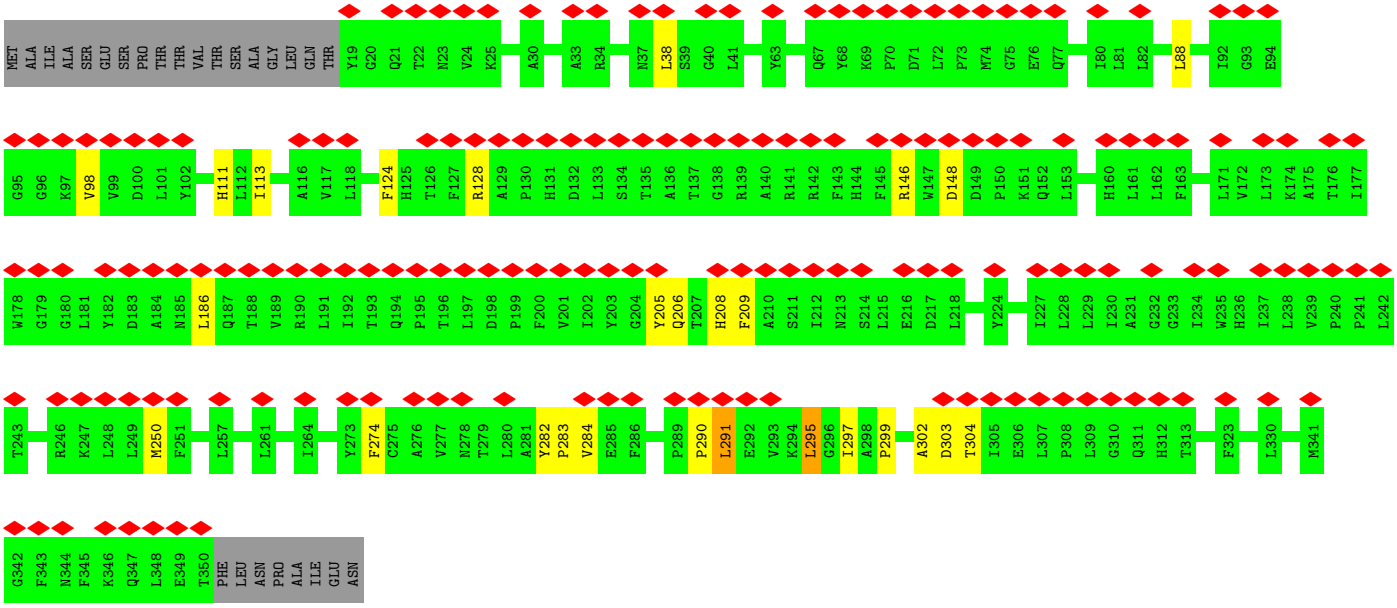
• Molecule 13: Iron stress in-duced protein A

Chain b4:



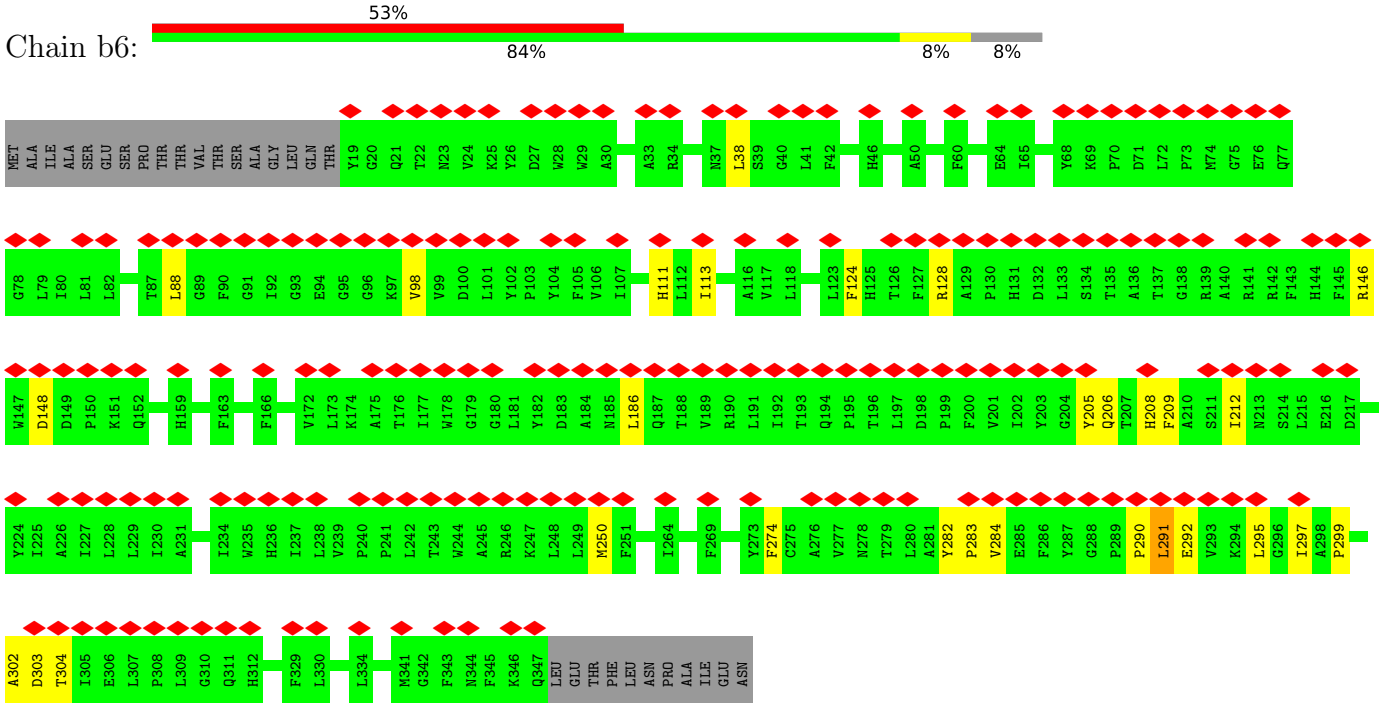
• Molecule 13: Iron stress in-duced protein A

Chain b5:



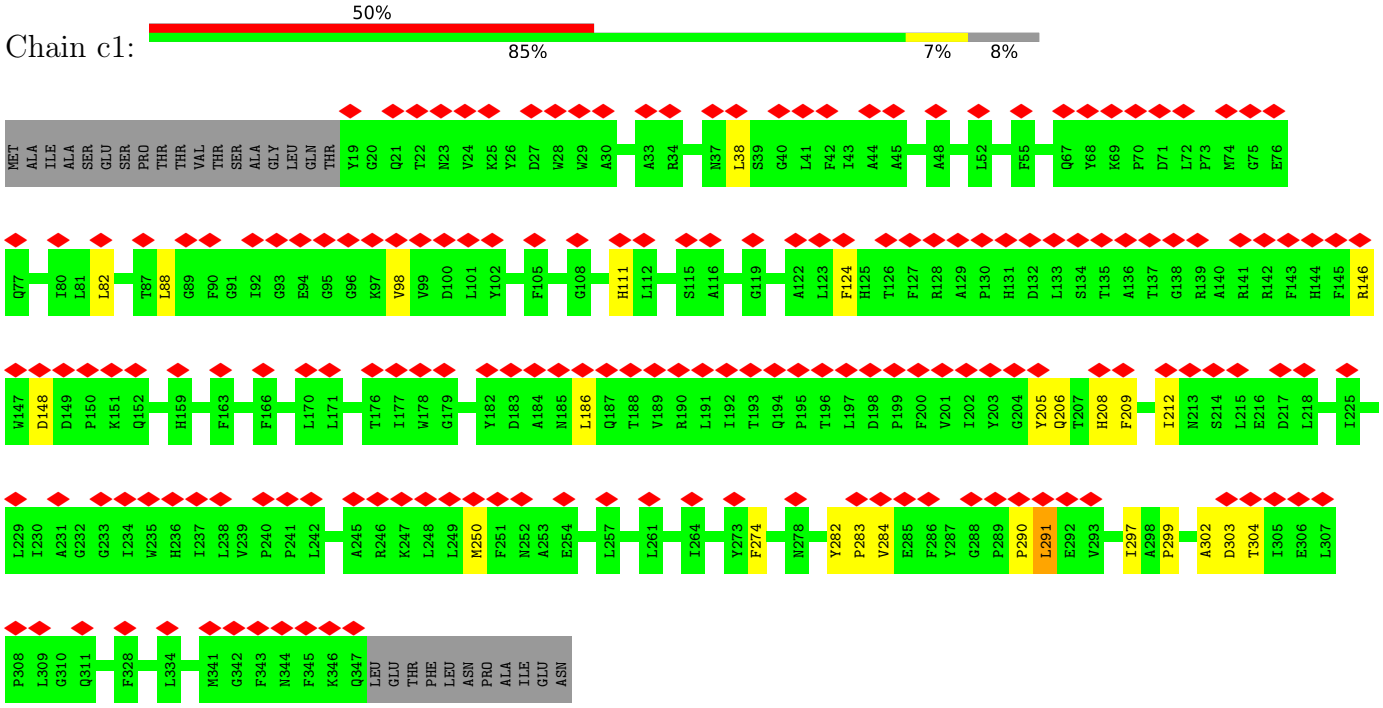
• Molecule 13: Iron stress in-duced protein A

Chain b6:



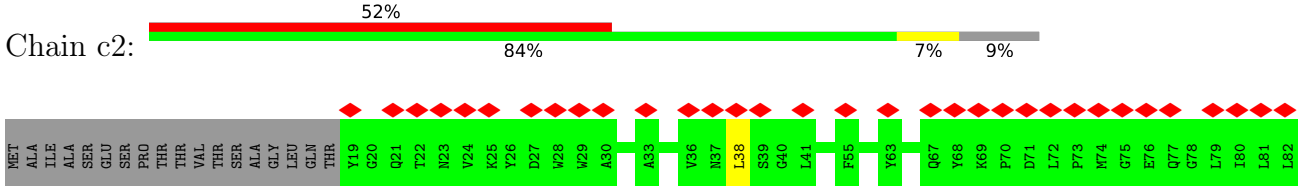
• Molecule 13: Iron stress in-duced protein A

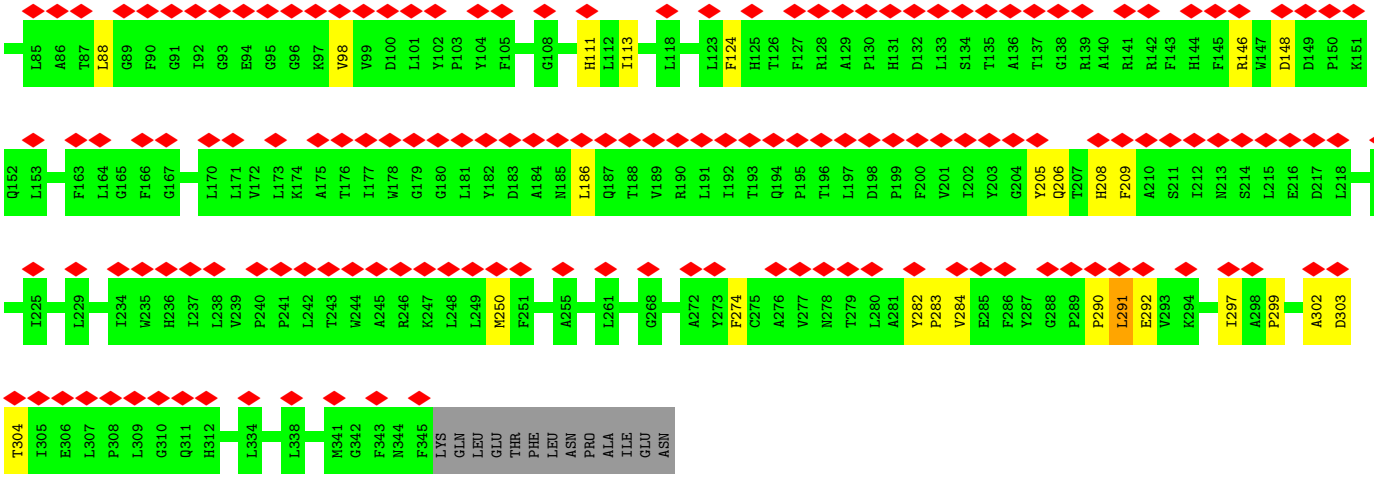
Chain c1:



• Molecule 13: Iron stress in-duced protein A

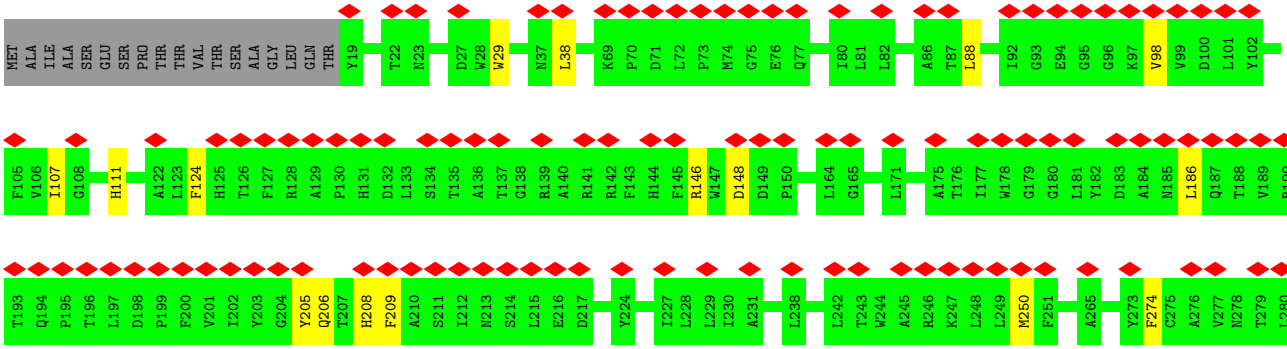
Chain c2:





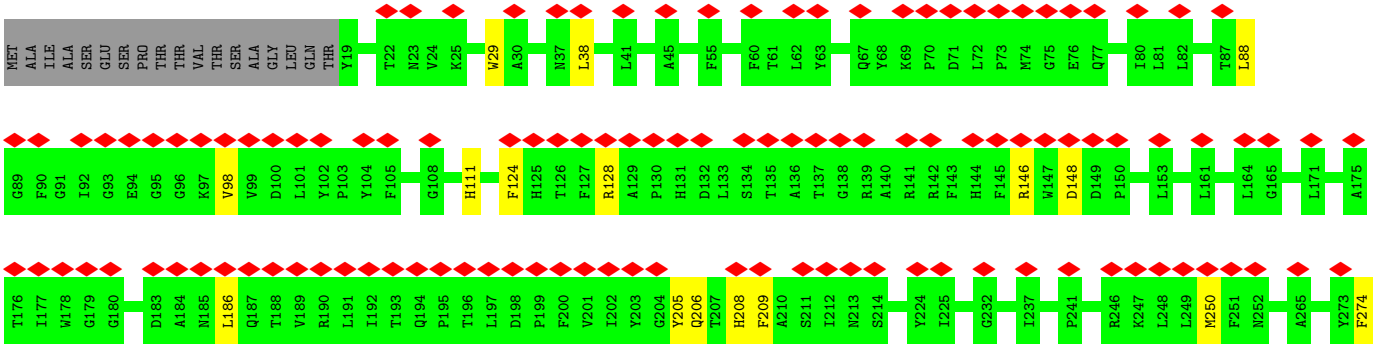
• Molecule 13: Iron stress in-duced protein A

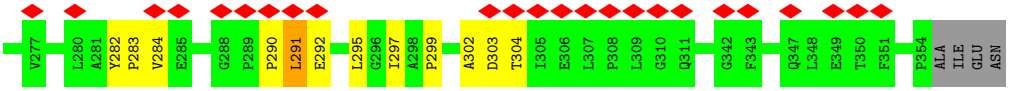
Chain c3:



• Molecule 13: Iron stress in-duced protein A

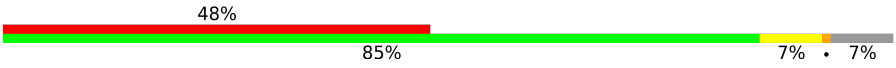
Chain c4:

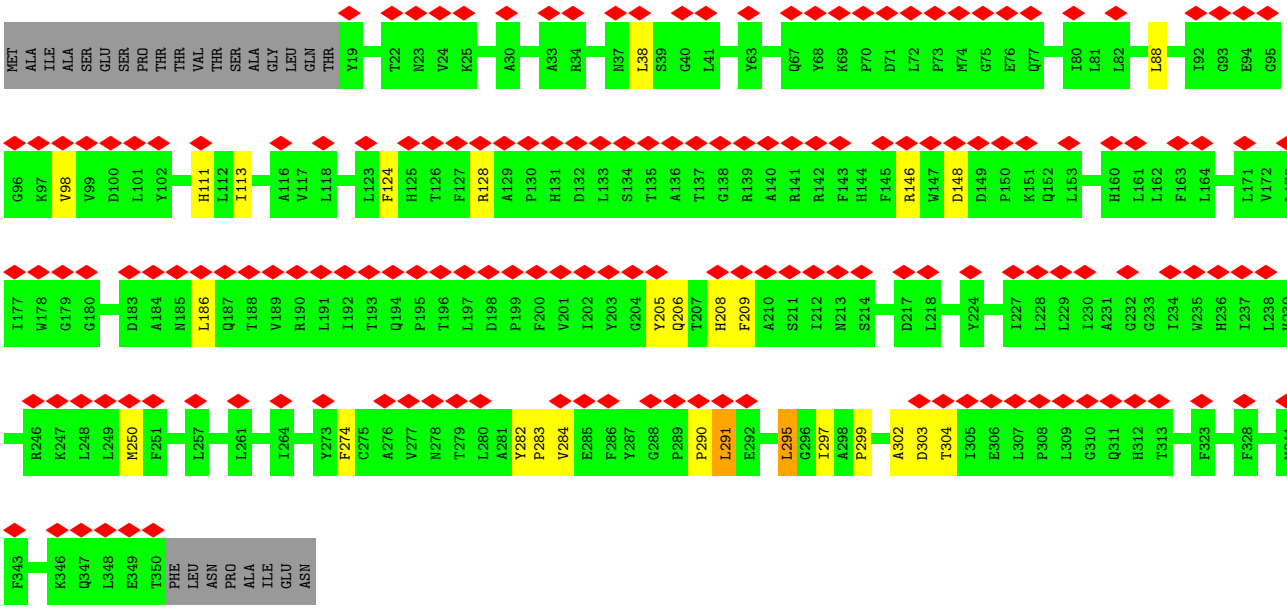




• Molecule 13: Iron stress in-duced protein A

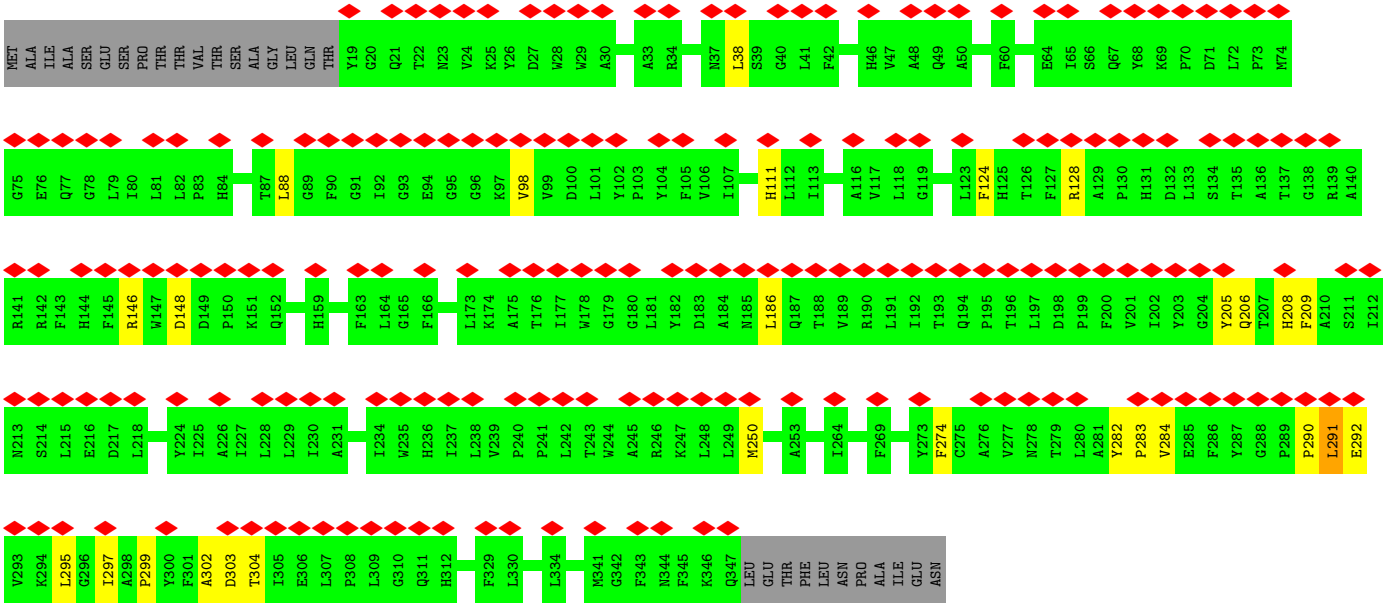
Chain c5:





• Molecule 13: Iron stress in-duced protein A

Chain c6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	303983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.291	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	534.24, 534.24, 534.24	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BCR, PQN, SF4, LMG, CLA, CL0, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	aA	0.58	1/6000 (0.0%)	0.55	0/8180
1	bA	0.58	1/6000 (0.0%)	0.55	0/8180
1	cA	0.58	1/6000 (0.0%)	0.55	0/8180
2	aB	0.58	1/6096 (0.0%)	0.58	1/8332 (0.0%)
2	bB	0.58	1/6096 (0.0%)	0.57	1/8332 (0.0%)
2	cB	0.58	1/6096 (0.0%)	0.57	1/8332 (0.0%)
3	aC	0.60	0/608	0.65	0/824
3	bC	0.60	0/608	0.65	0/824
3	cC	0.60	0/608	0.65	0/824
4	aD	0.49	0/1101	0.53	0/1492
4	bD	0.49	0/1101	0.53	0/1492
4	cD	0.49	0/1101	0.53	0/1492
5	aE	0.47	0/551	0.51	0/750
5	bE	0.47	0/551	0.51	0/750
5	cE	0.47	0/551	0.51	0/750
6	aF	0.43	0/1087	0.57	0/1476
6	bF	0.43	0/1087	0.57	0/1476
6	cF	0.43	0/1087	0.57	0/1476
7	aI	0.63	0/312	0.68	0/425
7	bI	0.63	0/312	0.68	0/425
7	cI	0.63	0/312	0.68	0/425
8	aJ	0.50	0/350	0.64	0/477
8	bJ	0.50	0/350	0.64	0/477
8	cJ	0.50	0/350	0.64	0/477
9	aK	0.25	0/206	0.36	0/281
9	bK	0.25	0/206	0.36	0/281
9	cK	0.25	0/206	0.36	0/281
10	aL	0.57	0/1148	0.54	0/1558
10	bL	0.57	0/1148	0.54	0/1558
10	cL	0.57	0/1148	0.54	0/1558
11	aM	0.45	0/244	0.59	0/332
11	bM	0.46	0/244	0.59	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	cM	0.45	0/244	0.59	0/332
12	aX	0.53	0/242	0.45	0/332
12	bX	0.53	0/242	0.45	0/332
12	cX	0.53	0/242	0.45	0/332
13	a1	0.47	1/2671 (0.0%)	0.68	4/3647 (0.1%)
13	a2	0.46	1/2653 (0.0%)	0.69	4/3624 (0.1%)
13	a3	0.49	2/2695 (0.1%)	0.69	5/3680 (0.1%)
13	a4	0.48	1/2731 (0.0%)	0.71	6/3730 (0.2%)
13	a5	0.47	1/2695 (0.0%)	0.73	7/3680 (0.2%)
13	a6	0.46	1/2671 (0.0%)	0.72	8/3647 (0.2%)
13	b1	0.47	1/2671 (0.0%)	0.68	4/3647 (0.1%)
13	b2	0.46	1/2653 (0.0%)	0.69	4/3624 (0.1%)
13	b3	0.48	2/2695 (0.1%)	0.68	4/3680 (0.1%)
13	b4	0.48	2/2731 (0.1%)	0.71	6/3730 (0.2%)
13	b5	0.47	1/2695 (0.0%)	0.73	7/3680 (0.2%)
13	b6	0.46	1/2671 (0.0%)	0.72	8/3647 (0.2%)
13	c1	0.47	1/2671 (0.0%)	0.68	4/3647 (0.1%)
13	c2	0.46	1/2653 (0.0%)	0.69	4/3624 (0.1%)
13	c3	0.49	2/2695 (0.1%)	0.69	4/3680 (0.1%)
13	c4	0.48	2/2731 (0.1%)	0.71	6/3730 (0.2%)
13	c5	0.47	1/2695 (0.0%)	0.73	7/3680 (0.2%)
13	c6	0.46	1/2671 (0.0%)	0.71	8/3647 (0.2%)
All	All	0.52	29/102183 (0.0%)	0.63	103/139401 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	aB	0	1
2	bB	0	1
2	cB	0	1
6	aF	0	1
6	bF	0	1
6	cF	0	1
11	aM	0	1
11	bM	0	1
11	cM	0	1
13	a1	0	3
13	a2	0	3
13	a3	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	a4	0	3
13	a5	0	3
13	a6	0	3
13	b1	0	3
13	b2	0	3
13	b3	0	3
13	b4	0	3
13	b5	0	3
13	b6	0	3
13	c1	0	3
13	c2	0	3
13	c3	0	3
13	c4	0	3
13	c5	0	3
13	c6	0	3
All	All	0	63

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	297	ILE	CB-CG2	-7.19	1.30	1.52
13	b1	297	ILE	CB-CG2	-7.19	1.30	1.52
13	c4	297	ILE	CB-CG2	-7.18	1.30	1.52
13	a4	297	ILE	CB-CG2	-7.16	1.30	1.52
13	b4	297	ILE	CB-CG2	-7.16	1.30	1.52
13	c1	297	ILE	CB-CG2	-7.11	1.30	1.52
13	b5	297	ILE	CB-CG2	-7.08	1.30	1.52
13	a5	297	ILE	CB-CG2	-7.06	1.30	1.52
13	c5	297	ILE	CB-CG2	-7.05	1.30	1.52
13	c3	297	ILE	CB-CG2	-7.00	1.31	1.52
13	a3	297	ILE	CB-CG2	-6.96	1.31	1.52
13	b3	297	ILE	CB-CG2	-6.96	1.31	1.52
13	c6	297	ILE	CB-CG2	-6.92	1.31	1.52
13	a6	297	ILE	CB-CG2	-6.87	1.31	1.52
13	b6	297	ILE	CB-CG2	-6.82	1.31	1.52
13	b2	297	ILE	CB-CG2	-6.65	1.32	1.52
13	c2	297	ILE	CB-CG2	-6.64	1.32	1.52
13	a2	297	ILE	CB-CG2	-6.55	1.32	1.52
13	a3	29	TRP	CB-CG	-6.24	1.39	1.50
1	bA	447	VAL	CB-CG2	-6.11	1.40	1.52
1	cA	447	VAL	CB-CG2	-6.09	1.40	1.52
1	aA	447	VAL	CB-CG2	-6.08	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c3	29	TRP	CB-CG	-5.82	1.39	1.50
13	c4	29	TRP	CB-CG	-5.56	1.40	1.50
13	b4	29	TRP	CB-CG	-5.15	1.41	1.50
2	aB	196	VAL	CB-CG2	-5.08	1.42	1.52
2	bB	196	VAL	CB-CG2	-5.07	1.42	1.52
2	cB	196	VAL	CB-CG2	-5.06	1.42	1.52
13	b3	29	TRP	CB-CG	-5.04	1.41	1.50

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a6	128	ARG	NE-CZ-NH1	-10.78	114.91	120.30
13	b6	128	ARG	NE-CZ-NH1	-10.05	115.28	120.30
13	c5	295	LEU	CA-CB-CG	9.71	137.64	115.30
13	b5	295	LEU	CA-CB-CG	9.67	137.54	115.30
13	a5	295	LEU	CA-CB-CG	9.58	137.32	115.30
13	b4	295	LEU	CA-CB-CG	9.47	137.08	115.30
13	c4	295	LEU	CA-CB-CG	9.42	136.97	115.30
13	a4	295	LEU	CA-CB-CG	9.41	136.94	115.30
13	b6	128	ARG	NE-CZ-NH2	9.30	124.95	120.30
13	b5	148	ASP	CB-CG-OD1	8.80	126.22	118.30
13	c6	128	ARG	NE-CZ-NH2	8.80	124.70	120.30
13	a5	148	ASP	CB-CG-OD1	8.78	126.20	118.30
13	c5	148	ASP	CB-CG-OD1	8.71	126.14	118.30
13	b3	291	LEU	CA-CB-CG	8.68	135.25	115.30
13	c3	291	LEU	CA-CB-CG	8.65	135.20	115.30
13	c2	148	ASP	CB-CG-OD1	8.65	126.08	118.30
13	b1	148	ASP	CB-CG-OD1	8.63	126.07	118.30
13	a3	291	LEU	CA-CB-CG	8.61	135.11	115.30
13	a4	148	ASP	CB-CG-OD1	8.61	126.05	118.30
13	c2	291	LEU	CA-CB-CG	8.61	135.10	115.30
13	b2	291	LEU	CA-CB-CG	8.60	135.09	115.30
13	c4	148	ASP	CB-CG-OD1	8.59	126.03	118.30
13	b3	148	ASP	CB-CG-OD1	8.59	126.03	118.30
13	b6	148	ASP	CB-CG-OD1	8.59	126.03	118.30
13	a2	148	ASP	CB-CG-OD1	8.58	126.03	118.30
13	b4	148	ASP	CB-CG-OD1	8.58	126.02	118.30
13	c1	148	ASP	CB-CG-OD1	8.58	126.02	118.30
13	a1	148	ASP	CB-CG-OD1	8.57	126.01	118.30
13	a2	291	LEU	CA-CB-CG	8.57	135.00	115.30
13	b2	148	ASP	CB-CG-OD1	8.55	126.00	118.30
13	a6	148	ASP	CB-CG-OD1	8.54	125.98	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b4	291	LEU	CA-CB-CG	8.54	134.94	115.30
13	a3	148	ASP	CB-CG-OD1	8.54	125.98	118.30
13	c4	291	LEU	CA-CB-CG	8.53	134.92	115.30
13	c6	291	LEU	CA-CB-CG	8.53	134.92	115.30
13	b6	291	LEU	CA-CB-CG	8.53	134.91	115.30
13	c6	148	ASP	CB-CG-OD1	8.52	125.97	118.30
13	b1	291	LEU	CA-CB-CG	8.52	134.89	115.30
13	c3	148	ASP	CB-CG-OD1	8.51	125.95	118.30
13	a6	291	LEU	CA-CB-CG	8.50	134.84	115.30
13	a4	291	LEU	CA-CB-CG	8.49	134.84	115.30
13	c1	291	LEU	CA-CB-CG	8.42	134.66	115.30
13	c5	291	LEU	CA-CB-CG	8.40	134.61	115.30
13	b5	291	LEU	CA-CB-CG	8.38	134.56	115.30
13	a1	291	LEU	CA-CB-CG	8.37	134.55	115.30
13	a5	291	LEU	CA-CB-CG	8.30	134.39	115.30
13	b4	128	ARG	NE-CZ-NH2	7.96	124.28	120.30
13	a4	128	ARG	NE-CZ-NH2	7.92	124.26	120.30
13	c4	128	ARG	NE-CZ-NH2	7.77	124.18	120.30
13	c6	128	ARG	NE-CZ-NH1	-7.58	116.51	120.30
13	a6	128	ARG	NE-CZ-NH2	7.36	123.98	120.30
13	a5	128	ARG	NE-CZ-NH2	7.34	123.97	120.30
13	c5	128	ARG	NE-CZ-NH2	7.32	123.96	120.30
13	b5	128	ARG	NE-CZ-NH2	7.31	123.95	120.30
13	b4	299	PRO	N-CD-CG	-6.91	92.83	103.20
13	a4	299	PRO	N-CD-CG	-6.89	92.86	103.20
13	c4	299	PRO	N-CD-CG	-6.87	92.89	103.20
13	a5	128	ARG	NE-CZ-NH1	-6.86	116.87	120.30
13	c5	128	ARG	NE-CZ-NH1	-6.80	116.90	120.30
13	b5	128	ARG	NE-CZ-NH1	-6.79	116.91	120.30
13	b5	299	PRO	N-CD-CG	-6.78	93.03	103.20
13	c5	299	PRO	N-CD-CG	-6.78	93.03	103.20
13	a5	299	PRO	N-CD-CG	-6.76	93.05	103.20
13	c3	299	PRO	N-CD-CG	-6.69	93.17	103.20
13	a3	299	PRO	N-CD-CG	-6.65	93.23	103.20
13	b3	299	PRO	N-CD-CG	-6.63	93.25	103.20
13	a2	299	PRO	N-CD-CG	-6.62	93.27	103.20
13	b2	299	PRO	N-CD-CG	-6.59	93.31	103.20
13	b6	299	PRO	N-CD-CG	-6.58	93.33	103.20
13	c2	299	PRO	N-CD-CG	-6.56	93.36	103.20
13	a6	299	PRO	N-CD-CG	-6.56	93.36	103.20
13	c6	299	PRO	N-CD-CG	-6.55	93.37	103.20
13	b1	299	PRO	N-CD-CG	-6.44	93.54	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c1	299	PRO	N-CD-CG	-6.35	93.68	103.20
13	a1	299	PRO	N-CD-CG	-6.25	93.83	103.20
13	b3	209	PHE	C-N-CA	5.58	135.65	121.70
13	c3	209	PHE	C-N-CA	5.55	135.58	121.70
13	a3	209	PHE	C-N-CA	5.53	135.53	121.70
13	a4	209	PHE	C-N-CA	5.48	135.40	121.70
13	c4	209	PHE	C-N-CA	5.47	135.38	121.70
13	b4	209	PHE	C-N-CA	5.46	135.35	121.70
13	b6	209	PHE	C-N-CA	5.43	135.29	121.70
13	a6	209	PHE	C-N-CA	5.41	135.22	121.70
13	c6	209	PHE	C-N-CA	5.41	135.23	121.70
13	c1	209	PHE	C-N-CA	5.38	135.16	121.70
13	a1	209	PHE	C-N-CA	5.36	135.09	121.70
13	b1	209	PHE	C-N-CA	5.35	135.08	121.70
2	aB	254	LEU	CB-CG-CD1	5.35	120.09	111.00
13	a5	209	PHE	C-N-CA	5.34	135.05	121.70
13	c5	209	PHE	C-N-CA	5.34	135.06	121.70
2	cB	254	LEU	CB-CG-CD1	5.34	120.08	111.00
13	b5	209	PHE	C-N-CA	5.34	135.04	121.70
13	b6	295	LEU	CA-CB-CG	5.33	127.56	115.30
13	a6	295	LEU	CA-CB-CG	5.32	127.53	115.30
2	bB	254	LEU	CB-CG-CD1	5.31	120.03	111.00
13	c6	295	LEU	CA-CB-CG	5.29	127.47	115.30
13	c6	291	LEU	CB-CG-CD2	5.18	119.81	111.00
13	c2	209	PHE	C-N-CA	5.17	134.63	121.70
13	a2	209	PHE	C-N-CA	5.15	134.58	121.70
13	b2	209	PHE	C-N-CA	5.13	134.52	121.70
13	a6	291	LEU	CB-CG-CD2	5.12	119.71	111.00
13	b6	291	LEU	CB-CG-CD2	5.07	119.62	111.00
13	a3	41	LEU	CB-CG-CD2	-5.04	102.44	111.00

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	a1	282	TYR	Peptide
13	a1	290	PRO	Peptide
13	a1	302	ALA	Peptide
13	a2	282	TYR	Peptide
13	a2	290	PRO	Peptide
13	a2	302	ALA	Peptide
13	a3	282	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
13	a3	290	PRO	Peptide
13	a3	302	ALA	Peptide
13	a4	282	TYR	Peptide
13	a4	290	PRO	Peptide
13	a4	302	ALA	Peptide
13	a5	282	TYR	Peptide
13	a5	290	PRO	Peptide
13	a5	302	ALA	Peptide
13	a6	282	TYR	Peptide
13	a6	290	PRO	Peptide
13	a6	302	ALA	Peptide
2	aB	234	GLN	Peptide
6	aF	125	ALA	Peptide
11	aM	29	LEU	Peptide
13	b1	282	TYR	Peptide
13	b1	290	PRO	Peptide
13	b1	302	ALA	Peptide
13	b2	282	TYR	Peptide
13	b2	290	PRO	Peptide
13	b2	302	ALA	Peptide
13	b3	282	TYR	Peptide
13	b3	290	PRO	Peptide
13	b3	302	ALA	Peptide
13	b4	282	TYR	Peptide
13	b4	290	PRO	Peptide
13	b4	302	ALA	Peptide
13	b5	282	TYR	Peptide
13	b5	290	PRO	Peptide
13	b5	302	ALA	Peptide
13	b6	282	TYR	Peptide
13	b6	290	PRO	Peptide
13	b6	302	ALA	Peptide
2	bB	234	GLN	Peptide
6	bF	125	ALA	Peptide
11	bM	29	LEU	Peptide
13	c1	282	TYR	Peptide
13	c1	290	PRO	Peptide
13	c1	302	ALA	Peptide
13	c2	282	TYR	Peptide
13	c2	290	PRO	Peptide
13	c2	302	ALA	Peptide
13	c3	282	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
13	c3	290	PRO	Peptide
13	c3	302	ALA	Peptide
13	c4	282	TYR	Peptide
13	c4	290	PRO	Peptide
13	c4	302	ALA	Peptide
13	c5	282	TYR	Peptide
13	c5	290	PRO	Peptide
13	c5	302	ALA	Peptide
13	c6	282	TYR	Peptide
13	c6	290	PRO	Peptide
13	c6	302	ALA	Peptide
2	cB	234	GLN	Peptide
6	cF	125	ALA	Peptide
11	cM	29	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5801	0	5660	0	0
1	bA	5801	0	5660	0	0
1	cA	5801	0	5660	0	0
2	aB	5879	0	5627	0	0
2	bB	5879	0	5627	0	0
2	cB	5879	0	5627	0	0
3	aC	598	0	580	0	0
3	bC	598	0	580	0	0
3	cC	598	0	580	0	0
4	aD	1075	0	1077	0	0
4	bD	1075	0	1077	0	0
4	cD	1075	0	1077	0	0
5	aE	539	0	528	0	0
5	bE	539	0	528	0	0
5	cE	539	0	528	0	0
6	aF	1065	0	1077	0	0
6	bF	1065	0	1077	0	0
6	cF	1065	0	1077	0	0
7	aI	301	0	306	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	bI	301	0	306	0	0
7	cI	301	0	306	0	0
8	aJ	338	0	347	0	0
8	bJ	338	0	347	0	0
8	cJ	338	0	347	0	0
9	aK	208	0	106	0	0
9	bK	208	0	106	0	0
9	cK	208	0	106	0	0
10	aL	1119	0	1125	0	0
10	bL	1119	0	1125	0	0
10	cL	1119	0	1125	0	0
11	aM	241	0	264	0	0
11	bM	241	0	264	0	0
11	cM	241	0	264	0	0
12	aX	233	0	231	0	0
12	bX	233	0	231	0	0
12	cX	233	0	231	0	0
13	a1	2583	0	2568	0	0
13	a2	2565	0	2545	0	0
13	a3	2607	0	2590	0	0
13	a4	2641	0	2624	0	0
13	a5	2607	0	2591	0	0
13	a6	2583	0	2567	0	0
13	b1	2583	0	2568	0	0
13	b2	2565	0	2545	0	0
13	b3	2607	0	2590	0	0
13	b4	2641	0	2624	0	0
13	b5	2607	0	2591	0	0
13	b6	2583	0	2567	0	0
13	c1	2583	0	2568	0	0
13	c2	2565	0	2545	0	0
13	c3	2607	0	2590	0	0
13	c4	2641	0	2624	0	0
13	c5	2607	0	2591	0	0
13	c6	2583	0	2567	0	0
14	aA	65	0	72	0	0
14	bA	65	0	72	0	0
14	cA	65	0	72	0	0
15	a1	895	0	790	0	0
15	a2	960	0	862	0	0
15	a3	895	0	790	0	0
15	a4	895	0	792	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	a5	895	0	792	0	0
15	a6	895	0	790	0	0
15	aA	2557	0	2532	0	0
15	aB	2414	0	2369	0	0
15	aJ	127	0	91	0	0
15	aK	45	0	33	0	0
15	aL	195	0	216	0	0
15	aX	45	0	33	0	0
15	b1	830	0	720	0	0
15	b2	960	0	862	0	0
15	b3	895	0	790	0	0
15	b4	895	0	792	0	0
15	b5	895	0	792	0	0
15	b6	895	0	790	0	0
15	bA	2557	0	2532	0	0
15	bB	2414	0	2369	0	0
15	bF	45	0	33	0	0
15	bJ	82	0	58	0	0
15	bK	45	0	33	0	0
15	bL	195	0	216	0	0
15	bX	45	0	33	0	0
15	c1	830	0	720	0	0
15	c2	960	0	862	0	0
15	c3	895	0	790	0	0
15	c4	895	0	792	0	0
15	c5	895	0	792	0	0
15	c6	830	0	720	0	0
15	cA	2506	0	2491	0	0
15	cB	2414	0	2369	0	0
15	cF	96	0	74	0	0
15	cJ	82	0	58	0	0
15	cK	45	0	33	0	0
15	cL	195	0	216	0	0
15	cX	45	0	33	0	0
16	aA	33	0	46	0	0
16	aB	33	0	46	0	0
16	bA	33	0	46	0	0
16	bB	33	0	46	0	0
16	cA	33	0	46	0	0
16	cB	33	0	46	0	0
17	aA	8	0	0	0	0
17	aC	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bA	8	0	0	0	0
17	bC	16	0	0	0	0
17	cA	8	0	0	0	0
17	cC	16	0	0	0	0
18	a1	200	0	280	0	0
18	a2	160	0	224	0	0
18	a3	160	0	224	0	0
18	a4	160	0	224	0	0
18	a5	120	0	168	0	0
18	a6	200	0	280	0	0
18	aA	200	0	278	0	0
18	aB	225	0	313	0	0
18	aF	120	0	168	0	0
18	aI	120	0	168	0	0
18	aJ	80	0	112	0	0
18	aK	40	0	56	0	0
18	aL	40	0	56	0	0
18	aM	40	0	56	0	0
18	b1	160	0	224	0	0
18	b2	160	0	224	0	0
18	b3	160	0	224	0	0
18	b4	160	0	224	0	0
18	b5	120	0	168	0	0
18	b6	200	0	280	0	0
18	bA	240	0	334	0	0
18	bB	265	0	369	0	0
18	bF	40	0	56	0	0
18	bI	80	0	112	0	0
18	bJ	120	0	168	0	0
18	bL	120	0	168	0	0
18	bM	40	0	56	0	0
18	c1	160	0	224	0	0
18	c2	160	0	224	0	0
18	c3	160	0	224	0	0
18	c4	160	0	224	0	0
18	c5	120	0	168	0	0
18	c6	160	0	224	0	0
18	cA	200	0	278	0	0
18	cB	225	0	313	0	0
18	cF	120	0	168	0	0
18	cI	80	0	112	0	0
18	cJ	80	0	112	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	cK	40	0	56	0	0
18	cL	40	0	56	0	0
18	cM	40	0	56	0	0
19	aA	76	0	98	0	0
19	aX	23	0	16	0	0
19	bA	76	0	98	0	0
19	bX	23	0	16	0	0
19	cA	76	0	98	0	0
19	cX	23	0	16	0	0
20	aB	55	0	86	0	0
20	bB	55	0	86	0	0
20	cB	55	0	86	0	0
21	aL	2	0	0	0	0
21	bL	1	0	0	0	0
22	aA	3	0	0	0	0
22	aB	3	0	0	0	0
22	aL	1	0	0	0	0
22	bA	3	0	0	0	0
22	bB	3	0	0	0	0
22	bL	1	0	0	0	0
22	cA	2	0	0	0	0
22	cB	3	0	0	0	0
22	cF	1	0	0	0	0
22	cL	1	0	0	0	0
All	All	137634	0	136044	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	51	75
1	bA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	51	75
1	cA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	51	75
2	aB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
2	bB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
2	cB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
3	aC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	5	8
3	bC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	5	8
3	cC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	5	8
4	aD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
4	bD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
4	cD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
5	aE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	bE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	cE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
6	aF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
6	bF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
6	cF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
7	aI	36/38 (95%)	36 (100%)	0	0	100	100
7	bI	36/38 (95%)	36 (100%)	0	0	100	100
7	cI	36/38 (95%)	36 (100%)	0	0	100	100
8	aJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	bJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	cJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	aK	39/85 (46%)	39 (100%)	0	0	100	100
9	bK	39/85 (46%)	39 (100%)	0	0	100	100
9	cK	39/85 (46%)	39 (100%)	0	0	100	100
10	aL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	bL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	cL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
11	aM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	bM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	cM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	aX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	bX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	cX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
13	a1	327/358 (91%)	301 (92%)	24 (7%)	2 (1%)	25	44
13	a2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	17	32
13	a3	330/358 (92%)	303 (92%)	24 (7%)	3 (1%)	17	32
13	a4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	17	32
13	a5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	25	44
13	a6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	17	32
13	b1	327/358 (91%)	299 (91%)	26 (8%)	2 (1%)	25	44
13	b2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	17	32
13	b3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	17	32
13	b4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	17	32
13	b5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	25	44
13	b6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	17	32
13	c1	327/358 (91%)	300 (92%)	25 (8%)	2 (1%)	25	44
13	c2	325/358 (91%)	298 (92%)	24 (7%)	3 (1%)	17	32
13	c3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	17	32
13	c4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	17	32
13	c5	330/358 (92%)	302 (92%)	26 (8%)	2 (1%)	25	44
13	c6	327/358 (91%)	298 (91%)	26 (8%)	3 (1%)	17	32
All	All	12561/13452 (93%)	11740 (94%)	764 (6%)	57 (0%)	32	48

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	aA	233	ALA
13	a1	283	PRO
13	a2	283	PRO
13	a3	283	PRO
13	a4	283	PRO
13	a5	283	PRO
13	a6	283	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	bA	233	ALA
13	b1	283	PRO
13	b2	283	PRO
13	b3	283	PRO
13	b4	283	PRO
13	b5	283	PRO
13	b6	283	PRO
1	cA	233	ALA
13	c1	283	PRO
13	c2	283	PRO
13	c3	283	PRO
13	c4	283	PRO
13	c5	283	PRO
13	c6	283	PRO
3	aC	61	PHE
3	bC	61	PHE
3	cC	61	PHE
3	aC	62	LEU
13	a2	292	GLU
13	a2	303	ASP
13	a3	303	ASP
13	a4	303	ASP
13	a5	303	ASP
13	a6	292	GLU
13	a6	303	ASP
3	bC	62	LEU
13	b2	292	GLU
13	b2	303	ASP
13	b3	303	ASP
13	b4	303	ASP
13	b5	303	ASP
13	b6	292	GLU
13	b6	303	ASP
3	cC	62	LEU
13	c2	292	GLU
13	c2	303	ASP
13	c4	303	ASP
13	c5	303	ASP
13	c6	292	GLU
13	c6	303	ASP
13	a1	303	ASP
13	a3	292	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	b1	303	ASP
13	c1	303	ASP
13	c3	303	ASP
13	a4	292	GLU
13	b3	292	GLU
13	b4	292	GLU
13	c3	292	GLU
13	c4	292	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	592/604 (98%)	558 (94%)	34 (6%)	20	36
1	bA	592/604 (98%)	558 (94%)	34 (6%)	20	36
1	cA	592/604 (98%)	558 (94%)	34 (6%)	20	36
2	aB	595/597 (100%)	568 (96%)	27 (4%)	27	47
2	bB	595/597 (100%)	568 (96%)	27 (4%)	27	47
2	cB	595/597 (100%)	568 (96%)	27 (4%)	27	47
3	aC	67/67 (100%)	60 (90%)	7 (10%)	7	12
3	bC	67/67 (100%)	60 (90%)	7 (10%)	7	12
3	cC	67/67 (100%)	60 (90%)	7 (10%)	7	12
4	aD	115/115 (100%)	107 (93%)	8 (7%)	15	27
4	bD	115/115 (100%)	107 (93%)	8 (7%)	15	27
4	cD	115/115 (100%)	107 (93%)	8 (7%)	15	27
5	aE	59/64 (92%)	53 (90%)	6 (10%)	7	13
5	bE	59/64 (92%)	53 (90%)	6 (10%)	7	13
5	cE	59/64 (92%)	53 (90%)	6 (10%)	7	13
6	aF	109/128 (85%)	103 (94%)	6 (6%)	21	37
6	bF	109/128 (85%)	103 (94%)	6 (6%)	21	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	cF	109/128 (85%)	103 (94%)	6 (6%)	21	37
7	aI	32/32 (100%)	30 (94%)	2 (6%)	18	31
7	bI	32/32 (100%)	30 (94%)	2 (6%)	18	31
7	cI	32/32 (100%)	30 (94%)	2 (6%)	18	31
8	aJ	36/36 (100%)	33 (92%)	3 (8%)	11	20
8	bJ	36/36 (100%)	33 (92%)	3 (8%)	11	20
8	cJ	36/36 (100%)	33 (92%)	3 (8%)	11	20
10	aL	117/119 (98%)	113 (97%)	4 (3%)	37	58
10	bL	117/119 (98%)	113 (97%)	4 (3%)	37	58
10	cL	117/119 (98%)	113 (97%)	4 (3%)	37	58
11	aM	26/26 (100%)	21 (81%)	5 (19%)	1	2
11	bM	26/26 (100%)	21 (81%)	5 (19%)	1	2
11	cM	26/26 (100%)	21 (81%)	5 (19%)	1	2
12	aX	20/24 (83%)	19 (95%)	1 (5%)	24	42
12	bX	20/24 (83%)	19 (95%)	1 (5%)	24	42
12	cX	20/24 (83%)	19 (95%)	1 (5%)	24	42
13	a1	255/279 (91%)	237 (93%)	18 (7%)	14	26
13	a2	253/279 (91%)	237 (94%)	16 (6%)	18	31
13	a3	258/279 (92%)	241 (93%)	17 (7%)	16	29
13	a4	262/279 (94%)	247 (94%)	15 (6%)	20	36
13	a5	258/279 (92%)	241 (93%)	17 (7%)	16	29
13	a6	255/279 (91%)	238 (93%)	17 (7%)	16	29
13	b1	255/279 (91%)	237 (93%)	18 (7%)	14	26
13	b2	253/279 (91%)	237 (94%)	16 (6%)	18	31
13	b3	258/279 (92%)	241 (93%)	17 (7%)	16	29
13	b4	262/279 (94%)	247 (94%)	15 (6%)	20	36
13	b5	258/279 (92%)	241 (93%)	17 (7%)	16	29
13	b6	255/279 (91%)	238 (93%)	17 (7%)	16	29
13	c1	255/279 (91%)	238 (93%)	17 (7%)	16	29
13	c2	253/279 (91%)	237 (94%)	16 (6%)	18	31
13	c3	258/279 (92%)	241 (93%)	17 (7%)	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	c4	262/279 (94%)	247 (94%)	15 (6%)	20	36
13	c5	258/279 (92%)	241 (93%)	17 (7%)	16	29
13	c6	255/279 (91%)	240 (94%)	15 (6%)	19	34
All	All	9927/10458 (95%)	9321 (94%)	606 (6%)	22	32

All (606) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aA	11	LYS
1	aA	15	VAL
1	aA	36	ARG
1	aA	59	ASP
1	aA	74	SER
1	aA	98	SER
1	aA	115	GLN
1	aA	120	ILE
1	aA	121	VAL
1	aA	130	VAL
1	aA	171	LEU
1	aA	205	LEU
1	aA	248	LEU
1	aA	249	MET
1	aA	257	ASP
1	aA	261	PHE
1	aA	277	ASP
1	aA	281	PHE
1	aA	307	LEU
1	aA	363	MET
1	aA	365	SER
1	aA	372	GLN
1	aA	383	LEU
1	aA	390	GLN
1	aA	463	ASP
1	aA	478	THR
1	aA	511	VAL
1	aA	549	THR
1	aA	566	ILE
1	aA	628	ASP
1	aA	645	THR
1	aA	692	SER
1	aA	718	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	aA	753	SER
2	aB	48	SER
2	aB	133	ASP
2	aB	146	SER
2	aB	159	LYS
2	aB	184	VAL
2	aB	256	PHE
2	aB	308	ASP
2	aB	312	THR
2	aB	318	PHE
2	aB	329	TYR
2	aB	357	SER
2	aB	416	GLN
2	aB	429	SER
2	aB	439	LEU
2	aB	440	TYR
2	aB	444	ASP
2	aB	479	THR
2	aB	481	LEU
2	aB	494	ASN
2	aB	535	THR
2	aB	542	LYS
2	aB	565	CYS
2	aB	582	PHE
2	aB	583	TYR
2	aB	646	THR
2	aB	651	VAL
2	aB	735	THR
3	aC	3	THR
3	aC	11	ILE
3	aC	16	CYS
3	aC	44	THR
3	aC	62	LEU
3	aC	73	THR
3	aC	76	MET
4	aD	4	THR
4	aD	6	GLN
4	aD	75	ARG
4	aD	88	ASP
4	aD	92	VAL
4	aD	93	LEU
4	aD	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	aD	129	LYS
5	aE	3	ARG
5	aE	22	THR
5	aE	28	GLN
5	aE	29	THR
5	aE	51	SER
5	aE	62	LEU
6	aF	2	VAL
6	aF	6	VAL
6	aF	36	GLU
6	aF	43	CYS
6	aF	104	PRO
6	aF	124	LEU
7	aI	1	MET
7	aI	18	VAL
8	aJ	2	LYS
8	aJ	14	LEU
8	aJ	31	ARG
10	aL	22	SER
10	aL	42	SER
10	aL	69	ARG
10	aL	131	SER
11	aM	1	MET
11	aM	5	ASP
11	aM	16	LEU
11	aM	27	THR
11	aM	30	TYR
12	aX	8	THR
13	a1	38	LEU
13	a1	82	LEU
13	a1	88	LEU
13	a1	98	VAL
13	a1	111	HIS
13	a1	124	PHE
13	a1	146	ARG
13	a1	186	LEU
13	a1	205	TYR
13	a1	206	GLN
13	a1	208	HIS
13	a1	212	ILE
13	a1	250	MET
13	a1	274	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a1	284	VAL
13	a1	291	LEU
13	a1	304	THR
13	a1	341	MET
13	a2	38	LEU
13	a2	88	LEU
13	a2	98	VAL
13	a2	111	HIS
13	a2	113	ILE
13	a2	124	PHE
13	a2	146	ARG
13	a2	186	LEU
13	a2	205	TYR
13	a2	206	GLN
13	a2	208	HIS
13	a2	250	MET
13	a2	274	PHE
13	a2	284	VAL
13	a2	291	LEU
13	a2	304	THR
13	a3	38	LEU
13	a3	88	LEU
13	a3	98	VAL
13	a3	107	ILE
13	a3	111	HIS
13	a3	124	PHE
13	a3	146	ARG
13	a3	186	LEU
13	a3	205	TYR
13	a3	206	GLN
13	a3	208	HIS
13	a3	250	MET
13	a3	274	PHE
13	a3	284	VAL
13	a3	291	LEU
13	a3	304	THR
13	a3	348	LEU
13	a4	38	LEU
13	a4	88	LEU
13	a4	98	VAL
13	a4	111	HIS
13	a4	124	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a4	146	ARG
13	a4	186	LEU
13	a4	205	TYR
13	a4	206	GLN
13	a4	208	HIS
13	a4	250	MET
13	a4	274	PHE
13	a4	284	VAL
13	a4	291	LEU
13	a4	304	THR
13	a5	38	LEU
13	a5	88	LEU
13	a5	98	VAL
13	a5	111	HIS
13	a5	113	ILE
13	a5	124	PHE
13	a5	146	ARG
13	a5	186	LEU
13	a5	205	TYR
13	a5	206	GLN
13	a5	208	HIS
13	a5	250	MET
13	a5	274	PHE
13	a5	284	VAL
13	a5	291	LEU
13	a5	295	LEU
13	a5	304	THR
13	a6	38	LEU
13	a6	88	LEU
13	a6	98	VAL
13	a6	111	HIS
13	a6	113	ILE
13	a6	124	PHE
13	a6	146	ARG
13	a6	186	LEU
13	a6	205	TYR
13	a6	206	GLN
13	a6	208	HIS
13	a6	212	ILE
13	a6	250	MET
13	a6	274	PHE
13	a6	284	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a6	291	LEU
13	a6	304	THR
1	bA	11	LYS
1	bA	15	VAL
1	bA	36	ARG
1	bA	59	ASP
1	bA	74	SER
1	bA	98	SER
1	bA	115	GLN
1	bA	120	ILE
1	bA	121	VAL
1	bA	130	VAL
1	bA	171	LEU
1	bA	205	LEU
1	bA	248	LEU
1	bA	249	MET
1	bA	257	ASP
1	bA	261	PHE
1	bA	277	ASP
1	bA	281	PHE
1	bA	307	LEU
1	bA	363	MET
1	bA	365	SER
1	bA	372	GLN
1	bA	383	LEU
1	bA	390	GLN
1	bA	463	ASP
1	bA	478	THR
1	bA	511	VAL
1	bA	549	THR
1	bA	566	ILE
1	bA	628	ASP
1	bA	645	THR
1	bA	692	SER
1	bA	718	GLN
1	bA	753	SER
2	bB	48	SER
2	bB	133	ASP
2	bB	146	SER
2	bB	159	LYS
2	bB	184	VAL
2	bB	256	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	bB	308	ASP
2	bB	312	THR
2	bB	318	PHE
2	bB	329	TYR
2	bB	357	SER
2	bB	416	GLN
2	bB	429	SER
2	bB	439	LEU
2	bB	440	TYR
2	bB	444	ASP
2	bB	479	THR
2	bB	481	LEU
2	bB	494	ASN
2	bB	535	THR
2	bB	542	LYS
2	bB	565	CYS
2	bB	582	PHE
2	bB	583	TYR
2	bB	646	THR
2	bB	651	VAL
2	bB	735	THR
3	bC	3	THR
3	bC	11	ILE
3	bC	16	CYS
3	bC	44	THR
3	bC	62	LEU
3	bC	73	THR
3	bC	76	MET
4	bD	4	THR
4	bD	6	GLN
4	bD	75	ARG
4	bD	88	ASP
4	bD	92	VAL
4	bD	93	LEU
4	bD	126	SER
4	bD	129	LYS
5	bE	3	ARG
5	bE	22	THR
5	bE	28	GLN
5	bE	29	THR
5	bE	51	SER
5	bE	62	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	bF	2	VAL
6	bF	6	VAL
6	bF	36	GLU
6	bF	43	CYS
6	bF	104	PRO
6	bF	124	LEU
7	bI	1	MET
7	bI	18	VAL
8	bJ	2	LYS
8	bJ	14	LEU
8	bJ	31	ARG
10	bL	22	SER
10	bL	42	SER
10	bL	69	ARG
10	bL	131	SER
11	bM	1	MET
11	bM	5	ASP
11	bM	16	LEU
11	bM	27	THR
11	bM	30	TYR
12	bX	8	THR
13	b1	38	LEU
13	b1	82	LEU
13	b1	88	LEU
13	b1	98	VAL
13	b1	111	HIS
13	b1	113	ILE
13	b1	124	PHE
13	b1	146	ARG
13	b1	186	LEU
13	b1	205	TYR
13	b1	206	GLN
13	b1	208	HIS
13	b1	212	ILE
13	b1	250	MET
13	b1	274	PHE
13	b1	284	VAL
13	b1	291	LEU
13	b1	304	THR
13	b2	38	LEU
13	b2	88	LEU
13	b2	98	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	b2	111	HIS
13	b2	113	ILE
13	b2	124	PHE
13	b2	146	ARG
13	b2	186	LEU
13	b2	205	TYR
13	b2	206	GLN
13	b2	208	HIS
13	b2	250	MET
13	b2	274	PHE
13	b2	284	VAL
13	b2	291	LEU
13	b2	304	THR
13	b3	38	LEU
13	b3	88	LEU
13	b3	98	VAL
13	b3	107	ILE
13	b3	111	HIS
13	b3	124	PHE
13	b3	146	ARG
13	b3	186	LEU
13	b3	205	TYR
13	b3	206	GLN
13	b3	208	HIS
13	b3	250	MET
13	b3	274	PHE
13	b3	284	VAL
13	b3	291	LEU
13	b3	304	THR
13	b3	348	LEU
13	b4	38	LEU
13	b4	88	LEU
13	b4	98	VAL
13	b4	111	HIS
13	b4	124	PHE
13	b4	146	ARG
13	b4	186	LEU
13	b4	205	TYR
13	b4	206	GLN
13	b4	208	HIS
13	b4	250	MET
13	b4	274	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	b4	284	VAL
13	b4	291	LEU
13	b4	304	THR
13	b5	38	LEU
13	b5	88	LEU
13	b5	98	VAL
13	b5	111	HIS
13	b5	113	ILE
13	b5	124	PHE
13	b5	146	ARG
13	b5	186	LEU
13	b5	205	TYR
13	b5	206	GLN
13	b5	208	HIS
13	b5	250	MET
13	b5	274	PHE
13	b5	284	VAL
13	b5	291	LEU
13	b5	295	LEU
13	b5	304	THR
13	b6	38	LEU
13	b6	88	LEU
13	b6	98	VAL
13	b6	111	HIS
13	b6	113	ILE
13	b6	124	PHE
13	b6	146	ARG
13	b6	186	LEU
13	b6	205	TYR
13	b6	206	GLN
13	b6	208	HIS
13	b6	212	ILE
13	b6	250	MET
13	b6	274	PHE
13	b6	284	VAL
13	b6	291	LEU
13	b6	304	THR
1	cA	11	LYS
1	cA	15	VAL
1	cA	36	ARG
1	cA	59	ASP
1	cA	74	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	cA	98	SER
1	cA	115	GLN
1	cA	120	ILE
1	cA	121	VAL
1	cA	130	VAL
1	cA	171	LEU
1	cA	205	LEU
1	cA	248	LEU
1	cA	249	MET
1	cA	257	ASP
1	cA	261	PHE
1	cA	277	ASP
1	cA	281	PHE
1	cA	307	LEU
1	cA	363	MET
1	cA	365	SER
1	cA	372	GLN
1	cA	383	LEU
1	cA	390	GLN
1	cA	463	ASP
1	cA	478	THR
1	cA	511	VAL
1	cA	549	THR
1	cA	566	ILE
1	cA	628	ASP
1	cA	645	THR
1	cA	692	SER
1	cA	718	GLN
1	cA	753	SER
2	cB	48	SER
2	cB	133	ASP
2	cB	146	SER
2	cB	159	LYS
2	cB	184	VAL
2	cB	256	PHE
2	cB	308	ASP
2	cB	312	THR
2	cB	318	PHE
2	cB	329	TYR
2	cB	357	SER
2	cB	416	GLN
2	cB	429	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	cB	439	LEU
2	cB	440	TYR
2	cB	444	ASP
2	cB	479	THR
2	cB	481	LEU
2	cB	494	ASN
2	cB	535	THR
2	cB	542	LYS
2	cB	565	CYS
2	cB	582	PHE
2	cB	583	TYR
2	cB	646	THR
2	cB	651	VAL
2	cB	735	THR
3	cC	3	THR
3	cC	11	ILE
3	cC	16	CYS
3	cC	44	THR
3	cC	62	LEU
3	cC	73	THR
3	cC	76	MET
4	cD	4	THR
4	cD	6	GLN
4	cD	75	ARG
4	cD	88	ASP
4	cD	92	VAL
4	cD	93	LEU
4	cD	126	SER
4	cD	129	LYS
5	cE	3	ARG
5	cE	22	THR
5	cE	28	GLN
5	cE	29	THR
5	cE	51	SER
5	cE	62	LEU
6	cF	2	VAL
6	cF	6	VAL
6	cF	36	GLU
6	cF	43	CYS
6	cF	104	PRO
6	cF	124	LEU
7	cI	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	cI	18	VAL
8	cJ	2	LYS
8	cJ	14	LEU
8	cJ	31	ARG
10	cL	22	SER
10	cL	42	SER
10	cL	69	ARG
10	cL	131	SER
11	cM	1	MET
11	cM	5	ASP
11	cM	16	LEU
11	cM	27	THR
11	cM	30	TYR
12	cX	8	THR
13	c1	38	LEU
13	c1	82	LEU
13	c1	88	LEU
13	c1	98	VAL
13	c1	111	HIS
13	c1	124	PHE
13	c1	146	ARG
13	c1	186	LEU
13	c1	205	TYR
13	c1	206	GLN
13	c1	208	HIS
13	c1	212	ILE
13	c1	250	MET
13	c1	274	PHE
13	c1	284	VAL
13	c1	291	LEU
13	c1	304	THR
13	c2	38	LEU
13	c2	88	LEU
13	c2	98	VAL
13	c2	111	HIS
13	c2	113	ILE
13	c2	124	PHE
13	c2	146	ARG
13	c2	186	LEU
13	c2	205	TYR
13	c2	206	GLN
13	c2	208	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	c2	250	MET
13	c2	274	PHE
13	c2	284	VAL
13	c2	291	LEU
13	c2	304	THR
13	c3	38	LEU
13	c3	88	LEU
13	c3	98	VAL
13	c3	107	ILE
13	c3	111	HIS
13	c3	124	PHE
13	c3	146	ARG
13	c3	186	LEU
13	c3	205	TYR
13	c3	206	GLN
13	c3	208	HIS
13	c3	250	MET
13	c3	274	PHE
13	c3	284	VAL
13	c3	291	LEU
13	c3	304	THR
13	c3	348	LEU
13	c4	38	LEU
13	c4	88	LEU
13	c4	98	VAL
13	c4	111	HIS
13	c4	124	PHE
13	c4	146	ARG
13	c4	186	LEU
13	c4	205	TYR
13	c4	206	GLN
13	c4	208	HIS
13	c4	250	MET
13	c4	274	PHE
13	c4	284	VAL
13	c4	291	LEU
13	c4	304	THR
13	c5	38	LEU
13	c5	88	LEU
13	c5	98	VAL
13	c5	111	HIS
13	c5	113	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	c5	124	PHE
13	c5	146	ARG
13	c5	186	LEU
13	c5	205	TYR
13	c5	206	GLN
13	c5	208	HIS
13	c5	250	MET
13	c5	274	PHE
13	c5	284	VAL
13	c5	291	LEU
13	c5	295	LEU
13	c5	304	THR
13	c6	38	LEU
13	c6	88	LEU
13	c6	98	VAL
13	c6	111	HIS
13	c6	124	PHE
13	c6	146	ARG
13	c6	186	LEU
13	c6	205	TYR
13	c6	206	GLN
13	c6	208	HIS
13	c6	250	MET
13	c6	274	PHE
13	c6	284	VAL
13	c6	291	LEU
13	c6	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	aA	18	ASN
1	aA	192	ASN
1	aA	216	GLN
1	aA	353	HIS
1	aA	359	ASN
1	aA	542	HIS
1	aA	618	GLN
2	aB	33	HIS
2	aB	136	GLN
2	aB	234	GLN
2	aB	261	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	aB	330	ASN
2	aB	340	HIS
2	aB	406	ASN
2	aB	455	GLN
2	aB	494	ASN
2	aB	614	GLN
2	aB	678	GLN
2	aB	688	HIS
4	aD	54	ASN
4	aD	71	GLN
5	aE	18	ASN
6	aF	15	GLN
10	aL	16	HIS
13	a1	206	GLN
13	a1	320	ASN
13	a2	206	GLN
13	a2	320	ASN
13	a3	206	GLN
13	a3	320	ASN
13	a4	206	GLN
13	a4	320	ASN
13	a5	206	GLN
13	a5	320	ASN
13	a6	206	GLN
13	a6	320	ASN
1	bA	18	ASN
1	bA	192	ASN
1	bA	216	GLN
1	bA	353	HIS
1	bA	359	ASN
1	bA	542	HIS
1	bA	618	GLN
2	bB	33	HIS
2	bB	136	GLN
2	bB	234	GLN
2	bB	261	HIS
2	bB	330	ASN
2	bB	340	HIS
2	bB	406	ASN
2	bB	455	GLN
2	bB	494	ASN
2	bB	614	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	bB	678	GLN
2	bB	688	HIS
4	bD	54	ASN
4	bD	71	GLN
5	bE	18	ASN
6	bF	15	GLN
10	bL	16	HIS
13	b1	206	GLN
13	b1	320	ASN
13	b2	206	GLN
13	b2	320	ASN
13	b3	206	GLN
13	b3	320	ASN
13	b4	206	GLN
13	b4	320	ASN
13	b5	206	GLN
13	b5	320	ASN
13	b6	206	GLN
13	b6	320	ASN
1	cA	18	ASN
1	cA	192	ASN
1	cA	216	GLN
1	cA	353	HIS
1	cA	359	ASN
1	cA	542	HIS
2	cB	33	HIS
2	cB	136	GLN
2	cB	234	GLN
2	cB	261	HIS
2	cB	330	ASN
2	cB	340	HIS
2	cB	406	ASN
2	cB	455	GLN
2	cB	494	ASN
2	cB	614	GLN
2	cB	678	GLN
2	cB	688	HIS
4	cD	54	ASN
4	cD	71	GLN
5	cE	18	ASN
6	cF	15	GLN
10	cL	16	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	c1	206	GLN
13	c1	320	ASN
13	c2	111	HIS
13	c2	206	GLN
13	c2	320	ASN
13	c3	206	GLN
13	c3	320	ASN
13	c4	206	GLN
13	c4	320	ASN
13	c5	206	GLN
13	c5	320	ASN
13	c6	206	GLN
13	c6	320	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 759 ligands modelled in this entry, 3 are monoatomic - leaving 756 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	c6	407	-	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cB	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.87	12 (15%)
15	CLA	c2	409	-	45,53,73	1.66	8 (17%)	52,89,113	1.80	9 (17%)
15	CLA	aB	820	22	65,73,73	1.43	9 (13%)	76,113,113	1.44	7 (9%)
15	CLA	aB	808	-	65,73,73	1.45	10 (15%)	76,113,113	1.58	10 (13%)
15	CLA	cB	821	-	47,55,73	1.72	9 (19%)	54,91,113	1.57	6 (11%)
15	CLA	b3	403	-	65,73,73	1.38	7 (10%)	76,113,113	1.59	9 (11%)
15	CLA	b6	414	-	45,53,73	1.81	8 (17%)	52,89,113	1.83	12 (23%)
15	CLA	a6	422	-	65,73,73	1.76	14 (21%)	76,113,113	2.25	20 (26%)
18	BCR	cJ	104	-	41,41,41	1.31	3 (7%)	56,56,56	1.43	7 (12%)
15	CLA	b2	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.56	9 (11%)
18	BCR	a5	418	-	41,41,41	1.39	6 (14%)	56,56,56	1.53	10 (17%)
15	CLA	aB	840	-	65,73,73	1.51	10 (15%)	76,113,113	1.74	11 (14%)
15	CLA	aB	811	2	65,73,73	1.39	12 (18%)	76,113,113	1.71	12 (15%)
15	CLA	aB	815	-	65,73,73	1.46	9 (13%)	76,113,113	1.53	9 (11%)
15	CLA	b1	405	-	45,53,73	1.81	6 (13%)	52,89,113	2.09	20 (38%)
15	CLA	c3	409	-	65,73,73	1.47	8 (12%)	76,113,113	1.46	8 (10%)
15	CLA	c5	406	-	45,53,73	1.74	7 (15%)	52,89,113	1.68	7 (13%)
15	CLA	cA	805	-	59,67,73	1.51	11 (18%)	68,105,113	1.70	10 (14%)
18	BCR	c2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	cA	836	-	54,62,73	1.61	10 (18%)	62,99,113	1.48	6 (9%)
15	CLA	c4	403	-	65,73,73	1.40	7 (10%)	76,113,113	1.53	7 (9%)
15	CLA	aB	826	22	46,54,73	1.64	10 (21%)	53,90,113	1.97	11 (20%)
15	CLA	b1	417	13	55,63,73	1.77	6 (10%)	64,101,113	2.13	12 (18%)
15	CLA	aB	837	-	65,73,73	1.43	10 (15%)	76,113,113	1.59	10 (13%)
15	CLA	c5	415	-	45,53,73	1.80	9 (20%)	52,89,113	2.06	11 (21%)
18	BCR	c5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	bA	840	-	47,55,73	1.65	11 (23%)	54,91,113	2.01	9 (16%)
18	BCR	aB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.35	9 (16%)
18	BCR	cB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
18	BCR	a5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	11 (19%)
18	BCR	cI	102	-	41,41,41	1.37	3 (7%)	56,56,56	1.41	9 (16%)
15	CLA	cA	839	-	65,73,73	1.50	11 (16%)	76,113,113	1.54	8 (10%)
18	BCR	b6	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.53	8 (14%)
15	CLA	bA	806	-	65,73,73	1.47	11 (16%)	76,113,113	1.73	9 (11%)
15	CLA	aA	808	-	51,59,73	1.63	9 (17%)	59,96,113	1.62	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a1	402	-	65,73,73	1.40	7 (10%)	76,113,113	1.56	9 (11%)
15	CLA	bB	801	-	65,73,73	1.51	11 (16%)	76,113,113	1.49	9 (11%)
15	CLA	b6	405	-	65,73,73	1.51	8 (12%)	76,113,113	1.45	9 (11%)
15	CLA	a3	403	-	65,73,73	1.40	7 (10%)	76,113,113	1.57	9 (11%)
18	BCR	c3	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
15	CLA	b1	413	-	45,53,73	1.80	8 (17%)	52,89,113	1.53	5 (9%)
15	CLA	cB	823	-	55,63,73	1.48	6 (10%)	64,101,113	1.67	8 (12%)
15	CLA	b3	412	-	45,53,73	1.82	10 (22%)	52,89,113	1.73	14 (26%)
15	CLA	a2	411	13	64,72,73	1.48	8 (12%)	74,111,113	1.71	14 (18%)
18	BCR	aI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
15	CLA	cB	805	-	54,62,73	1.55	10 (18%)	62,99,113	1.66	7 (11%)
15	CLA	bA	827	22	65,73,73	1.42	9 (13%)	76,113,113	1.61	12 (15%)
15	CLA	bA	817	-	49,57,73	1.69	8 (16%)	55,93,113	1.59	6 (10%)
15	CLA	bB	835	-	45,53,73	1.68	10 (22%)	52,89,113	1.87	8 (15%)
18	BCR	bA	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
15	CLA	c4	412	-	45,53,73	1.81	10 (22%)	52,89,113	1.71	14 (26%)
15	CLA	aB	825	2	54,62,73	1.52	9 (16%)	62,99,113	1.76	10 (16%)
15	CLA	bA	820	-	65,73,73	1.47	10 (15%)	76,113,113	1.67	10 (13%)
15	CLA	cB	841	-	45,53,73	1.82	9 (20%)	52,89,113	1.67	9 (17%)
18	BCR	bL	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.45	9 (16%)
18	BCR	c1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.65	12 (21%)
15	CLA	b4	411	13	45,53,73	1.77	7 (15%)	52,89,113	1.89	8 (15%)
15	CLA	c3	407	-	45,53,73	1.70	8 (17%)	52,89,113	1.71	8 (15%)
15	CLA	cA	837	1	45,53,73	1.76	8 (17%)	52,89,113	1.74	7 (13%)
15	CLA	b3	413	-	45,53,73	1.76	9 (20%)	52,89,113	1.63	5 (9%)
15	CLA	a1	406	-	45,53,73	1.71	7 (15%)	52,89,113	1.74	9 (17%)
15	CLA	a5	417	13	55,63,73	1.77	6 (10%)	64,101,113	2.13	11 (17%)
15	CLA	b6	406	-	45,53,73	1.84	6 (13%)	52,89,113	2.11	19 (36%)
17	SF4	cC	101	3	0,12,12	-	-	-		
15	CLA	bB	831	-	45,53,73	1.67	10 (22%)	52,89,113	1.65	6 (11%)
15	CLA	cA	819	-	54,62,73	1.59	9 (16%)	62,99,113	1.68	10 (16%)
15	CLA	b2	413	-	45,53,73	1.83	10 (22%)	52,89,113	1.77	15 (28%)
15	CLA	cL	201	10	65,73,73	1.47	10 (15%)	76,113,113	1.33	8 (10%)
15	CLA	cA	802	22	65,73,73	1.58	12 (18%)	76,113,113	1.59	10 (13%)
15	CLA	bB	821	-	47,55,73	1.71	9 (19%)	54,91,113	1.57	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a3	416	-	50,58,73	1.65	10 (20%)	58,95,113	2.51	18 (31%)
15	CLA	a3	417	13	55,63,73	1.77	5 (9%)	64,101,113	2.12	14 (21%)
15	CLA	bB	816	-	45,53,73	1.62	9 (20%)	52,89,113	1.96	7 (13%)
15	CLA	bA	814	-	60,68,73	1.50	10 (16%)	70,107,113	1.48	8 (11%)
15	CLA	c4	413	-	45,53,73	1.79	8 (17%)	52,89,113	1.61	5 (9%)
15	CLA	a4	412	-	45,53,73	1.81	10 (22%)	52,89,113	1.72	14 (26%)
15	CLA	cA	808	-	51,59,73	1.63	9 (17%)	59,96,113	1.62	9 (15%)
18	BCR	a4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.49	11 (19%)
15	CLA	aB	809	-	65,73,73	1.45	11 (16%)	76,113,113	1.62	10 (13%)
15	CLA	c1	414	-	41,49,73	1.86	7 (17%)	47,84,113	1.77	7 (14%)
15	CLA	a1	410	13	45,53,73	1.75	8 (17%)	52,89,113	1.87	7 (13%)
15	CLA	b6	410	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	8 (10%)
15	CLA	b3	408	-	45,53,73	1.67	8 (17%)	52,89,113	1.82	10 (19%)
20	LMG	bB	851	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	c5	413	-	45,53,73	1.77	10 (22%)	52,89,113	1.63	5 (9%)
15	CLA	aB	842	-	45,53,73	1.82	7 (15%)	52,89,113	1.55	5 (9%)
15	CLA	a6	406	-	45,53,73	1.83	6 (13%)	52,89,113	2.11	19 (36%)
15	CLA	aB	807	-	65,73,73	1.49	11 (16%)	76,113,113	1.59	9 (11%)
15	CLA	aA	811	-	45,53,73	1.74	10 (22%)	52,89,113	1.62	7 (13%)
15	CLA	cA	825	-	59,67,73	1.53	10 (16%)	68,105,113	1.49	9 (13%)
15	CLA	c1	412	-	45,53,73	1.79	10 (22%)	52,89,113	1.79	14 (26%)
15	CLA	b1	409	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	a5	408	-	45,53,73	1.69	8 (17%)	52,89,113	1.84	9 (17%)
18	BCR	a1	417	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	8 (14%)
15	CLA	aA	842	22	51,59,73	1.66	8 (15%)	59,96,113	1.42	10 (16%)
15	CLA	bB	823	-	55,63,73	1.48	7 (12%)	64,101,113	1.67	8 (12%)
15	CLA	c1	402	-	65,73,73	1.43	7 (10%)	76,113,113	1.46	7 (9%)
15	CLA	bB	806	-	65,73,73	1.40	10 (15%)	76,113,113	1.68	10 (13%)
15	CLA	a2	407	-	45,53,73	1.72	6 (13%)	52,89,113	1.65	7 (13%)
15	CLA	cB	825	2	54,62,73	1.53	9 (16%)	62,99,113	1.76	10 (16%)
15	CLA	aA	809	1	65,73,73	1.43	10 (15%)	76,113,113	1.54	10 (13%)
14	CL0	cA	801	-	65,73,73	1.92	17 (26%)	76,113,113	2.78	33 (43%)
18	BCR	aB	847	-	25,25,41	1.18	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	cA	818	-	54,62,73	1.56	8 (14%)	62,99,113	1.76	8 (12%)
18	BCR	bI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c6	403	-	65,73,73	1.42	6 (9%)	76,113,113	1.46	7 (9%)
15	CLA	aA	806	-	65,73,73	1.47	11 (16%)	76,113,113	1.73	10 (13%)
15	CLA	a4	408	-	45,53,73	1.66	8 (17%)	52,89,113	1.81	8 (15%)
15	CLA	bA	808	-	51,59,73	1.63	9 (17%)	59,96,113	1.62	9 (15%)
15	CLA	b6	408	-	45,53,73	1.72	7 (15%)	52,89,113	1.72	9 (17%)
15	CLA	bB	828	-	65,73,73	1.39	12 (18%)	76,113,113	1.67	8 (10%)
15	CLA	a1	404	-	45,53,73	1.79	9 (20%)	52,89,113	2.09	19 (36%)
18	BCR	cA	850	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	c2	402	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
15	CLA	bA	804	-	65,73,73	1.50	9 (13%)	76,113,113	1.55	11 (14%)
15	CLA	bB	802	-	65,73,73	1.51	12 (18%)	76,113,113	1.52	9 (11%)
15	CLA	a2	413	-	45,53,73	1.81	10 (22%)	52,89,113	1.76	15 (28%)
15	CLA	bA	813	-	54,62,73	1.62	9 (16%)	62,99,113	1.53	9 (14%)
15	CLA	aL	201	10	65,73,73	1.48	10 (15%)	76,113,113	1.33	8 (10%)
18	BCR	cK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
15	CLA	a6	412	13	45,53,73	1.70	8 (17%)	52,89,113	1.87	10 (19%)
15	CLA	b4	402	-	65,73,73	1.41	7 (10%)	76,113,113	1.49	8 (10%)
15	CLA	bB	827	-	65,73,73	1.42	9 (13%)	76,113,113	1.69	13 (17%)
15	CLA	c5	409	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	7 (9%)
15	CLA	b3	411	13	45,53,73	1.75	8 (17%)	52,89,113	1.86	9 (17%)
15	CLA	a4	405	-	45,53,73	1.78	9 (20%)	52,89,113	2.16	21 (40%)
15	CLA	a5	404	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	9 (11%)
15	CLA	aB	803	-	65,73,73	1.42	9 (13%)	76,113,113	1.67	13 (17%)
15	CLA	b6	416	-	45,53,73	1.83	9 (20%)	52,89,113	2.06	10 (19%)
15	CLA	a4	404	-	65,73,73	1.47	8 (12%)	76,113,113	1.42	8 (10%)
15	CLA	bB	810	2	65,73,73	1.47	12 (18%)	76,113,113	1.66	10 (13%)
15	CLA	aJ	201	-	45,53,73	1.73	10 (22%)	52,89,113	1.83	10 (19%)
18	BCR	bB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	c3	405	-	45,53,73	1.78	10 (22%)	52,89,113	2.11	20 (38%)
18	BCR	b1	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	8 (14%)
15	CLA	bB	840	-	65,73,73	1.52	10 (15%)	76,113,113	1.73	11 (14%)
15	CLA	bB	838	-	47,55,73	1.67	10 (21%)	54,91,113	1.85	9 (16%)
15	CLA	bA	832	-	50,58,73	1.58	11 (22%)	58,95,113	1.81	10 (17%)
18	BCR	b1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
15	CLA	bA	833	-	65,73,73	1.40	12 (18%)	76,113,113	1.49	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	bA	852	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	bA	831	-	65,73,73	1.53	11 (16%)	76,113,113	1.63	9 (11%)
15	CLA	aA	807	-	65,73,73	1.50	12 (18%)	76,113,113	1.59	12 (15%)
18	BCR	b6	401	-	41,41,41	1.18	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	b3	407	-	45,53,73	1.69	8 (17%)	52,89,113	1.71	8 (15%)
15	CLA	aA	844	-	42,49,73	1.72	7 (16%)	48,83,113	1.76	6 (12%)
19	LHG	bA	854	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	c3	415	-	45,53,73	1.77	10 (22%)	52,89,113	2.04	10 (19%)
15	CLA	b2	411	13	64,72,73	1.47	9 (14%)	74,111,113	1.70	14 (18%)
15	CLA	c5	416	-	50,58,73	1.60	9 (18%)	58,95,113	2.53	16 (27%)
15	CLA	b1	415	-	45,53,73	1.77	9 (20%)	52,89,113	2.03	10 (19%)
15	CLA	a3	409	-	65,73,73	1.47	8 (12%)	76,113,113	1.45	8 (10%)
15	CLA	c5	417	13	55,63,73	1.76	5 (9%)	64,101,113	2.14	11 (17%)
18	BCR	b2	419	-	41,41,41	1.36	5 (12%)	56,56,56	1.55	9 (16%)
19	LHG	bA	855	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	bA	802	22	65,73,73	1.58	13 (20%)	76,113,113	1.59	10 (13%)
15	CLA	c3	412	-	45,53,73	1.80	10 (22%)	52,89,113	1.74	14 (26%)
15	CLA	b4	409	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
17	SF4	bA	847	2,1	0,12,12	-	-	-		
15	CLA	aB	819	-	60,68,73	1.44	11 (18%)	70,107,113	1.74	8 (11%)
15	CLA	aB	836	-	60,68,73	1.52	10 (16%)	70,107,113	1.55	11 (15%)
15	CLA	a6	408	-	45,53,73	1.73	7 (15%)	52,89,113	1.71	9 (17%)
15	CLA	aA	839	-	65,73,73	1.49	11 (16%)	76,113,113	1.54	8 (10%)
15	CLA	c1	416	-	50,58,73	1.61	10 (20%)	58,95,113	2.54	17 (29%)
15	CLA	a6	418	13	55,63,73	1.80	5 (9%)	64,101,113	2.09	10 (15%)
15	CLA	cA	830	-	65,73,73	1.42	11 (16%)	76,113,113	1.67	10 (13%)
15	CLA	a3	415	-	45,53,73	1.76	11 (24%)	52,89,113	2.05	10 (19%)
15	CLA	cA	803	-	65,73,73	1.42	11 (16%)	76,113,113	1.90	14 (18%)
18	BCR	a6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	bA	834	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	11 (14%)
15	CLA	bL	204	22	65,73,73	1.44	10 (15%)	76,113,113	1.41	8 (10%)
15	CLA	aA	841	-	65,73,73	1.52	9 (13%)	76,113,113	1.45	8 (10%)
15	CLA	c4	402	-	65,73,73	1.42	6 (9%)	76,113,113	1.49	8 (10%)
15	CLA	bL	202	10	65,73,73	1.48	10 (15%)	76,113,113	1.33	8 (10%)
15	CLA	b1	414	-	41,49,73	1.87	7 (17%)	47,84,113	1.76	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b4	412	-	45,53,73	1.81	10 (22%)	52,89,113	1.73	14 (26%)
15	CLA	aA	830	-	65,73,73	1.41	11 (16%)	76,113,113	1.67	10 (13%)
18	BCR	aA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
15	CLA	aL	202	-	65,73,73	1.43	11 (16%)	76,113,113	1.71	10 (13%)
18	BCR	a1	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.59	9 (16%)
15	CLA	c1	413	-	45,53,73	1.79	8 (17%)	52,89,113	1.55	5 (9%)
15	CLA	aA	820	-	65,73,73	1.46	10 (15%)	76,113,113	1.67	9 (11%)
15	CLA	bF	201	-	45,53,73	1.73	11 (24%)	52,89,113	1.83	10 (19%)
15	CLA	a2	415	-	41,49,73	1.85	7 (17%)	47,84,113	1.77	7 (14%)
15	CLA	aA	815	-	45,53,73	1.74	10 (22%)	52,89,113	1.64	10 (19%)
15	CLA	b6	409	-	45,53,73	1.70	8 (17%)	52,89,113	1.85	8 (15%)
15	CLA	a6	404	-	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
15	CLA	c5	420	-	65,73,73	1.61	10 (15%)	76,113,113	1.94	18 (23%)
15	CLA	aA	826	-	65,73,73	1.35	8 (12%)	76,113,113	1.63	10 (13%)
18	BCR	bA	849	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	b5	413	-	45,53,73	1.76	9 (20%)	52,89,113	1.60	5 (9%)
18	BCR	bM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	bA	828	-	65,73,73	1.51	10 (15%)	76,113,113	1.40	8 (10%)
15	CLA	b4	413	-	45,53,73	1.78	8 (17%)	52,89,113	1.60	5 (9%)
15	CLA	a5	410	13	64,72,73	1.48	8 (12%)	74,111,113	1.74	14 (18%)
15	CLA	a1	414	-	45,53,73	1.77	10 (22%)	52,89,113	2.06	10 (19%)
15	CLA	bA	829	-	65,73,73	1.40	8 (12%)	76,113,113	1.65	12 (15%)
18	BCR	a2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.44	8 (14%)
15	CLA	cB	819	-	60,68,73	1.44	11 (18%)	70,107,113	1.74	8 (11%)
15	CLA	bB	833	-	65,73,73	1.53	9 (13%)	76,113,113	1.46	13 (17%)
18	BCR	a3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	c5	402	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	7 (9%)
15	CLA	a1	407	-	45,53,73	1.68	8 (17%)	52,89,113	1.83	8 (15%)
15	CLA	a6	411	13	64,72,73	1.50	8 (12%)	74,111,113	1.68	14 (18%)
15	CLA	a6	416	-	45,53,73	1.84	9 (20%)	52,89,113	2.05	10 (19%)
15	CLA	a4	411	13	45,53,73	1.75	7 (15%)	52,89,113	1.88	8 (15%)
15	CLA	aB	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.87	12 (15%)
15	CLA	aA	822	-	65,73,73	1.42	11 (16%)	76,113,113	1.53	8 (10%)
18	BCR	bB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	cF	203	-	45,53,73	1.72	11 (24%)	52,89,113	1.83	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b1	406	-	45,53,73	1.75	7 (15%)	52,89,113	1.66	7 (13%)
18	BCR	b1	401	-	41,41,41	1.16	4 (9%)	56,56,56	1.54	10 (17%)
15	CLA	cB	835	-	45,53,73	1.68	9 (20%)	52,89,113	1.86	8 (15%)
15	CLA	aB	816	-	45,53,73	1.61	9 (20%)	52,89,113	1.96	7 (13%)
15	CLA	bB	814	-	65,73,73	1.43	8 (12%)	76,113,113	1.71	15 (19%)
18	BCR	b3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	aA	819	-	54,62,73	1.59	9 (16%)	62,99,113	1.67	10 (16%)
15	CLA	aA	836	-	54,62,73	1.60	10 (18%)	62,99,113	1.48	7 (11%)
18	BCR	a6	421	-	41,41,41	1.11	4 (9%)	56,56,56	1.55	9 (16%)
15	CLA	cA	815	-	45,53,73	1.74	10 (22%)	52,89,113	1.65	10 (19%)
15	CLA	a4	403	-	65,73,73	1.40	7 (10%)	76,113,113	1.53	8 (10%)
15	CLA	bX	102	12	45,53,73	1.80	9 (20%)	52,89,113	1.82	11 (21%)
15	CLA	c4	409	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
15	CLA	bA	839	-	65,73,73	1.50	11 (16%)	76,113,113	1.54	8 (10%)
15	CLA	cB	810	2	65,73,73	1.47	12 (18%)	76,113,113	1.67	10 (13%)
15	CLA	c2	412	13	45,53,73	1.77	9 (20%)	52,89,113	1.88	9 (17%)
15	CLA	aA	831	-	65,73,73	1.54	11 (16%)	76,113,113	1.63	9 (11%)
15	CLA	b2	415	-	41,49,73	1.85	7 (17%)	47,84,113	1.77	7 (14%)
15	CLA	aA	821	-	61,69,73	1.52	11 (18%)	71,108,113	1.50	9 (12%)
15	CLA	c1	404	-	65,73,73	1.48	8 (12%)	76,113,113	1.44	8 (10%)
18	BCR	c6	419	-	41,41,41	1.36	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	cA	809	1	65,73,73	1.43	10 (15%)	76,113,113	1.55	10 (13%)
15	CLA	a5	402	-	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
18	BCR	cA	847	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	c1	411	13	45,53,73	1.75	8 (17%)	52,89,113	1.87	8 (15%)
18	BCR	cM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.34	9 (16%)
17	SF4	aA	847	2,1	0,12,12	-	-	-		
15	CLA	bB	822	-	45,53,73	1.68	6 (13%)	52,89,113	1.81	7 (13%)
15	CLA	a5	416	-	50,58,73	1.60	9 (18%)	58,95,113	2.54	16 (27%)
15	CLA	c6	417	-	50,58,73	1.61	9 (18%)	58,95,113	2.55	18 (31%)
15	CLA	cB	826	22	46,54,73	1.63	10 (21%)	53,90,113	1.98	11 (20%)
18	BCR	c4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	c2	404	-	65,73,73	1.48	9 (13%)	76,113,113	1.46	9 (11%)
15	CLA	b5	411	13	45,53,73	1.74	8 (17%)	52,89,113	1.88	9 (17%)
15	CLA	b1	416	-	50,58,73	1.62	9 (18%)	58,95,113	2.52	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	cB	848	-	41,41,41	1.33	4 (9%)	56,56,56	1.50	8 (14%)
18	BCR	cI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.28	5 (8%)
15	CLA	b3	415	-	45,53,73	1.77	11 (24%)	52,89,113	2.05	10 (19%)
15	CLA	cA	841	-	65,73,73	1.53	9 (13%)	76,113,113	1.46	9 (11%)
15	CLA	b4	417	13	55,63,73	1.79	7 (12%)	64,101,113	2.14	12 (18%)
15	CLA	b2	412	13	45,53,73	1.76	9 (20%)	52,89,113	1.89	9 (17%)
18	BCR	b2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	c6	408	-	45,53,73	1.73	7 (15%)	52,89,113	1.69	8 (15%)
15	CLA	cA	816	-	45,53,73	1.68	8 (17%)	52,89,113	1.88	6 (11%)
15	CLA	cA	828	-	65,73,73	1.50	10 (15%)	76,113,113	1.41	8 (10%)
15	CLA	cB	838	-	47,55,73	1.67	10 (21%)	54,91,113	1.87	9 (16%)
15	CLA	c4	408	-	45,53,73	1.67	8 (17%)	52,89,113	1.82	8 (15%)
15	CLA	c6	414	-	45,53,73	1.80	7 (15%)	52,89,113	1.77	10 (19%)
15	CLA	b4	403	-	65,73,73	1.40	7 (10%)	76,113,113	1.53	7 (9%)
15	CLA	a1	401	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	7 (9%)
15	CLA	bA	843	-	65,73,73	1.54	10 (15%)	76,113,113	1.57	9 (11%)
15	CLA	cA	807	-	65,73,73	1.50	12 (18%)	76,113,113	1.59	12 (15%)
15	CLA	c2	418	13	55,63,73	1.80	6 (10%)	64,101,113	2.11	11 (17%)
18	BCR	a6	402	-	41,41,41	1.24	4 (9%)	56,56,56	1.71	10 (17%)
15	CLA	bB	834	-	58,66,73	1.56	10 (17%)	67,104,113	1.61	12 (17%)
15	CLA	b4	410	13	64,72,73	1.50	9 (14%)	74,111,113	1.72	14 (18%)
15	CLA	b2	408	-	45,53,73	1.72	8 (17%)	52,89,113	1.68	9 (17%)
15	CLA	b5	412	-	45,53,73	1.79	10 (22%)	52,89,113	1.76	13 (25%)
15	CLA	a1	412	-	45,53,73	1.80	8 (17%)	52,89,113	1.55	5 (9%)
15	CLA	bA	825	-	59,67,73	1.53	10 (16%)	68,105,113	1.49	10 (14%)
15	CLA	aA	816	-	45,53,73	1.68	8 (17%)	52,89,113	1.87	6 (11%)
15	CLA	aA	828	-	65,73,73	1.51	10 (15%)	76,113,113	1.40	8 (10%)
16	PQN	cB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
18	BCR	a3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.67	9 (16%)
18	BCR	c4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	aB	810	2	65,73,73	1.48	12 (18%)	76,113,113	1.66	10 (13%)
15	CLA	c3	417	13	55,63,73	1.79	5 (9%)	64,101,113	2.12	14 (21%)
18	BCR	a3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	9 (16%)
15	CLA	c2	422	-	65,73,73	1.60	10 (15%)	76,113,113	1.87	18 (23%)
15	CLA	a2	416	-	45,53,73	1.77	10 (22%)	52,89,113	2.03	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a2	417	-	50,58,73	1.62	9 (18%)	58,95,113	2.64	20 (34%)
18	BCR	c5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.41	11 (19%)
15	CLA	aA	803	-	65,73,73	1.42	11 (16%)	76,113,113	1.90	14 (18%)
15	CLA	b4	407	-	45,53,73	1.71	8 (17%)	52,89,113	1.70	8 (15%)
15	CLA	cB	832	-	49,57,73	1.60	11 (22%)	55,93,113	1.71	7 (12%)
14	CL0	aA	801	-	65,73,73	1.92	17 (26%)	76,113,113	2.77	33 (43%)
15	CLA	aA	827	22	65,73,73	1.42	9 (13%)	76,113,113	1.61	12 (15%)
15	CLA	aB	823	-	55,63,73	1.47	6 (10%)	64,101,113	1.67	8 (12%)
15	CLA	b3	405	-	45,53,73	1.78	10 (22%)	52,89,113	2.11	19 (36%)
15	CLA	bB	812	-	45,53,73	1.70	7 (15%)	52,89,113	1.63	8 (15%)
15	CLA	bL	203	-	65,73,73	1.43	11 (16%)	76,113,113	1.72	10 (13%)
15	CLA	a3	408	-	45,53,73	1.67	8 (17%)	52,89,113	1.82	10 (19%)
15	CLA	b2	410	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	8 (10%)
15	CLA	c2	407	-	45,53,73	1.73	6 (13%)	52,89,113	1.65	7 (13%)
15	CLA	bB	837	-	65,73,73	1.44	10 (15%)	76,113,113	1.60	9 (11%)
15	CLA	b1	410	13	64,72,73	1.50	8 (12%)	74,111,113	1.73	14 (18%)
15	CLA	b4	421	-	65,73,73	1.65	13 (20%)	76,113,113	1.75	16 (21%)
15	CLA	b6	403	-	65,73,73	1.42	6 (9%)	76,113,113	1.46	7 (9%)
15	CLA	bB	817	-	55,63,73	1.48	8 (14%)	64,101,113	1.74	11 (17%)
18	BCR	a5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
15	CLA	cB	837	-	65,73,73	1.44	10 (15%)	76,113,113	1.60	8 (10%)
15	CLA	c1	410	13	64,72,73	1.48	9 (14%)	74,111,113	1.72	14 (18%)
15	CLA	c3	414	-	41,49,73	1.86	8 (19%)	47,84,113	1.79	7 (14%)
15	CLA	a2	422	-	65,73,73	1.61	10 (15%)	76,113,113	1.87	18 (23%)
15	CLA	cB	802	-	65,73,73	1.52	13 (20%)	76,113,113	1.52	10 (13%)
15	CLA	aB	822	-	45,53,73	1.67	6 (13%)	52,89,113	1.81	7 (13%)
15	CLA	cB	807	-	65,73,73	1.49	11 (16%)	76,113,113	1.60	9 (11%)
15	CLA	aB	817	-	55,63,73	1.48	8 (14%)	64,101,113	1.73	10 (15%)
15	CLA	c4	404	-	65,73,73	1.49	8 (12%)	76,113,113	1.41	8 (10%)
18	BCR	b2	401	-	41,41,41	1.24	4 (9%)	56,56,56	1.82	12 (21%)
15	CLA	c4	414	-	41,49,73	1.88	9 (21%)	47,84,113	1.76	7 (14%)
15	CLA	bA	816	-	45,53,73	1.68	8 (17%)	52,89,113	1.87	6 (11%)
15	CLA	cA	826	-	65,73,73	1.35	8 (12%)	76,113,113	1.63	10 (13%)
15	CLA	c6	406	-	45,53,73	1.83	7 (15%)	52,89,113	2.11	19 (36%)
15	CLA	a3	405	-	45,53,73	1.78	10 (22%)	52,89,113	2.11	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cA	842	-	65,73,73	1.53	10 (15%)	76,113,113	1.58	9 (11%)
15	CLA	cB	834	-	58,66,73	1.55	10 (17%)	67,104,113	1.60	12 (17%)
15	CLA	cB	804	-	65,73,73	1.47	9 (13%)	76,113,113	2.05	16 (21%)
15	CLA	aA	817	-	49,57,73	1.69	8 (16%)	55,93,113	1.60	6 (10%)
15	CLA	b2	422	-	65,73,73	1.60	10 (15%)	76,113,113	1.87	18 (23%)
18	BCR	aB	845	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	6 (10%)
18	BCR	aA	851	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	c6	415	-	41,49,73	1.88	7 (17%)	47,84,113	1.76	7 (14%)
15	CLA	cB	813	-	45,53,73	1.78	9 (20%)	52,89,113	1.74	7 (13%)
15	CLA	b4	414	-	41,49,73	1.87	8 (19%)	47,84,113	1.77	7 (14%)
15	CLA	cB	809	-	65,73,73	1.45	11 (16%)	76,113,113	1.62	10 (13%)
15	CLA	c3	402	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	7 (9%)
15	CLA	b5	403	-	65,73,73	1.40	7 (10%)	76,113,113	1.56	10 (13%)
15	CLA	aB	813	-	45,53,73	1.79	9 (20%)	52,89,113	1.73	7 (13%)
18	BCR	a2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	a2	410	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	8 (10%)
15	CLA	cJ	102	-	38,45,73	1.82	9 (23%)	43,78,113	1.83	7 (16%)
15	CLA	b6	417	-	50,58,73	1.62	9 (18%)	58,95,113	2.55	18 (31%)
15	CLA	c5	404	-	65,73,73	1.47	8 (12%)	76,113,113	1.45	9 (11%)
15	CLA	cA	810	1	65,73,73	1.43	9 (13%)	76,113,113	1.56	8 (10%)
15	CLA	c6	410	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
15	CLA	b1	404	-	65,73,73	1.48	7 (10%)	76,113,113	1.45	9 (11%)
18	BCR	b3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	10 (17%)
18	BCR	cB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	cL	202	-	65,73,73	1.43	11 (16%)	76,113,113	1.71	10 (13%)
15	CLA	aB	824	-	45,53,73	1.74	8 (17%)	52,89,113	1.63	11 (21%)
15	CLA	cB	812	-	45,53,73	1.69	6 (13%)	52,89,113	1.63	7 (13%)
15	CLA	aB	838	-	47,55,73	1.67	11 (23%)	54,91,113	1.86	9 (16%)
15	CLA	c2	414	-	45,53,73	1.77	9 (20%)	52,89,113	1.61	5 (9%)
15	CLA	bB	818	-	59,67,73	1.43	8 (13%)	68,105,113	1.66	12 (17%)
15	CLA	b2	402	-	65,73,73	1.45	6 (9%)	76,113,113	1.47	7 (9%)
15	CLA	bA	805	-	59,67,73	1.50	11 (18%)	68,105,113	1.70	10 (14%)
15	CLA	c5	408	-	45,53,73	1.68	8 (17%)	52,89,113	1.83	9 (17%)
15	CLA	b6	413	-	45,53,73	1.81	10 (22%)	52,89,113	1.70	14 (26%)
15	CLA	aA	810	1	65,73,73	1.43	9 (13%)	76,113,113	1.55	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cB	818	-	59,67,73	1.43	9 (15%)	68,105,113	1.66	12 (17%)
15	CLA	bA	821	-	61,69,73	1.50	11 (18%)	71,108,113	1.50	9 (12%)
15	CLA	c3	406	-	45,53,73	1.74	7 (15%)	52,89,113	1.66	7 (13%)
15	CLA	aB	832	-	49,57,73	1.59	11 (22%)	55,93,113	1.71	7 (12%)
15	CLA	aB	833	-	65,73,73	1.53	9 (13%)	76,113,113	1.47	13 (17%)
15	CLA	a1	413	-	41,49,73	1.85	7 (17%)	47,84,113	1.76	8 (17%)
18	BCR	cA	849	-	41,41,41	1.19	2 (4%)	56,56,56	1.44	9 (16%)
18	BCR	cF	204	-	41,41,41	1.20	3 (7%)	56,56,56	1.43	10 (17%)
15	CLA	aB	831	-	45,53,73	1.68	11 (24%)	52,89,113	1.65	6 (11%)
15	CLA	bA	841	-	65,73,73	1.53	9 (13%)	76,113,113	1.45	9 (11%)
15	CLA	aK	102	-	45,53,73	1.67	8 (17%)	52,89,113	1.64	10 (19%)
15	CLA	c6	412	13	45,53,73	1.71	7 (15%)	52,89,113	1.87	10 (19%)
18	BCR	bL	206	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	b2	416	-	45,53,73	1.78	10 (22%)	52,89,113	2.03	10 (19%)
15	CLA	b2	417	-	50,58,73	1.63	9 (18%)	58,95,113	2.60	18 (31%)
15	CLA	aA	823	-	49,57,73	1.62	9 (18%)	55,93,113	1.58	7 (12%)
17	SF4	cA	846	2,1	0,12,12	-	-	-		
15	CLA	bA	830	-	65,73,73	1.42	10 (15%)	76,113,113	1.67	10 (13%)
15	CLA	b3	409	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	8 (10%)
15	CLA	c4	421	-	65,73,73	1.63	12 (18%)	76,113,113	1.75	16 (21%)
15	CLA	a2	414	-	45,53,73	1.78	8 (17%)	52,89,113	1.61	5 (9%)
15	CLA	cB	811	2	65,73,73	1.39	11 (16%)	76,113,113	1.72	12 (15%)
15	CLA	cB	815	-	65,73,73	1.45	9 (13%)	76,113,113	1.53	9 (11%)
15	CLA	cB	840	-	65,73,73	1.52	10 (15%)	76,113,113	1.74	11 (14%)
15	CLA	c4	406	-	45,53,73	1.74	7 (15%)	52,89,113	1.66	7 (13%)
17	SF4	cC	102	3	0,12,12	-	-	-		
18	BCR	c4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.49	10 (17%)
15	CLA	a3	402	-	65,73,73	1.42	7 (10%)	76,113,113	1.48	7 (9%)
15	CLA	a5	414	-	41,49,73	1.86	7 (17%)	47,84,113	1.79	8 (17%)
15	CLA	a3	410	13	64,72,73	1.47	9 (14%)	74,111,113	1.72	14 (18%)
15	CLA	c2	411	13	64,72,73	1.49	8 (12%)	74,111,113	1.71	14 (18%)
15	CLA	c6	413	-	45,53,73	1.82	10 (22%)	52,89,113	1.71	14 (26%)
15	CLA	a6	403	-	65,73,73	1.43	6 (9%)	76,113,113	1.46	7 (9%)
15	CLA	c5	407	-	45,53,73	1.73	7 (15%)	52,89,113	1.70	9 (17%)
15	CLA	b1	407	-	45,53,73	1.70	7 (15%)	52,89,113	1.74	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	aB	801	-	65,73,73	1.51	11 (16%)	76,113,113	1.50	10 (13%)
15	CLA	c4	410	13	64,72,73	1.49	9 (14%)	74,111,113	1.70	14 (18%)
15	CLA	bB	839	22	65,73,73	1.43	10 (15%)	76,113,113	1.53	10 (13%)
15	CLA	cB	820	22	65,73,73	1.43	9 (13%)	76,113,113	1.43	7 (9%)
15	CLA	bA	819	-	54,62,73	1.58	9 (16%)	62,99,113	1.68	10 (16%)
15	CLA	cA	835	-	65,73,73	1.51	10 (15%)	76,113,113	1.63	11 (14%)
18	BCR	bA	853	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	6 (10%)
15	CLA	a3	406	-	45,53,73	1.75	7 (15%)	52,89,113	1.66	7 (13%)
15	CLA	a4	409	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
15	CLA	aA	813	-	54,62,73	1.62	9 (16%)	62,99,113	1.53	10 (16%)
18	BCR	a1	420	-	41,41,41	1.14	3 (7%)	56,56,56	1.51	10 (17%)
18	BCR	c3	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.54	10 (17%)
15	CLA	b4	415	-	45,53,73	1.76	10 (22%)	52,89,113	2.09	12 (23%)
15	CLA	bB	820	22	65,73,73	1.43	9 (13%)	76,113,113	1.43	7 (9%)
15	CLA	cB	822	-	45,53,73	1.69	6 (13%)	52,89,113	1.81	7 (13%)
15	CLA	cB	814	-	65,73,73	1.43	8 (12%)	76,113,113	1.71	15 (19%)
15	CLA	bA	803	-	65,73,73	1.42	11 (16%)	76,113,113	1.89	14 (18%)
18	BCR	b4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	a2	406	-	65,73,73	1.67	11 (16%)	76,113,113	1.98	19 (25%)
15	CLA	bB	826	22	46,54,73	1.63	10 (21%)	53,90,113	1.98	11 (20%)
15	CLA	cB	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.67	13 (17%)
18	BCR	cA	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	a1	416	13	55,63,73	1.74	7 (12%)	64,101,113	2.15	14 (21%)
15	CLA	a5	406	-	45,53,73	1.75	7 (15%)	52,89,113	1.68	8 (15%)
19	LHG	cA	853	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
18	BCR	c3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.40	8 (14%)
15	CLA	c5	410	13	64,72,73	1.48	8 (12%)	74,111,113	1.75	14 (18%)
15	CLA	aA	832	-	50,58,73	1.58	11 (22%)	58,95,113	1.81	10 (17%)
15	CLA	c1	405	-	45,53,73	1.80	8 (17%)	52,89,113	2.08	19 (36%)
15	CLA	aA	833	-	65,73,73	1.39	13 (20%)	76,113,113	1.48	7 (9%)
18	BCR	cF	205	-	41,41,41	1.21	5 (12%)	56,56,56	1.34	8 (14%)
18	BCR	cL	204	-	41,41,41	1.30	4 (9%)	56,56,56	1.45	9 (16%)
18	BCR	a6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	b2	414	-	45,53,73	1.78	8 (17%)	52,89,113	1.63	6 (11%)
18	BCR	a4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c3	410	13	64,72,73	1.48	9 (14%)	74,111,113	1.73	14 (18%)
15	CLA	aB	814	-	65,73,73	1.43	8 (12%)	76,113,113	1.71	15 (19%)
14	CL0	bA	801	-	65,73,73	1.91	17 (26%)	76,113,113	2.78	33 (43%)
17	SF4	aC	101	3	0,12,12	-	-	-		
15	CLA	cB	842	-	45,53,73	1.82	7 (15%)	52,89,113	1.55	5 (9%)
18	BCR	c5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.53	12 (21%)
18	BCR	bJ	105	-	41,41,41	1.20	5 (12%)	56,56,56	1.35	9 (16%)
18	BCR	aF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	b3	416	-	50,58,73	1.65	10 (20%)	58,95,113	2.51	18 (31%)
15	CLA	b3	417	13	55,63,73	1.78	6 (10%)	64,101,113	2.12	14 (21%)
15	CLA	a1	422	-	65,73,73	1.67	12 (18%)	76,113,113	2.07	20 (26%)
18	BCR	bB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	9 (16%)
18	BCR	aI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
15	CLA	a5	405	-	45,53,73	1.80	8 (17%)	52,89,113	2.17	21 (40%)
15	CLA	c4	405	-	45,53,73	1.79	10 (22%)	52,89,113	2.15	21 (40%)
18	BCR	b5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	10 (17%)
15	CLA	b6	411	13	64,72,73	1.49	8 (12%)	74,111,113	1.69	14 (18%)
15	CLA	bA	845	19	52,60,73	1.64	10 (19%)	60,97,113	2.18	15 (25%)
15	CLA	a5	420	-	65,73,73	1.61	10 (15%)	76,113,113	1.93	18 (23%)
15	CLA	cA	823	-	49,57,73	1.61	9 (18%)	55,93,113	1.58	7 (12%)
18	BCR	bA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	cB	824	-	45,53,73	1.74	8 (17%)	52,89,113	1.64	11 (21%)
15	CLA	b6	412	13	45,53,73	1.71	7 (15%)	52,89,113	1.87	10 (19%)
18	BCR	aF	203	-	41,41,41	1.20	4 (9%)	56,56,56	1.35	9 (16%)
18	BCR	a3	418	-	41,41,41	1.44	5 (12%)	56,56,56	1.55	10 (17%)
15	CLA	c2	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.54	8 (10%)
16	PQN	aA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	a6	409	-	45,53,73	1.71	8 (17%)	52,89,113	1.85	7 (13%)
15	CLA	cK	102	-	45,53,73	1.67	8 (17%)	52,89,113	1.64	10 (19%)
15	CLA	cB	829	-	65,73,73	1.40	11 (16%)	76,113,113	1.52	8 (10%)
18	BCR	bB	849	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	10 (17%)
18	BCR	c6	401	-	41,41,41	1.18	4 (9%)	56,56,56	1.53	11 (19%)
18	BCR	a4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	7 (12%)
15	CLA	c2	413	-	45,53,73	1.83	10 (22%)	52,89,113	1.74	15 (28%)
15	CLA	b3	414	-	41,49,73	1.86	8 (19%)	47,84,113	1.79	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b6	407	-	45,53,73	1.74	7 (15%)	52,89,113	1.67	7 (13%)
18	BCR	bA	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.41	9 (16%)
15	CLA	aB	829	-	65,73,73	1.41	11 (16%)	76,113,113	1.51	8 (10%)
15	CLA	c5	411	13	45,53,73	1.73	7 (15%)	52,89,113	1.88	9 (17%)
15	CLA	bB	825	2	54,62,73	1.52	9 (16%)	62,99,113	1.76	10 (16%)
15	CLA	b5	404	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	9 (11%)
15	CLA	aA	843	-	65,73,73	1.53	10 (15%)	76,113,113	1.58	9 (11%)
15	CLA	c3	403	-	65,73,73	1.40	7 (10%)	76,113,113	1.59	9 (11%)
18	BCR	aB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	cA	831	-	65,73,73	1.53	11 (16%)	76,113,113	1.63	9 (11%)
15	CLA	aA	804	-	65,73,73	1.50	9 (13%)	76,113,113	1.56	11 (14%)
15	CLA	aA	812	-	65,73,73	1.46	11 (16%)	76,113,113	1.44	10 (13%)
15	CLA	a2	408	-	45,53,73	1.74	8 (17%)	52,89,113	1.67	9 (17%)
15	CLA	a4	417	13	55,63,73	1.78	7 (12%)	64,101,113	2.15	12 (18%)
19	LHG	aX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	cA	821	-	61,69,73	1.51	11 (18%)	71,108,113	1.51	9 (12%)
15	CLA	c3	413	-	45,53,73	1.76	9 (20%)	52,89,113	1.61	5 (9%)
15	CLA	c4	415	-	45,53,73	1.76	9 (20%)	52,89,113	2.07	11 (21%)
18	BCR	b5	419	-	41,41,41	1.16	2 (4%)	56,56,56	1.41	10 (17%)
18	BCR	a1	419	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
15	CLA	a6	405	-	65,73,73	1.51	8 (12%)	76,113,113	1.44	8 (10%)
18	BCR	c6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
15	CLA	b2	406	-	65,73,73	1.67	10 (15%)	76,113,113	1.97	20 (26%)
15	CLA	cA	827	22	65,73,73	1.43	10 (15%)	76,113,113	1.61	12 (15%)
15	CLA	aB	841	-	45,53,73	1.82	8 (17%)	52,89,113	1.68	9 (17%)
15	CLA	a5	413	-	45,53,73	1.78	9 (20%)	52,89,113	1.61	5 (9%)
18	BCR	cA	851	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
15	CLA	b3	402	-	65,73,73	1.42	6 (9%)	76,113,113	1.45	7 (9%)
15	CLA	c3	408	-	45,53,73	1.66	8 (17%)	52,89,113	1.82	9 (17%)
15	CLA	a6	407	-	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
15	CLA	c3	404	-	65,73,73	1.48	8 (12%)	76,113,113	1.44	8 (10%)
18	BCR	c6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	bA	844	-	42,49,73	1.72	7 (16%)	48,83,113	1.75	6 (12%)
18	BCR	c3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
16	PQN	bB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a4	414	-	41,49,73	1.87	8 (19%)	47,84,113	1.77	7 (14%)
15	CLA	b1	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.58	9 (11%)
15	CLA	bA	835	-	65,73,73	1.51	11 (16%)	76,113,113	1.64	11 (14%)
15	CLA	cA	838	-	51,59,73	1.53	12 (23%)	59,96,113	1.87	10 (16%)
15	CLA	aA	814	-	60,68,73	1.51	11 (18%)	70,107,113	1.48	8 (11%)
15	CLA	c6	416	-	45,53,73	1.84	9 (20%)	52,89,113	2.06	10 (19%)
15	CLA	cF	201	22	51,59,73	1.66	9 (17%)	59,96,113	1.42	10 (16%)
15	CLA	bB	824	-	45,53,73	1.75	8 (17%)	52,89,113	1.63	10 (19%)
15	CLA	c4	416	-	50,58,73	1.63	9 (18%)	58,95,113	2.55	17 (29%)
15	CLA	bA	837	1	45,53,73	1.76	8 (17%)	52,89,113	1.73	8 (15%)
18	BCR	b2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	bB	807	-	65,73,73	1.49	11 (16%)	76,113,113	1.59	8 (10%)
15	CLA	b3	406	-	45,53,73	1.75	7 (15%)	52,89,113	1.67	7 (13%)
15	CLA	b5	409	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	7 (9%)
18	BCR	b3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
18	BCR	a6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	a4	402	-	65,73,73	1.41	7 (10%)	76,113,113	1.48	8 (10%)
18	BCR	bJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
18	BCR	bF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	cB	836	-	60,68,73	1.52	10 (16%)	70,107,113	1.55	11 (15%)
15	CLA	c6	405	-	65,73,73	1.51	9 (13%)	76,113,113	1.46	9 (11%)
15	CLA	b5	415	-	45,53,73	1.78	9 (20%)	52,89,113	2.06	11 (21%)
15	CLA	a3	404	-	65,73,73	1.48	9 (13%)	76,113,113	1.45	9 (11%)
15	CLA	bB	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.88	12 (15%)
18	BCR	bB	850	-	41,41,41	1.41	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	aA	829	-	65,73,73	1.40	9 (13%)	76,113,113	1.65	12 (15%)
15	CLA	bB	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.67	13 (17%)
15	CLA	b4	405	-	45,53,73	1.79	9 (20%)	52,89,113	2.15	19 (36%)
18	BCR	aA	852	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
15	CLA	aA	818	-	54,62,73	1.57	8 (14%)	62,99,113	1.78	7 (11%)
15	CLA	c5	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.56	10 (13%)
15	CLA	aB	827	-	65,73,73	1.41	8 (12%)	76,113,113	1.70	13 (17%)
15	CLA	c3	416	-	50,58,73	1.65	10 (20%)	58,95,113	2.51	18 (31%)
18	BCR	c1	401	-	41,41,41	1.16	3 (7%)	56,56,56	1.54	9 (16%)
18	BCR	b4	420	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a4	406	-	45,53,73	1.74	7 (15%)	52,89,113	1.66	7 (13%)
15	CLA	a2	402	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
15	CLA	bA	812	-	65,73,73	1.46	11 (16%)	76,113,113	1.44	11 (14%)
15	CLA	c1	407	-	45,53,73	1.71	8 (17%)	52,89,113	1.73	9 (17%)
15	CLA	a4	415	-	45,53,73	1.76	9 (20%)	52,89,113	2.08	12 (23%)
18	BCR	a4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	a2	409	-	45,53,73	1.66	8 (17%)	52,89,113	1.79	8 (15%)
15	CLA	bA	810	1	65,73,73	1.42	9 (13%)	76,113,113	1.56	8 (10%)
15	CLA	aX	102	12	45,53,73	1.79	9 (20%)	52,89,113	1.81	12 (23%)
15	CLA	cA	824	-	51,59,73	1.60	10 (19%)	59,96,113	1.58	7 (11%)
15	CLA	cA	840	-	47,55,73	1.66	11 (23%)	54,91,113	2.01	9 (16%)
15	CLA	c1	415	-	45,53,73	1.77	9 (20%)	52,89,113	2.07	10 (19%)
15	CLA	bA	818	-	54,62,73	1.57	9 (16%)	62,99,113	1.77	8 (12%)
15	CLA	b4	408	-	45,53,73	1.67	8 (17%)	52,89,113	1.83	8 (15%)
18	BCR	a2	401	-	41,41,41	1.26	4 (9%)	56,56,56	1.83	12 (21%)
15	CLA	a5	409	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	7 (9%)
15	CLA	cA	813	-	54,62,73	1.62	9 (16%)	62,99,113	1.52	10 (16%)
15	CLA	cA	806	-	65,73,73	1.47	11 (16%)	76,113,113	1.73	10 (13%)
18	BCR	c1	418	-	41,41,41	1.37	5 (12%)	56,56,56	1.54	11 (19%)
15	CLA	a5	411	13	45,53,73	1.73	8 (17%)	52,89,113	1.88	9 (17%)
16	PQN	aB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
19	LHG	aA	853	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
18	BCR	b3	418	-	41,41,41	1.43	5 (12%)	56,56,56	1.55	10 (17%)
15	CLA	aA	834	-	65,73,73	1.44	12 (18%)	76,113,113	1.71	11 (14%)
15	CLA	aB	839	22	65,73,73	1.42	10 (15%)	76,113,113	1.52	10 (13%)
15	CLA	b1	408	-	45,53,73	1.68	7 (15%)	52,89,113	1.83	9 (17%)
15	CLA	cX	102	12	45,53,73	1.79	9 (20%)	52,89,113	1.82	11 (21%)
18	BCR	aL	205	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	bB	808	-	65,73,73	1.45	9 (13%)	76,113,113	1.58	10 (13%)
15	CLA	c5	412	-	45,53,73	1.80	9 (20%)	52,89,113	1.74	14 (26%)
15	CLA	aA	840	-	47,55,73	1.65	11 (23%)	54,91,113	2.01	9 (16%)
18	BCR	a1	418	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
15	CLA	cB	808	-	65,73,73	1.44	9 (13%)	76,113,113	1.57	10 (13%)
15	CLA	b5	408	-	45,53,73	1.68	8 (17%)	52,89,113	1.85	9 (17%)
15	CLA	bA	811	-	45,53,73	1.73	10 (22%)	52,89,113	1.61	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	bA	815	-	45,53,73	1.75	10 (22%)	52,89,113	1.65	10 (19%)
18	BCR	bB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
18	BCR	cJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	b5	420	-	65,73,73	1.61	10 (15%)	76,113,113	1.93	18 (23%)
18	BCR	aJ	204	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	a2	412	13	45,53,73	1.75	9 (20%)	52,89,113	1.89	9 (17%)
18	BCR	b6	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.41	10 (17%)
19	LHG	cX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	a1	403	-	65,73,73	1.48	8 (12%)	76,113,113	1.45	9 (11%)
15	CLA	a5	412	-	45,53,73	1.79	10 (22%)	52,89,113	1.75	13 (25%)
15	CLA	bA	826	-	65,73,73	1.36	8 (12%)	76,113,113	1.64	10 (13%)
15	CLA	bB	819	-	60,68,73	1.44	11 (18%)	70,107,113	1.75	8 (11%)
15	CLA	bB	836	-	60,68,73	1.52	10 (16%)	70,107,113	1.55	11 (15%)
15	CLA	cA	820	-	65,73,73	1.47	10 (15%)	76,113,113	1.66	10 (13%)
15	CLA	bA	842	22	51,59,73	1.66	10 (19%)	59,96,113	1.42	10 (16%)
15	CLA	cA	832	-	50,58,73	1.57	11 (22%)	58,95,113	1.81	10 (17%)
15	CLA	c2	416	-	45,53,73	1.78	10 (22%)	52,89,113	2.05	10 (19%)
15	CLA	c3	421	-	65,73,73	1.62	10 (15%)	76,113,113	1.66	15 (19%)
15	CLA	a1	415	-	50,58,73	1.61	10 (20%)	58,95,113	2.55	18 (31%)
18	BCR	cB	846	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
15	CLA	cB	839	22	65,73,73	1.43	10 (15%)	76,113,113	1.53	10 (13%)
15	CLA	cB	816	-	45,53,73	1.63	9 (20%)	52,89,113	1.95	7 (13%)
15	CLA	cB	828	-	65,73,73	1.40	12 (18%)	76,113,113	1.68	8 (10%)
15	CLA	bA	809	1	65,73,73	1.44	10 (15%)	76,113,113	1.55	10 (13%)
18	BCR	aA	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
19	LHG	aA	854	15	26,26,48	0.97	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	a5	407	-	45,53,73	1.72	7 (15%)	52,89,113	1.71	9 (17%)
15	CLA	a1	408	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
15	CLA	aA	835	-	65,73,73	1.52	11 (16%)	76,113,113	1.64	11 (14%)
15	CLA	a4	407	-	45,53,73	1.71	8 (17%)	52,89,113	1.70	8 (15%)
15	CLA	bA	838	-	51,59,73	1.54	11 (21%)	59,96,113	1.87	10 (16%)
15	CLA	c3	411	13	45,53,73	1.74	8 (17%)	52,89,113	1.86	9 (17%)
18	BCR	b4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.50	9 (16%)
15	CLA	aB	802	-	65,73,73	1.51	12 (18%)	76,113,113	1.52	9 (11%)
15	CLA	b3	410	13	64,72,73	1.47	9 (14%)	74,111,113	1.73	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c6	404	-	65,73,73	1.40	7 (10%)	76,113,113	1.56	9 (11%)
19	LHG	bX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	a6	415	-	41,49,73	1.88	7 (17%)	47,84,113	1.76	7 (14%)
15	CLA	cL	203	22	65,73,73	1.44	10 (15%)	76,113,113	1.42	8 (10%)
15	CLA	c2	417	-	50,58,73	1.63	9 (18%)	58,95,113	2.63	19 (32%)
15	CLA	bB	832	-	49,57,73	1.59	11 (22%)	55,93,113	1.70	8 (14%)
18	BCR	c2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	cA	843	-	42,49,73	1.73	7 (16%)	48,83,113	1.75	6 (12%)
18	BCR	c4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	cA	804	-	65,73,73	1.50	9 (13%)	76,113,113	1.55	11 (14%)
15	CLA	cA	812	-	65,73,73	1.46	11 (16%)	76,113,113	1.45	10 (13%)
18	BCR	bB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	cB	806	-	65,73,73	1.40	11 (16%)	76,113,113	1.68	10 (13%)
15	CLA	a1	405	-	45,53,73	1.75	7 (15%)	52,89,113	1.65	7 (13%)
15	CLA	a3	413	-	45,53,73	1.77	10 (22%)	52,89,113	1.61	5 (9%)
15	CLA	cA	817	-	49,57,73	1.69	8 (16%)	55,93,113	1.59	6 (10%)
15	CLA	b1	411	13	45,53,73	1.74	7 (15%)	52,89,113	1.89	8 (15%)
15	CLA	a2	405	-	45,53,73	1.85	6 (13%)	52,89,113	2.13	19 (36%)
15	CLA	a4	410	13	64,72,73	1.49	9 (14%)	74,111,113	1.71	14 (18%)
18	BCR	b6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
15	CLA	c6	418	13	55,63,73	1.80	5 (9%)	64,101,113	2.10	10 (15%)
17	SF4	bC	101	3	0,12,12	-	-	-		
15	CLA	bA	807	-	65,73,73	1.49	12 (18%)	76,113,113	1.60	12 (15%)
18	BCR	aM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
18	BCR	cF	202	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	9 (16%)
15	CLA	cB	827	-	65,73,73	1.41	8 (12%)	76,113,113	1.69	13 (17%)
15	CLA	aB	818	-	59,67,73	1.43	8 (13%)	68,105,113	1.66	12 (17%)
15	CLA	cB	817	-	55,63,73	1.48	8 (14%)	64,101,113	1.73	10 (15%)
15	CLA	aL	203	22	65,73,73	1.45	10 (15%)	76,113,113	1.42	8 (10%)
15	CLA	c4	407	-	45,53,73	1.70	8 (17%)	52,89,113	1.71	8 (15%)
15	CLA	bB	805	-	54,62,73	1.55	10 (18%)	62,99,113	1.67	7 (11%)
18	BCR	c2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.52	9 (16%)
15	CLA	b2	405	-	45,53,73	1.85	6 (13%)	52,89,113	2.13	19 (36%)
15	CLA	b3	404	-	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
15	CLA	a3	421	-	65,73,73	1.63	10 (15%)	76,113,113	1.66	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	bB	813	-	45,53,73	1.78	9 (20%)	52,89,113	1.74	7 (13%)
15	CLA	b4	416	-	50,58,73	1.63	9 (18%)	58,95,113	2.53	17 (29%)
15	CLA	bB	809	-	65,73,73	1.45	11 (16%)	76,113,113	1.63	10 (13%)
15	CLA	b1	412	-	45,53,73	1.79	10 (22%)	52,89,113	1.79	14 (26%)
15	CLA	cA	814	-	60,68,73	1.50	9 (15%)	70,107,113	1.48	8 (11%)
15	CLA	a2	404	-	65,73,73	1.49	8 (12%)	76,113,113	1.46	9 (11%)
18	BCR	aF	201	-	41,41,41	1.31	4 (9%)	56,56,56	1.37	9 (16%)
18	BCR	c1	420	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
15	CLA	b2	407	-	45,53,73	1.72	6 (13%)	52,89,113	1.66	7 (13%)
15	CLA	bA	824	-	51,59,73	1.60	10 (19%)	59,96,113	1.58	7 (11%)
15	CLA	a5	415	-	45,53,73	1.78	9 (20%)	52,89,113	2.07	11 (21%)
15	CLA	cA	844	19	52,60,73	1.64	10 (19%)	60,97,113	2.17	15 (25%)
20	LMG	aB	850	-	55,55,55	1.07	4 (7%)	63,63,63	1.62	8 (12%)
18	BCR	b5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
15	CLA	aB	834	-	58,66,73	1.55	10 (17%)	67,104,113	1.61	12 (17%)
15	CLA	cA	811	-	45,53,73	1.74	10 (22%)	52,89,113	1.61	7 (13%)
15	CLA	aB	804	-	65,73,73	1.48	9 (13%)	76,113,113	2.04	16 (21%)
15	CLA	a6	414	-	45,53,73	1.77	10 (22%)	52,89,113	1.80	11 (21%)
15	CLA	c1	406	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	7 (13%)
15	CLA	c1	408	-	45,53,73	1.67	8 (17%)	52,89,113	1.82	8 (15%)
15	CLA	a6	413	-	45,53,73	1.82	10 (22%)	52,89,113	1.72	14 (26%)
18	BCR	bL	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	bA	823	-	49,57,73	1.62	10 (20%)	55,93,113	1.57	7 (12%)
15	CLA	a2	418	13	55,63,73	1.80	6 (10%)	64,101,113	2.10	11 (17%)
15	CLA	a4	413	-	45,53,73	1.79	8 (17%)	52,89,113	1.59	5 (9%)
18	BCR	b4	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.56	9 (16%)
15	CLA	aA	802	22	65,73,73	1.58	11 (16%)	76,113,113	1.59	10 (13%)
16	PQN	bA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	c4	417	13	55,63,73	1.79	7 (12%)	64,101,113	2.15	12 (18%)
15	CLA	b2	409	-	45,53,73	1.66	8 (17%)	52,89,113	1.81	10 (19%)
15	CLA	bK	101	-	45,53,73	1.68	8 (17%)	52,89,113	1.65	10 (19%)
15	CLA	cA	822	-	65,73,73	1.43	11 (16%)	76,113,113	1.53	8 (10%)
15	CLA	b5	410	13	64,72,73	1.48	8 (12%)	74,111,113	1.73	14 (18%)
15	CLA	cA	829	-	65,73,73	1.40	9 (13%)	76,113,113	1.65	12 (15%)
15	CLA	cA	833	-	65,73,73	1.39	13 (20%)	76,113,113	1.49	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	aJ	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	bB	811	2	65,73,73	1.40	12 (18%)	76,113,113	1.72	12 (15%)
15	CLA	c5	405	-	45,53,73	1.80	8 (17%)	52,89,113	2.16	21 (40%)
15	CLA	bJ	102	-	38,45,73	1.81	11 (28%)	43,78,113	1.81	7 (16%)
15	CLA	a5	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.56	9 (11%)
15	CLA	a1	409	13	64,72,73	1.49	9 (14%)	74,111,113	1.73	13 (17%)
16	PQN	cA	845	-	34,34,34	1.40	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	a3	411	13	45,53,73	1.75	8 (17%)	52,89,113	1.86	9 (17%)
18	BCR	aB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
18	BCR	aK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
15	CLA	b6	422	-	65,73,73	1.72	12 (18%)	76,113,113	2.08	20 (26%)
15	CLA	aB	821	-	47,55,73	1.71	9 (19%)	54,91,113	1.59	6 (11%)
15	CLA	aA	824	-	51,59,73	1.60	10 (19%)	59,96,113	1.58	7 (11%)
15	CLA	aA	838	-	51,59,73	1.53	11 (21%)	59,96,113	1.86	10 (16%)
15	CLA	b5	405	-	45,53,73	1.80	8 (17%)	52,89,113	2.16	21 (40%)
18	BCR	aI	103	-	41,41,41	1.31	4 (9%)	56,56,56	1.44	9 (16%)
18	BCR	bI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
15	CLA	b5	416	-	50,58,73	1.60	9 (18%)	58,95,113	2.54	16 (27%)
18	BCR	cB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	b5	417	13	55,63,73	1.76	5 (9%)	64,101,113	2.13	12 (18%)
15	CLA	aA	805	-	59,67,73	1.51	10 (16%)	68,105,113	1.70	10 (14%)
18	BCR	b6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	c1	417	13	55,63,73	1.76	6 (10%)	64,101,113	2.13	14 (21%)
15	CLA	aA	837	1	45,53,73	1.76	8 (17%)	52,89,113	1.73	7 (13%)
15	CLA	a1	411	-	45,53,73	1.79	10 (22%)	52,89,113	1.81	15 (28%)
15	CLA	b5	407	-	45,53,73	1.71	7 (15%)	52,89,113	1.71	9 (17%)
15	CLA	bB	842	-	45,53,73	1.83	7 (15%)	52,89,113	1.55	5 (9%)
15	CLA	c6	409	-	45,53,73	1.71	8 (17%)	52,89,113	1.84	8 (15%)
15	CLA	a3	407	-	45,53,73	1.70	8 (17%)	52,89,113	1.71	8 (15%)
15	CLA	bB	815	-	65,73,73	1.46	9 (13%)	76,113,113	1.53	9 (11%)
15	CLA	bA	822	-	65,73,73	1.43	11 (16%)	76,113,113	1.53	8 (10%)
15	CLA	a3	412	-	45,53,73	1.80	10 (22%)	52,89,113	1.75	14 (26%)
15	CLA	b4	406	-	45,53,73	1.75	7 (15%)	52,89,113	1.66	7 (13%)
15	CLA	c2	405	-	45,53,73	1.85	7 (15%)	52,89,113	2.11	19 (36%)
18	BCR	a2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	SF4	aC	102	3	0,12,12	-	-	-		
15	CLA	c2	406	-	65,73,73	1.67	10 (15%)	76,113,113	1.97	19 (25%)
18	BCR	c2	401	-	41,41,41	1.25	4 (9%)	56,56,56	1.84	11 (19%)
15	CLA	aJ	202	8	45,53,73	1.70	10 (22%)	52,89,113	1.80	9 (17%)
15	CLA	bA	836	-	54,62,73	1.60	10 (18%)	62,99,113	1.48	7 (11%)
15	CLA	aB	806	-	65,73,73	1.40	11 (16%)	76,113,113	1.67	10 (13%)
19	LHG	cA	852	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	a6	410	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
15	CLA	c1	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.57	9 (11%)
15	CLA	a4	416	-	50,58,73	1.62	9 (18%)	58,95,113	2.54	17 (29%)
15	CLA	bB	829	-	65,73,73	1.40	11 (16%)	76,113,113	1.51	8 (10%)
15	CLA	c2	415	-	41,49,73	1.86	7 (17%)	47,84,113	1.77	7 (14%)
15	CLA	c6	411	13	64,72,73	1.49	8 (12%)	74,111,113	1.69	14 (18%)
15	CLA	cB	833	-	65,73,73	1.53	9 (13%)	76,113,113	1.47	13 (17%)
15	CLA	aA	825	-	59,67,73	1.53	10 (16%)	68,105,113	1.49	10 (14%)
15	CLA	b1	402	-	65,73,73	1.42	7 (10%)	76,113,113	1.47	7 (9%)
15	CLA	cB	831	-	45,53,73	1.67	10 (22%)	52,89,113	1.66	6 (11%)
15	CLA	b2	418	13	55,63,73	1.81	6 (10%)	64,101,113	2.10	11 (17%)
15	CLA	c2	410	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	8 (10%)
15	CLA	a2	403	-	65,73,73	1.41	7 (10%)	76,113,113	1.55	7 (9%)
15	CLA	aB	828	-	65,73,73	1.40	12 (18%)	76,113,113	1.67	8 (10%)
20	LMG	cB	850	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	b5	402	-	65,73,73	1.46	7 (10%)	76,113,113	1.49	7 (9%)
15	CLA	aA	845	19	52,60,73	1.64	10 (19%)	60,97,113	2.17	16 (26%)
15	CLA	bB	804	-	65,73,73	1.48	9 (13%)	76,113,113	2.05	16 (21%)
15	CLA	cA	834	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	11 (14%)
15	CLA	b6	404	-	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
15	CLA	aB	805	-	54,62,73	1.56	10 (18%)	62,99,113	1.66	7 (11%)
15	CLA	b3	421	-	65,73,73	1.62	10 (15%)	76,113,113	1.65	15 (19%)
15	CLA	b6	415	-	41,49,73	1.87	7 (17%)	47,84,113	1.76	7 (14%)
15	CLA	c2	408	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	9 (17%)
15	CLA	a6	417	-	50,58,73	1.61	9 (18%)	58,95,113	2.55	17 (29%)
15	CLA	c5	414	-	41,49,73	1.86	7 (17%)	47,84,113	1.80	8 (17%)
15	CLA	aJ	203	-	38,45,73	1.82	10 (26%)	43,78,113	1.82	7 (16%)
15	CLA	a3	414	-	41,49,73	1.87	8 (19%)	47,84,113	1.79	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cB	801	-	65,73,73	1.52	11 (16%)	76,113,113	1.50	9 (11%)
18	BCR	aA	848	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	b2	404	-	65,73,73	1.49	8 (12%)	76,113,113	1.45	9 (11%)
15	CLA	b5	414	-	41,49,73	1.87	7 (17%)	47,84,113	1.81	7 (14%)
18	BCR	b1	420	-	41,41,41	1.20	4 (9%)	56,56,56	1.45	11 (19%)
15	CLA	b6	418	13	55,63,73	1.80	5 (9%)	64,101,113	2.10	11 (17%)
15	CLA	c1	409	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
18	BCR	bJ	104	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	aB	835	-	45,53,73	1.68	10 (22%)	52,89,113	1.86	8 (15%)
15	CLA	a4	421	-	65,73,73	1.65	13 (20%)	76,113,113	1.74	16 (21%)
15	CLA	b5	406	-	45,53,73	1.75	7 (15%)	52,89,113	1.68	8 (15%)
18	BCR	aB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	c4	411	13	45,53,73	1.75	7 (15%)	52,89,113	1.89	8 (15%)
17	SF4	bC	102	3	0,12,12	-	-	-		
15	CLA	cJ	101	8	45,53,73	1.70	9 (20%)	52,89,113	1.79	9 (17%)
15	CLA	aB	812	-	45,53,73	1.70	7 (15%)	52,89,113	1.62	8 (15%)
15	CLA	bB	841	-	45,53,73	1.83	8 (17%)	52,89,113	1.68	9 (17%)
15	CLA	bJ	101	8	45,53,73	1.71	10 (22%)	52,89,113	1.81	9 (17%)
18	BCR	cB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	9 (16%)
15	CLA	b4	404	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	7 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c6	407	-	1/1/11/20	4/13/91/115	-
15	CLA	cB	830	-	1/1/15/20	6/37/115/115	-
15	CLA	c2	409	-	1/1/11/20	5/13/91/115	-
15	CLA	aB	820	22	1/1/15/20	8/37/115/115	-
15	CLA	aB	808	-	-	12/37/115/115	-
15	CLA	cB	821	-	1/1/11/20	11/16/94/115	-
15	CLA	b3	403	-	1/1/15/20	13/37/115/115	-
15	CLA	b6	414	-	1/1/11/20	2/13/91/115	-
15	CLA	a6	422	-	1/1/15/20	17/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	cJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	b2	403	-	1/1/15/20	14/37/115/115	-
18	BCR	a5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	840	-	1/1/15/20	14/37/115/115	-
15	CLA	aB	811	2	1/1/15/20	11/37/115/115	-
15	CLA	aB	815	-	1/1/15/20	17/37/115/115	-
15	CLA	b1	405	-	1/1/11/20	3/13/91/115	-
15	CLA	c3	409	-	-	6/37/115/115	-
15	CLA	c5	406	-	1/1/11/20	4/13/91/115	-
15	CLA	cA	805	-	1/1/13/20	11/30/108/115	-
18	BCR	c2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	836	-	1/1/12/20	6/24/102/115	-
15	CLA	c4	403	-	1/1/15/20	14/37/115/115	-
15	CLA	aB	826	22	1/1/11/20	8/15/93/115	-
15	CLA	b1	417	13	1/1/13/20	11/25/103/115	-
15	CLA	aB	837	-	1/1/15/20	15/37/115/115	-
15	CLA	c5	415	-	-	5/13/91/115	-
18	BCR	c5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	840	-	1/1/11/20	5/16/94/115	-
18	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
18	BCR	cB	847	-	-	9/18/35/63	0/1/1/2
18	BCR	a5	419	-	-	12/29/63/63	0/2/2/2
18	BCR	cI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	839	-	1/1/15/20	14/37/115/115	-
18	BCR	b6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	bA	806	-	1/1/15/20	23/37/115/115	-
15	CLA	aA	808	-	-	2/21/99/115	-
15	CLA	a1	402	-	1/1/15/20	14/37/115/115	-
15	CLA	bB	801	-	1/1/15/20	10/37/115/115	-
15	CLA	b6	405	-	1/1/15/20	9/37/115/115	-
15	CLA	a3	403	-	1/1/15/20	13/37/115/115	-
18	BCR	c3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b1	413	-	1/1/11/20	2/13/91/115	-
15	CLA	cB	823	-	1/1/13/20	5/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b3	412	-	1/1/11/20	9/13/91/115	-
15	CLA	a2	411	13	1/1/14/20	11/36/114/115	-
18	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	805	-	1/1/12/20	5/24/102/115	-
15	CLA	bA	827	22	1/1/15/20	10/37/115/115	-
15	CLA	bA	817	-	-	4/18/96/115	-
15	CLA	bB	835	-	1/1/11/20	7/13/91/115	-
18	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
15	CLA	c4	412	-	1/1/11/20	9/13/91/115	-
15	CLA	aB	825	2	1/1/12/20	10/24/102/115	-
15	CLA	bA	820	-	1/1/15/20	18/37/115/115	-
15	CLA	cB	841	-	1/1/11/20	2/13/91/115	-
18	BCR	bL	205	-	-	9/29/63/63	0/2/2/2
18	BCR	c1	419	-	-	11/29/63/63	0/2/2/2
15	CLA	b4	411	13	1/1/11/20	5/13/91/115	-
15	CLA	c3	407	-	1/1/11/20	6/13/91/115	-
15	CLA	cA	837	1	-	7/13/91/115	-
15	CLA	b3	413	-	1/1/11/20	1/13/91/115	-
15	CLA	a1	406	-	1/1/11/20	6/13/91/115	-
15	CLA	a5	417	13	1/1/13/20	8/25/103/115	-
15	CLA	b6	406	-	1/1/11/20	3/13/91/115	-
17	SF4	cC	101	3	-	-	0/6/5/5
15	CLA	bB	831	-	1/1/11/20	6/13/91/115	-
15	CLA	cA	819	-	1/1/12/20	8/24/102/115	-
15	CLA	b2	413	-	1/1/11/20	9/13/91/115	-
15	CLA	cL	201	10	1/1/15/20	13/37/115/115	-
15	CLA	cA	802	22	1/1/15/20	16/37/115/115	-
15	CLA	bB	821	-	1/1/11/20	11/16/94/115	-
15	CLA	a3	416	-	1/1/12/20	9/19/97/115	-
15	CLA	a3	417	13	1/1/13/20	11/25/103/115	-
15	CLA	bB	816	-	1/1/11/20	6/13/91/115	-
15	CLA	bA	814	-	1/1/14/20	14/31/109/115	-
15	CLA	c4	413	-	1/1/11/20	2/13/91/115	-
15	CLA	a4	412	-	1/1/11/20	9/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cA	808	-	-	2/21/99/115	-
18	BCR	a4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	809	-	1/1/15/20	11/37/115/115	-
15	CLA	c1	414	-	1/1/10/20	2/8/86/115	-
15	CLA	a1	410	13	1/1/11/20	4/13/91/115	-
15	CLA	b6	410	-	1/1/15/20	6/37/115/115	-
15	CLA	b3	408	-	1/1/11/20	5/13/91/115	-
20	LMG	bB	851	-	-	26/50/70/70	0/1/1/1
15	CLA	c5	413	-	1/1/11/20	1/13/91/115	-
15	CLA	aB	842	-	-	0/13/91/115	-
15	CLA	a6	406	-	1/1/11/20	3/13/91/115	-
15	CLA	aB	807	-	1/1/15/20	15/37/115/115	-
15	CLA	aA	811	-	1/1/11/20	8/13/91/115	-
15	CLA	cA	825	-	1/1/13/20	15/30/108/115	-
15	CLA	c1	412	-	1/1/11/20	9/13/91/115	-
15	CLA	b1	409	-	1/1/15/20	6/37/115/115	-
15	CLA	a5	408	-	1/1/11/20	5/13/91/115	-
18	BCR	a1	417	-	-	9/29/63/63	0/2/2/2
15	CLA	aA	842	22	1/1/12/20	8/21/99/115	-
15	CLA	bB	823	-	1/1/13/20	5/25/103/115	-
15	CLA	c1	402	-	1/1/15/20	17/37/115/115	-
15	CLA	bB	806	-	1/1/15/20	21/37/115/115	-
15	CLA	a2	407	-	1/1/11/20	4/13/91/115	-
15	CLA	cB	825	2	1/1/12/20	10/24/102/115	-
15	CLA	aA	809	1	1/1/15/20	19/37/115/115	-
14	CL0	cA	801	-	3/3/20/25	6/37/135/135	-
18	BCR	aB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	cA	818	-	1/1/12/20	6/24/102/115	-
18	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	c6	403	-	1/1/15/20	17/37/115/115	-
15	CLA	aA	806	-	1/1/15/20	23/37/115/115	-
15	CLA	a4	408	-	1/1/11/20	5/13/91/115	-
15	CLA	bA	808	-	-	2/21/99/115	-
15	CLA	b6	408	-	1/1/11/20	6/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	828	-	1/1/15/20	21/37/115/115	-
15	CLA	a1	404	-	1/1/11/20	3/13/91/115	-
18	BCR	cA	850	-	-	8/29/63/63	0/2/2/2
15	CLA	c2	402	-	1/1/15/20	17/37/115/115	-
15	CLA	bA	804	-	1/1/15/20	10/37/115/115	-
15	CLA	bB	802	-	1/1/15/20	11/37/115/115	-
15	CLA	a2	413	-	1/1/11/20	9/13/91/115	-
15	CLA	bA	813	-	1/1/12/20	8/24/102/115	-
15	CLA	aL	201	10	1/1/15/20	13/37/115/115	-
18	BCR	cK	101	-	-	10/29/63/63	0/2/2/2
15	CLA	a6	412	13	1/1/11/20	4/13/91/115	-
15	CLA	b4	402	-	1/1/15/20	17/37/115/115	-
15	CLA	bB	827	-	1/1/15/20	15/37/115/115	-
15	CLA	c5	409	-	1/1/15/20	6/37/115/115	-
15	CLA	b3	411	13	1/1/11/20	5/13/91/115	-
15	CLA	a4	405	-	1/1/11/20	4/13/91/115	-
15	CLA	a5	404	-	1/1/15/20	9/37/115/115	-
15	CLA	aB	803	-	1/1/15/20	11/37/115/115	-
15	CLA	b6	416	-	-	5/13/91/115	-
15	CLA	a4	404	-	1/1/15/20	10/37/115/115	-
15	CLA	bB	810	2	1/1/15/20	14/37/115/115	-
15	CLA	aJ	201	-	1/1/11/20	8/13/91/115	-
18	BCR	bB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	c3	405	-	1/1/11/20	3/13/91/115	-
18	BCR	b1	418	-	-	9/29/63/63	0/2/2/2
15	CLA	bB	840	-	1/1/15/20	14/37/115/115	-
15	CLA	bB	838	-	1/1/11/20	2/16/94/115	-
15	CLA	bA	832	-	1/1/12/20	6/19/97/115	-
18	BCR	b1	419	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	833	-	1/1/15/20	11/37/115/115	-
18	BCR	bA	852	-	-	8/29/63/63	0/2/2/2
15	CLA	bA	831	-	1/1/15/20	8/37/115/115	-
15	CLA	aA	807	-	1/1/15/20	9/37/115/115	-
18	BCR	b6	401	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b3	407	-	1/1/11/20	6/13/91/115	-
15	CLA	aA	844	-	1/1/9/20	5/7/81/115	-
19	LHG	bA	854	-	-	19/53/53/53	-
15	CLA	c3	415	-	-	5/13/91/115	-
15	CLA	b2	411	13	1/1/14/20	11/36/114/115	-
15	CLA	c5	416	-	1/1/12/20	9/19/97/115	-
15	CLA	b1	415	-	-	5/13/91/115	-
15	CLA	a3	409	-	1/1/15/20	5/37/115/115	-
15	CLA	c5	417	13	1/1/13/20	9/25/103/115	-
18	BCR	b2	419	-	-	10/29/63/63	0/2/2/2
19	LHG	bA	855	15	-	15/31/31/53	-
15	CLA	bA	802	22	1/1/15/20	16/37/115/115	-
15	CLA	c3	412	-	1/1/11/20	9/13/91/115	-
15	CLA	b4	409	-	1/1/15/20	6/37/115/115	-
17	SF4	bA	847	2,1	-	-	0/6/5/5
15	CLA	aB	819	-	1/1/14/20	12/31/109/115	-
15	CLA	aB	836	-	1/1/14/20	9/31/109/115	-
15	CLA	a6	408	-	1/1/11/20	6/13/91/115	-
15	CLA	aA	839	-	1/1/15/20	14/37/115/115	-
15	CLA	c1	416	-	1/1/12/20	9/19/97/115	-
15	CLA	a6	418	13	1/1/13/20	10/25/103/115	-
15	CLA	cA	830	-	1/1/15/20	13/37/115/115	-
15	CLA	a3	415	-	-	5/13/91/115	-
15	CLA	cA	803	-	1/1/15/20	16/37/115/115	-
18	BCR	a6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	834	-	1/1/15/20	12/37/115/115	-
15	CLA	bL	204	22	1/1/15/20	13/37/115/115	-
15	CLA	aA	841	-	1/1/15/20	15/37/115/115	-
15	CLA	c4	402	-	1/1/15/20	17/37/115/115	-
15	CLA	bL	202	10	1/1/15/20	13/37/115/115	-
15	CLA	b1	414	-	1/1/10/20	2/8/86/115	-
15	CLA	b4	412	-	1/1/11/20	9/13/91/115	-
15	CLA	aA	830	-	1/1/15/20	13/37/115/115	-
18	BCR	aA	850	-	-	13/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aL	202	-	1/1/15/20	8/37/115/115	-
18	BCR	a1	421	-	-	14/29/63/63	0/2/2/2
15	CLA	c1	413	-	1/1/11/20	2/13/91/115	-
15	CLA	aA	820	-	1/1/15/20	18/37/115/115	-
15	CLA	bF	201	-	1/1/11/20	8/13/91/115	-
15	CLA	a2	415	-	1/1/10/20	2/8/86/115	-
15	CLA	aA	815	-	1/1/11/20	2/13/91/115	-
15	CLA	b6	409	-	1/1/11/20	5/13/91/115	-
15	CLA	a6	404	-	1/1/15/20	14/37/115/115	-
15	CLA	c5	420	-	1/1/15/20	10/37/115/115	-
15	CLA	aA	826	-	1/1/15/20	10/37/115/115	-
18	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	413	-	1/1/11/20	1/13/91/115	-
18	BCR	bM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	828	-	1/1/15/20	12/37/115/115	-
15	CLA	b4	413	-	1/1/11/20	2/13/91/115	-
15	CLA	a5	410	13	1/1/14/20	12/36/114/115	-
15	CLA	a1	414	-	-	5/13/91/115	-
15	CLA	bA	829	-	1/1/15/20	22/37/115/115	-
18	BCR	a2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	819	-	1/1/14/20	12/31/109/115	-
15	CLA	bB	833	-	1/1/15/20	18/37/115/115	-
18	BCR	a3	419	-	-	11/29/63/63	0/2/2/2
15	CLA	c5	402	-	1/1/15/20	17/37/115/115	-
15	CLA	a1	407	-	1/1/11/20	5/13/91/115	-
15	CLA	a6	411	13	1/1/14/20	11/36/114/115	-
15	CLA	a6	416	-	-	5/13/91/115	-
15	CLA	a4	411	13	1/1/11/20	5/13/91/115	-
15	CLA	aB	830	-	1/1/15/20	6/37/115/115	-
15	CLA	aA	822	-	1/1/15/20	16/37/115/115	-
18	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	cF	203	-	1/1/11/20	8/13/91/115	-
15	CLA	b1	406	-	1/1/11/20	4/13/91/115	-
18	BCR	b1	401	-	-	12/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	835	-	1/1/11/20	7/13/91/115	-
15	CLA	aB	816	-	1/1/11/20	6/13/91/115	-
15	CLA	bB	814	-	1/1/15/20	25/37/115/115	-
18	BCR	b3	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	819	-	1/1/12/20	8/24/102/115	-
15	CLA	aA	836	-	1/1/12/20	6/24/102/115	-
18	BCR	a6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	815	-	1/1/11/20	2/13/91/115	-
15	CLA	a4	403	-	1/1/15/20	14/37/115/115	-
15	CLA	bX	102	12	1/1/11/20	6/13/91/115	-
15	CLA	c4	409	-	1/1/15/20	6/37/115/115	-
15	CLA	bA	839	-	1/1/15/20	14/37/115/115	-
15	CLA	cB	810	2	1/1/15/20	14/37/115/115	-
15	CLA	c2	412	13	1/1/11/20	3/13/91/115	-
15	CLA	aA	831	-	1/1/15/20	8/37/115/115	-
15	CLA	b2	415	-	1/1/10/20	2/8/86/115	-
15	CLA	aA	821	-	1/1/14/20	13/33/111/115	-
15	CLA	c1	404	-	1/1/15/20	11/37/115/115	-
18	BCR	c6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	cA	809	1	1/1/15/20	19/37/115/115	-
15	CLA	a5	402	-	1/1/15/20	17/37/115/115	-
18	BCR	cA	847	-	-	11/29/63/63	0/2/2/2
15	CLA	c1	411	13	1/1/11/20	5/13/91/115	-
18	BCR	cM	101	-	-	11/29/63/63	0/2/2/2
17	SF4	aA	847	2,1	-	-	0/6/5/5
15	CLA	bB	822	-	1/1/11/20	2/13/91/115	-
15	CLA	a5	416	-	1/1/12/20	9/19/97/115	-
15	CLA	c6	417	-	1/1/12/20	9/19/97/115	-
15	CLA	cB	826	22	1/1/11/20	8/15/93/115	-
18	BCR	c4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	c2	404	-	1/1/15/20	9/37/115/115	-
15	CLA	b5	411	13	1/1/11/20	3/13/91/115	-
15	CLA	b1	416	-	1/1/12/20	9/19/97/115	-
18	BCR	cB	848	-	-	13/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	cI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	841	-	1/1/15/20	15/37/115/115	-
15	CLA	b3	415	-	-	5/13/91/115	-
15	CLA	b4	417	13	1/1/13/20	8/25/103/115	-
15	CLA	b2	412	13	1/1/11/20	3/13/91/115	-
18	BCR	b2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	c6	408	-	1/1/11/20	6/13/91/115	-
15	CLA	cB	838	-	1/1/11/20	2/16/94/115	-
15	CLA	cA	828	-	1/1/15/20	12/37/115/115	-
15	CLA	cA	816	-	-	3/13/91/115	-
15	CLA	c4	408	-	1/1/11/20	5/13/91/115	-
15	CLA	c6	414	-	1/1/11/20	2/13/91/115	-
15	CLA	b4	403	-	1/1/15/20	14/37/115/115	-
15	CLA	a1	401	-	1/1/15/20	17/37/115/115	-
15	CLA	bA	843	-	1/1/15/20	14/37/115/115	-
15	CLA	cA	807	-	1/1/15/20	9/37/115/115	-
15	CLA	c2	418	13	1/1/13/20	10/25/103/115	-
18	BCR	a6	402	-	-	14/29/63/63	0/2/2/2
15	CLA	bB	834	-	1/1/13/20	13/29/107/115	-
15	CLA	b4	410	13	1/1/14/20	11/36/114/115	-
15	CLA	b2	408	-	1/1/11/20	6/13/91/115	-
15	CLA	b5	412	-	1/1/11/20	9/13/91/115	-
15	CLA	a1	412	-	1/1/11/20	2/13/91/115	-
15	CLA	bA	825	-	1/1/13/20	15/30/108/115	-
15	CLA	aA	816	-	-	3/13/91/115	-
15	CLA	aA	828	-	1/1/15/20	12/37/115/115	-
16	PQN	cB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	a3	401	-	-	12/29/63/63	0/2/2/2
18	BCR	c4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	810	2	1/1/15/20	14/37/115/115	-
15	CLA	c3	417	13	1/1/13/20	10/25/103/115	-
18	BCR	a3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	c2	422	-	1/1/15/20	11/37/115/115	-
15	CLA	a2	416	-	-	5/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a2	417	-	1/1/12/20	9/19/97/115	-
18	BCR	c5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	803	-	1/1/15/20	16/37/115/115	-
15	CLA	b4	407	-	1/1/11/20	6/13/91/115	-
15	CLA	cB	832	-	1/1/11/20	8/18/96/115	-
14	CL0	aA	801	-	3/3/20/25	6/37/135/135	-
15	CLA	aA	827	22	1/1/15/20	10/37/115/115	-
15	CLA	aB	823	-	1/1/13/20	5/25/103/115	-
15	CLA	b3	405	-	1/1/11/20	3/13/91/115	-
15	CLA	bB	812	-	1/1/11/20	3/13/91/115	-
15	CLA	bL	203	-	1/1/15/20	8/37/115/115	-
15	CLA	a3	408	-	1/1/11/20	5/13/91/115	-
15	CLA	b2	410	-	1/1/15/20	7/37/115/115	-
15	CLA	c2	407	-	1/1/11/20	4/13/91/115	-
15	CLA	bB	837	-	1/1/15/20	15/37/115/115	-
15	CLA	b1	410	13	1/1/14/20	12/36/114/115	-
15	CLA	b4	421	-	1/1/15/20	11/37/115/115	-
15	CLA	b6	403	-	1/1/15/20	17/37/115/115	-
15	CLA	bB	817	-	1/1/13/20	10/25/103/115	-
18	BCR	a5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cB	837	-	1/1/15/20	15/37/115/115	-
15	CLA	c1	410	13	1/1/14/20	13/36/114/115	-
15	CLA	c3	414	-	1/1/10/20	2/8/86/115	-
15	CLA	a2	422	-	1/1/15/20	11/37/115/115	-
15	CLA	cB	802	-	1/1/15/20	11/37/115/115	-
15	CLA	aB	822	-	1/1/11/20	2/13/91/115	-
15	CLA	cB	807	-	1/1/15/20	15/37/115/115	-
15	CLA	aB	817	-	1/1/13/20	10/25/103/115	-
15	CLA	c4	404	-	1/1/15/20	9/37/115/115	-
18	BCR	b2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	c4	414	-	1/1/10/20	2/8/86/115	-
15	CLA	bA	816	-	-	3/13/91/115	-
15	CLA	cA	826	-	1/1/15/20	10/37/115/115	-
15	CLA	c6	406	-	1/1/11/20	3/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a3	405	-	1/1/11/20	3/13/91/115	-
15	CLA	cA	842	-	1/1/15/20	14/37/115/115	-
15	CLA	cB	834	-	1/1/13/20	13/29/107/115	-
15	CLA	cB	804	-	1/1/15/20	12/37/115/115	-
15	CLA	aA	817	-	-	4/18/96/115	-
15	CLA	b2	422	-	1/1/15/20	10/37/115/115	-
18	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
18	BCR	aA	851	-	-	8/29/63/63	0/2/2/2
15	CLA	c6	415	-	1/1/10/20	2/8/86/115	-
15	CLA	cB	813	-	1/1/11/20	4/13/91/115	-
15	CLA	b4	414	-	1/1/10/20	2/8/86/115	-
15	CLA	cB	809	-	1/1/15/20	11/37/115/115	-
15	CLA	c3	402	-	1/1/15/20	17/37/115/115	-
15	CLA	b5	403	-	1/1/15/20	14/37/115/115	-
15	CLA	aB	813	-	1/1/11/20	4/13/91/115	-
18	BCR	a2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	a2	410	-	1/1/15/20	6/37/115/115	-
15	CLA	cJ	102	-	1/1/8/20	0/2/76/115	-
15	CLA	b6	417	-	1/1/12/20	9/19/97/115	-
15	CLA	c5	404	-	1/1/15/20	9/37/115/115	-
15	CLA	cA	810	1	1/1/15/20	16/37/115/115	-
15	CLA	c6	410	-	1/1/15/20	6/37/115/115	-
15	CLA	b1	404	-	1/1/15/20	12/37/115/115	-
18	BCR	b3	420	-	-	12/29/63/63	0/2/2/2
18	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	cL	202	-	1/1/15/20	8/37/115/115	-
15	CLA	aB	824	-	1/1/11/20	5/13/91/115	-
15	CLA	cB	812	-	1/1/11/20	3/13/91/115	-
15	CLA	aB	838	-	1/1/11/20	2/16/94/115	-
15	CLA	c2	414	-	1/1/11/20	2/13/91/115	-
15	CLA	bB	818	-	1/1/13/20	10/30/108/115	-
15	CLA	b2	402	-	1/1/15/20	17/37/115/115	-
15	CLA	bA	805	-	1/1/13/20	11/30/108/115	-
15	CLA	c5	408	-	1/1/11/20	5/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b6	413	-	1/1/11/20	9/13/91/115	-
15	CLA	aA	810	1	1/1/15/20	16/37/115/115	-
15	CLA	cB	818	-	1/1/13/20	10/30/108/115	-
15	CLA	bA	821	-	1/1/14/20	13/33/111/115	-
15	CLA	c3	406	-	1/1/11/20	4/13/91/115	-
15	CLA	aB	832	-	1/1/11/20	8/18/96/115	-
15	CLA	aB	833	-	1/1/15/20	18/37/115/115	-
15	CLA	a1	413	-	1/1/10/20	2/8/86/115	-
18	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
18	BCR	cF	204	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	831	-	1/1/11/20	6/13/91/115	-
15	CLA	bA	841	-	1/1/15/20	15/37/115/115	-
15	CLA	aK	102	-	1/1/11/20	8/13/91/115	-
15	CLA	c6	412	13	1/1/11/20	4/13/91/115	-
18	BCR	bL	206	-	-	14/29/63/63	0/2/2/2
15	CLA	b2	416	-	-	5/13/91/115	-
15	CLA	b2	417	-	1/1/12/20	9/19/97/115	-
15	CLA	aA	823	-	1/1/11/20	4/18/96/115	-
17	SF4	cA	846	2,1	-	-	0/6/5/5
15	CLA	bA	830	-	1/1/15/20	13/37/115/115	-
15	CLA	b3	409	-	1/1/15/20	5/37/115/115	-
15	CLA	c4	421	-	1/1/15/20	10/37/115/115	-
15	CLA	a2	414	-	1/1/11/20	1/13/91/115	-
15	CLA	cB	811	2	1/1/15/20	11/37/115/115	-
15	CLA	cB	815	-	1/1/15/20	17/37/115/115	-
15	CLA	cB	840	-	1/1/15/20	14/37/115/115	-
15	CLA	c4	406	-	1/1/11/20	4/13/91/115	-
18	BCR	c4	401	-	-	13/29/63/63	0/2/2/2
17	SF4	cC	102	3	-	-	0/6/5/5
15	CLA	a3	402	-	1/1/15/20	17/37/115/115	-
15	CLA	a5	414	-	1/1/10/20	2/8/86/115	-
15	CLA	a3	410	13	1/1/14/20	10/36/114/115	-
15	CLA	c2	411	13	1/1/14/20	10/36/114/115	-
15	CLA	c6	413	-	1/1/11/20	9/13/91/115	-
15	CLA	a6	403	-	1/1/15/20	17/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c5	407	-	1/1/11/20	6/13/91/115	-
15	CLA	b1	407	-	1/1/11/20	6/13/91/115	-
15	CLA	aB	801	-	1/1/15/20	10/37/115/115	-
15	CLA	c4	410	13	1/1/14/20	11/36/114/115	-
15	CLA	bB	839	22	1/1/15/20	8/37/115/115	-
15	CLA	cB	820	22	1/1/15/20	8/37/115/115	-
15	CLA	bA	819	-	1/1/12/20	8/24/102/115	-
15	CLA	cA	835	-	1/1/15/20	12/37/115/115	-
18	BCR	bA	853	-	-	22/29/63/63	0/2/2/2
15	CLA	a3	406	-	1/1/11/20	4/13/91/115	-
15	CLA	a4	409	-	1/1/15/20	5/37/115/115	-
15	CLA	aA	813	-	1/1/12/20	8/24/102/115	-
18	BCR	a1	420	-	-	12/29/63/63	0/2/2/2
18	BCR	c3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	b4	415	-	-	5/13/91/115	-
15	CLA	bB	820	22	1/1/15/20	8/37/115/115	-
15	CLA	cB	822	-	1/1/11/20	2/13/91/115	-
15	CLA	cB	814	-	1/1/15/20	25/37/115/115	-
15	CLA	bA	803	-	1/1/15/20	16/37/115/115	-
18	BCR	b4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	a2	406	-	1/1/15/20	9/37/115/115	-
15	CLA	bB	826	22	1/1/11/20	8/15/93/115	-
15	CLA	cB	803	-	1/1/15/20	11/37/115/115	-
18	BCR	cA	848	-	-	13/29/63/63	0/2/2/2
15	CLA	a1	416	13	1/1/13/20	9/25/103/115	-
15	CLA	a5	406	-	1/1/11/20	4/13/91/115	-
19	LHG	cA	853	15	-	15/31/31/53	-
18	BCR	c3	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c5	410	13	1/1/14/20	11/36/114/115	-
15	CLA	aA	832	-	1/1/12/20	6/19/97/115	-
15	CLA	c1	405	-	1/1/11/20	3/13/91/115	-
15	CLA	aA	833	-	1/1/15/20	11/37/115/115	-
18	BCR	cF	205	-	-	11/29/63/63	0/2/2/2
18	BCR	cL	204	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	a6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	414	-	1/1/11/20	1/13/91/115	-
18	BCR	a4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	c3	410	13	1/1/14/20	10/36/114/115	-
15	CLA	aB	814	-	1/1/15/20	25/37/115/115	-
14	CL0	bA	801	-	3/3/20/25	6/37/135/135	-
17	SF4	aC	101	3	-	-	0/6/5/5
15	CLA	cB	842	-	-	0/13/91/115	-
18	BCR	c5	401	-	-	13/29/63/63	0/2/2/2
18	BCR	bJ	105	-	-	11/29/63/63	0/2/2/2
18	BCR	aF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	416	-	1/1/12/20	9/19/97/115	-
15	CLA	b3	417	13	1/1/13/20	10/25/103/115	-
15	CLA	a1	422	-	1/1/15/20	14/37/115/115	-
18	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
18	BCR	aI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	405	-	1/1/11/20	4/13/91/115	-
15	CLA	c4	405	-	1/1/11/20	4/13/91/115	-
18	BCR	b5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	b6	411	13	1/1/14/20	12/36/114/115	-
15	CLA	bA	845	19	1/1/12/20	13/22/100/115	-
15	CLA	a5	420	-	1/1/15/20	10/37/115/115	-
15	CLA	cA	823	-	1/1/11/20	4/18/96/115	-
18	BCR	bA	850	-	-	13/29/63/63	0/2/2/2
15	CLA	cB	824	-	1/1/11/20	5/13/91/115	-
15	CLA	b6	412	13	1/1/11/20	4/13/91/115	-
18	BCR	aF	203	-	-	11/29/63/63	0/2/2/2
18	BCR	a3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	c2	403	-	1/1/15/20	14/37/115/115	-
16	PQN	aA	846	-	-	5/23/43/43	0/2/2/2
15	CLA	a6	409	-	1/1/11/20	5/13/91/115	-
15	CLA	cK	102	-	1/1/11/20	8/13/91/115	-
15	CLA	cB	829	-	1/1/15/20	16/37/115/115	-
18	BCR	bB	849	-	-	14/29/63/63	0/2/2/2
18	BCR	c6	401	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	a4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	c2	413	-	1/1/11/20	9/13/91/115	-
15	CLA	b3	414	-	1/1/10/20	2/8/86/115	-
15	CLA	b6	407	-	1/1/11/20	4/13/91/115	-
18	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
15	CLA	aB	829	-	1/1/15/20	16/37/115/115	-
15	CLA	c5	411	13	1/1/11/20	3/13/91/115	-
15	CLA	bB	825	2	1/1/12/20	10/24/102/115	-
15	CLA	b5	404	-	1/1/15/20	9/37/115/115	-
15	CLA	aA	843	-	1/1/15/20	14/37/115/115	-
15	CLA	c3	403	-	1/1/15/20	13/37/115/115	-
18	BCR	aB	849	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	831	-	1/1/15/20	8/37/115/115	-
15	CLA	aA	804	-	1/1/15/20	10/37/115/115	-
15	CLA	aA	812	-	1/1/15/20	11/37/115/115	-
15	CLA	a2	408	-	1/1/11/20	6/13/91/115	-
15	CLA	a4	417	13	1/1/13/20	8/25/103/115	-
19	LHG	aX	101	-	-	11/26/26/53	-
15	CLA	cA	821	-	1/1/14/20	13/33/111/115	-
15	CLA	c3	413	-	1/1/11/20	2/13/91/115	-
15	CLA	c4	415	-	-	5/13/91/115	-
18	BCR	b5	419	-	-	12/29/63/63	0/2/2/2
18	BCR	a1	419	-	-	12/29/63/63	0/2/2/2
15	CLA	a6	405	-	1/1/15/20	9/37/115/115	-
18	BCR	c6	402	-	-	13/29/63/63	0/2/2/2
15	CLA	b2	406	-	1/1/15/20	8/37/115/115	-
15	CLA	cA	827	22	1/1/15/20	10/37/115/115	-
15	CLA	aB	841	-	1/1/11/20	2/13/91/115	-
15	CLA	a5	413	-	1/1/11/20	1/13/91/115	-
18	BCR	cA	851	-	-	22/29/63/63	0/2/2/2
15	CLA	b3	402	-	1/1/15/20	17/37/115/115	-
15	CLA	c3	408	-	1/1/11/20	5/13/91/115	-
15	CLA	a6	407	-	1/1/11/20	4/13/91/115	-
15	CLA	c3	404	-	1/1/15/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	c6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	844	-	1/1/9/20	5/7/81/115	-
18	BCR	c3	401	-	-	13/29/63/63	0/2/2/2
16	PQN	bB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	a4	414	-	1/1/10/20	2/8/86/115	-
15	CLA	b1	403	-	1/1/15/20	14/37/115/115	-
15	CLA	bA	835	-	1/1/15/20	12/37/115/115	-
15	CLA	cA	838	-	1/1/12/20	8/21/99/115	-
15	CLA	aA	814	-	1/1/14/20	14/31/109/115	-
15	CLA	c6	416	-	-	5/13/91/115	-
15	CLA	cF	201	22	1/1/12/20	8/21/99/115	-
15	CLA	bB	824	-	1/1/11/20	5/13/91/115	-
15	CLA	c4	416	-	1/1/12/20	9/19/97/115	-
15	CLA	bA	837	1	-	7/13/91/115	-
18	BCR	b2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	bB	807	-	1/1/15/20	15/37/115/115	-
15	CLA	b3	406	-	1/1/11/20	4/13/91/115	-
15	CLA	b5	409	-	1/1/15/20	6/37/115/115	-
18	BCR	b3	401	-	-	13/29/63/63	0/2/2/2
18	BCR	a6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	a4	402	-	1/1/15/20	17/37/115/115	-
18	BCR	bJ	103	-	-	14/29/63/63	0/2/2/2
18	BCR	bF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	cB	836	-	1/1/14/20	9/31/109/115	-
15	CLA	c6	405	-	1/1/15/20	9/37/115/115	-
15	CLA	b5	415	-	-	5/13/91/115	-
15	CLA	a3	404	-	1/1/15/20	10/37/115/115	-
15	CLA	bB	830	-	1/1/15/20	6/37/115/115	-
18	BCR	bB	850	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	829	-	1/1/15/20	22/37/115/115	-
15	CLA	bB	803	-	1/1/15/20	11/37/115/115	-
15	CLA	b4	405	-	1/1/11/20	4/13/91/115	-
18	BCR	aA	852	-	-	22/29/63/63	0/2/2/2
15	CLA	aA	818	-	1/1/12/20	6/24/102/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c5	403	-	1/1/15/20	14/37/115/115	-
15	CLA	aB	827	-	1/1/15/20	15/37/115/115	-
15	CLA	c3	416	-	1/1/12/20	9/19/97/115	-
18	BCR	c1	401	-	-	12/29/63/63	0/2/2/2
18	BCR	b4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	a4	406	-	1/1/11/20	4/13/91/115	-
15	CLA	a2	402	-	1/1/15/20	17/37/115/115	-
15	CLA	bA	812	-	1/1/15/20	11/37/115/115	-
15	CLA	c1	407	-	1/1/11/20	6/13/91/115	-
15	CLA	a4	415	-	-	5/13/91/115	-
18	BCR	a4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	a2	409	-	1/1/11/20	5/13/91/115	-
15	CLA	bA	810	1	1/1/15/20	16/37/115/115	-
15	CLA	aX	102	12	1/1/11/20	6/13/91/115	-
15	CLA	cA	824	-	1/1/12/20	12/21/99/115	-
15	CLA	cA	840	-	1/1/11/20	5/16/94/115	-
15	CLA	c1	415	-	-	5/13/91/115	-
15	CLA	bA	818	-	1/1/12/20	6/24/102/115	-
15	CLA	b4	408	-	1/1/11/20	5/13/91/115	-
18	BCR	a2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a5	409	-	1/1/15/20	6/37/115/115	-
15	CLA	cA	813	-	1/1/12/20	8/24/102/115	-
15	CLA	cA	806	-	1/1/15/20	23/37/115/115	-
18	BCR	c1	418	-	-	8/29/63/63	0/2/2/2
15	CLA	a5	411	13	1/1/11/20	3/13/91/115	-
16	PQN	aB	843	-	-	10/23/43/43	0/2/2/2
19	LHG	aA	853	-	-	19/53/53/53	-
18	BCR	b3	418	-	-	10/29/63/63	0/2/2/2
15	CLA	aA	834	-	1/1/15/20	12/37/115/115	-
15	CLA	aB	839	22	1/1/15/20	8/37/115/115	-
15	CLA	b1	408	-	1/1/11/20	5/13/91/115	-
15	CLA	cX	102	12	1/1/11/20	6/13/91/115	-
18	BCR	aL	205	-	-	14/29/63/63	0/2/2/2
15	CLA	bB	808	-	-	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c5	412	-	1/1/11/20	9/13/91/115	-
15	CLA	aA	840	-	1/1/11/20	4/16/94/115	-
18	BCR	a1	418	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	808	-	-	12/37/115/115	-
15	CLA	b5	408	-	1/1/11/20	5/13/91/115	-
15	CLA	bA	811	-	1/1/11/20	8/13/91/115	-
15	CLA	bA	815	-	1/1/11/20	2/13/91/115	-
18	BCR	bB	848	-	-	13/29/63/63	0/2/2/2
18	BCR	cJ	103	-	-	14/29/63/63	0/2/2/2
15	CLA	b5	420	-	1/1/15/20	10/37/115/115	-
18	BCR	aJ	204	-	-	14/29/63/63	0/2/2/2
15	CLA	a2	412	13	1/1/11/20	3/13/91/115	-
18	BCR	b6	420	-	-	12/29/63/63	0/2/2/2
19	LHG	cX	101	-	-	11/26/26/53	-
15	CLA	a1	403	-	1/1/15/20	11/37/115/115	-
15	CLA	a5	412	-	1/1/11/20	9/13/91/115	-
15	CLA	bA	826	-	1/1/15/20	10/37/115/115	-
15	CLA	bB	819	-	1/1/14/20	12/31/109/115	-
15	CLA	bB	836	-	1/1/14/20	9/31/109/115	-
15	CLA	cA	820	-	1/1/15/20	18/37/115/115	-
15	CLA	bA	842	22	1/1/12/20	8/21/99/115	-
15	CLA	cA	832	-	1/1/12/20	6/19/97/115	-
15	CLA	c3	421	-	1/1/15/20	10/37/115/115	-
15	CLA	c2	416	-	-	5/13/91/115	-
15	CLA	a1	415	-	1/1/12/20	9/19/97/115	-
18	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	cB	839	22	1/1/15/20	8/37/115/115	-
15	CLA	cB	816	-	1/1/11/20	6/13/91/115	-
15	CLA	cB	828	-	1/1/15/20	21/37/115/115	-
15	CLA	bA	809	1	1/1/15/20	19/37/115/115	-
18	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
19	LHG	aA	854	15	-	15/31/31/53	-
15	CLA	a5	407	-	1/1/11/20	6/13/91/115	-
15	CLA	a1	408	-	1/1/15/20	6/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	835	-	1/1/15/20	12/37/115/115	-
15	CLA	a4	407	-	1/1/11/20	6/13/91/115	-
15	CLA	bA	838	-	1/1/12/20	8/21/99/115	-
15	CLA	c3	411	13	1/1/11/20	5/13/91/115	-
18	BCR	b4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	802	-	1/1/15/20	11/37/115/115	-
15	CLA	b3	410	13	1/1/14/20	10/36/114/115	-
15	CLA	c6	404	-	1/1/15/20	14/37/115/115	-
19	LHG	bX	101	-	-	11/26/26/53	-
15	CLA	a6	415	-	1/1/10/20	2/8/86/115	-
15	CLA	cL	203	22	1/1/15/20	13/37/115/115	-
15	CLA	c2	417	-	1/1/12/20	9/19/97/115	-
15	CLA	bB	832	-	1/1/11/20	8/18/96/115	-
18	BCR	c2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	843	-	1/1/9/20	5/7/81/115	-
18	BCR	c4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	804	-	1/1/15/20	10/37/115/115	-
15	CLA	cA	812	-	1/1/15/20	11/37/115/115	-
18	BCR	bB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	cB	806	-	1/1/15/20	21/37/115/115	-
15	CLA	a1	405	-	1/1/11/20	4/13/91/115	-
15	CLA	a3	413	-	1/1/11/20	1/13/91/115	-
15	CLA	cA	817	-	-	4/18/96/115	-
15	CLA	b1	411	13	1/1/11/20	5/13/91/115	-
15	CLA	a2	405	-	1/1/11/20	4/13/91/115	-
15	CLA	a4	410	13	1/1/14/20	11/36/114/115	-
18	BCR	b6	402	-	-	14/29/63/63	0/2/2/2
15	CLA	c6	418	13	1/1/13/20	10/25/103/115	-
17	SF4	bC	101	3	-	-	0/6/5/5
15	CLA	bA	807	-	1/1/15/20	9/37/115/115	-
18	BCR	aM	101	-	-	11/29/63/63	0/2/2/2
18	BCR	cF	202	-	-	14/29/63/63	0/2/2/2
15	CLA	cB	827	-	1/1/15/20	15/37/115/115	-
15	CLA	aB	818	-	1/1/13/20	10/30/108/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	817	-	1/1/13/20	10/25/103/115	-
15	CLA	aL	203	22	1/1/15/20	13/37/115/115	-
15	CLA	c4	407	-	1/1/11/20	6/13/91/115	-
15	CLA	bB	805	-	1/1/12/20	5/24/102/115	-
18	BCR	c2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b2	405	-	1/1/11/20	4/13/91/115	-
15	CLA	b3	404	-	1/1/15/20	10/37/115/115	-
15	CLA	a3	421	-	1/1/15/20	10/37/115/115	-
15	CLA	bB	813	-	1/1/11/20	4/13/91/115	-
15	CLA	b4	416	-	1/1/12/20	9/19/97/115	-
15	CLA	bB	809	-	1/1/15/20	11/37/115/115	-
15	CLA	b1	412	-	1/1/11/20	9/13/91/115	-
15	CLA	cA	814	-	1/1/14/20	14/31/109/115	-
15	CLA	a2	404	-	1/1/15/20	10/37/115/115	-
18	BCR	aF	201	-	-	14/29/63/63	0/2/2/2
18	BCR	c1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	407	-	1/1/11/20	4/13/91/115	-
15	CLA	bA	824	-	1/1/12/20	12/21/99/115	-
15	CLA	a5	415	-	-	5/13/91/115	-
15	CLA	cA	844	19	1/1/12/20	13/22/100/115	-
20	LMG	aB	850	-	-	26/50/70/70	0/1/1/1
18	BCR	b5	401	-	-	14/29/63/63	0/2/2/2
15	CLA	aB	834	-	1/1/13/20	13/29/107/115	-
15	CLA	cA	811	-	1/1/11/20	8/13/91/115	-
15	CLA	aB	804	-	1/1/15/20	12/37/115/115	-
15	CLA	a6	414	-	1/1/11/20	2/13/91/115	-
15	CLA	c1	406	-	1/1/11/20	4/13/91/115	-
15	CLA	c1	408	-	1/1/11/20	5/13/91/115	-
15	CLA	a6	413	-	1/1/11/20	9/13/91/115	-
18	BCR	bL	201	-	-	14/29/63/63	0/2/2/2
15	CLA	bA	823	-	1/1/11/20	4/18/96/115	-
15	CLA	a2	418	13	1/1/13/20	10/25/103/115	-
15	CLA	a4	413	-	1/1/11/20	2/13/91/115	-
18	BCR	b4	418	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	802	22	1/1/15/20	16/37/115/115	-
16	PQN	bA	846	-	-	5/23/43/43	0/2/2/2
15	CLA	c4	417	13	1/1/13/20	8/25/103/115	-
15	CLA	b2	409	-	1/1/11/20	5/13/91/115	-
15	CLA	bK	101	-	1/1/11/20	8/13/91/115	-
15	CLA	cA	822	-	1/1/15/20	16/37/115/115	-
15	CLA	b5	410	13	1/1/14/20	12/36/114/115	-
15	CLA	cA	829	-	1/1/15/20	22/37/115/115	-
15	CLA	cA	833	-	1/1/15/20	11/37/115/115	-
18	BCR	aJ	205	-	-	10/29/63/63	0/2/2/2
15	CLA	bB	811	2	1/1/15/20	11/37/115/115	-
15	CLA	c5	405	-	1/1/11/20	4/13/91/115	-
15	CLA	bJ	102	-	1/1/8/20	0/2/76/115	-
15	CLA	a5	403	-	1/1/15/20	14/37/115/115	-
15	CLA	a1	409	13	1/1/14/20	12/36/114/115	-
16	PQN	cA	845	-	-	5/23/43/43	0/2/2/2
15	CLA	a3	411	13	1/1/11/20	5/13/91/115	-
18	BCR	aB	848	-	-	13/29/63/63	0/2/2/2
18	BCR	aK	101	-	-	10/29/63/63	0/2/2/2
15	CLA	b6	422	-	1/1/15/20	15/37/115/115	-
15	CLA	aB	821	-	1/1/11/20	11/16/94/115	-
15	CLA	aA	824	-	1/1/12/20	12/21/99/115	-
15	CLA	aA	838	-	1/1/12/20	8/21/99/115	-
15	CLA	b5	405	-	1/1/11/20	4/13/91/115	-
18	BCR	aI	103	-	-	9/29/63/63	0/2/2/2
18	BCR	bI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	416	-	1/1/12/20	9/19/97/115	-
18	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	b5	417	13	1/1/13/20	9/25/103/115	-
15	CLA	aA	805	-	1/1/13/20	11/30/108/115	-
18	BCR	b6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c1	417	13	1/1/13/20	8/25/103/115	-
15	CLA	a1	411	-	1/1/11/20	9/13/91/115	-
15	CLA	aA	837	1	-	7/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b5	407	-	1/1/11/20	6/13/91/115	-
15	CLA	bB	842	-	-	0/13/91/115	-
15	CLA	c6	409	-	1/1/11/20	5/13/91/115	-
15	CLA	a3	407	-	1/1/11/20	6/13/91/115	-
15	CLA	bB	815	-	1/1/15/20	17/37/115/115	-
15	CLA	bA	822	-	1/1/15/20	16/37/115/115	-
15	CLA	a3	412	-	1/1/11/20	9/13/91/115	-
15	CLA	b4	406	-	1/1/11/20	4/13/91/115	-
15	CLA	c2	405	-	1/1/11/20	3/13/91/115	-
18	BCR	a2	421	-	-	12/29/63/63	0/2/2/2
17	SF4	aC	102	3	-	-	0/6/5/5
15	CLA	c2	406	-	1/1/15/20	9/37/115/115	-
18	BCR	c2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	aJ	202	8	1/1/11/20	6/13/91/115	-
15	CLA	bA	836	-	1/1/12/20	6/24/102/115	-
15	CLA	aB	806	-	1/1/15/20	21/37/115/115	-
19	LHG	cA	852	-	-	19/53/53/53	-
15	CLA	a6	410	-	1/1/15/20	6/37/115/115	-
15	CLA	c1	403	-	1/1/15/20	14/37/115/115	-
15	CLA	a4	416	-	1/1/12/20	9/19/97/115	-
15	CLA	bB	829	-	1/1/15/20	16/37/115/115	-
15	CLA	c2	415	-	1/1/10/20	2/8/86/115	-
15	CLA	c6	411	13	1/1/14/20	10/36/114/115	-
15	CLA	cB	833	-	1/1/15/20	18/37/115/115	-
15	CLA	aA	825	-	1/1/13/20	15/30/108/115	-
15	CLA	b1	402	-	1/1/15/20	17/37/115/115	-
15	CLA	cB	831	-	1/1/11/20	6/13/91/115	-
15	CLA	b2	418	13	1/1/13/20	10/25/103/115	-
15	CLA	c2	410	-	1/1/15/20	6/37/115/115	-
15	CLA	a2	403	-	1/1/15/20	14/37/115/115	-
15	CLA	aB	828	-	1/1/15/20	21/37/115/115	-
20	LMG	cB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	b5	402	-	1/1/15/20	17/37/115/115	-
15	CLA	aA	845	19	1/1/12/20	13/22/100/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	804	-	1/1/15/20	12/37/115/115	-
15	CLA	cA	834	-	1/1/15/20	12/37/115/115	-
15	CLA	b6	404	-	1/1/15/20	14/37/115/115	-
15	CLA	aB	805	-	1/1/12/20	5/24/102/115	-
15	CLA	b3	421	-	1/1/15/20	10/37/115/115	-
15	CLA	b6	415	-	1/1/10/20	2/8/86/115	-
15	CLA	c2	408	-	1/1/11/20	6/13/91/115	-
15	CLA	a6	417	-	1/1/12/20	9/19/97/115	-
15	CLA	c5	414	-	1/1/10/20	2/8/86/115	-
15	CLA	aJ	203	-	1/1/8/20	0/2/76/115	-
15	CLA	a3	414	-	1/1/10/20	2/8/86/115	-
15	CLA	cB	801	-	1/1/15/20	10/37/115/115	-
18	BCR	aA	848	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	404	-	1/1/15/20	9/37/115/115	-
15	CLA	b5	414	-	1/1/10/20	2/8/86/115	-
18	BCR	b1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b6	418	13	1/1/13/20	10/25/103/115	-
15	CLA	c1	409	-	1/1/15/20	6/37/115/115	-
18	BCR	bJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	aB	835	-	1/1/11/20	7/13/91/115	-
15	CLA	a4	421	-	1/1/15/20	11/37/115/115	-
15	CLA	b5	406	-	1/1/11/20	4/13/91/115	-
18	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	c4	411	13	1/1/11/20	4/13/91/115	-
17	SF4	bC	102	3	-	-	0/6/5/5
15	CLA	cJ	101	8	1/1/11/20	6/13/91/115	-
15	CLA	aB	812	-	1/1/11/20	3/13/91/115	-
15	CLA	bB	841	-	1/1/11/20	2/13/91/115	-
15	CLA	bJ	101	8	1/1/11/20	6/13/91/115	-
18	BCR	cB	849	-	-	11/29/63/63	0/2/2/2
15	CLA	b4	404	-	1/1/15/20	10/37/115/115	-

All (5761) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	417	CLA	C4B-NB	9.16	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c4	417	CLA	C4B-NB	9.15	1.43	1.35
15	b3	417	CLA	C4B-NB	9.07	1.43	1.35
15	c3	417	CLA	C4B-NB	9.06	1.43	1.35
15	a4	417	CLA	C4B-NB	9.06	1.43	1.35
15	a2	418	CLA	C4B-NB	9.03	1.43	1.35
15	b2	418	CLA	C4B-NB	9.01	1.43	1.35
15	c2	418	CLA	C4B-NB	9.00	1.43	1.35
15	b6	418	CLA	C4B-NB	8.98	1.43	1.35
15	c6	418	CLA	C4B-NB	8.94	1.43	1.35
15	a6	418	CLA	C4B-NB	8.94	1.43	1.35
15	a3	417	CLA	C4B-NB	8.87	1.43	1.35
15	a5	417	CLA	C4B-NB	8.86	1.43	1.35
15	b5	417	CLA	C4B-NB	8.82	1.43	1.35
15	c5	417	CLA	C4B-NB	8.80	1.43	1.35
15	b1	417	CLA	C4B-NB	8.79	1.43	1.35
15	c1	417	CLA	C4B-NB	8.72	1.43	1.35
15	a1	416	CLA	C4B-NB	8.51	1.42	1.35
15	b6	422	CLA	C4B-NB	8.25	1.42	1.35
15	b5	420	CLA	C4B-NB	8.17	1.42	1.35
15	a4	421	CLA	C4B-NB	8.15	1.42	1.35
15	a5	420	CLA	C4B-NB	8.12	1.42	1.35
15	b4	421	CLA	C4B-NB	8.09	1.42	1.35
15	c5	420	CLA	C4B-NB	8.09	1.42	1.35
15	c2	406	CLA	C4B-NB	8.08	1.42	1.35
15	a6	422	CLA	C4B-NB	8.06	1.42	1.35
15	b2	406	CLA	C4B-NB	8.04	1.42	1.35
15	a2	406	CLA	C4B-NB	8.04	1.42	1.35
15	a6	415	CLA	C4B-NB	8.01	1.42	1.35
15	c6	415	CLA	C4B-NB	7.97	1.42	1.35
15	c4	421	CLA	C4B-NB	7.95	1.42	1.35
15	b6	415	CLA	C4B-NB	7.94	1.42	1.35
15	a3	414	CLA	C4B-NB	7.94	1.42	1.35
15	b1	414	CLA	C4B-NB	7.91	1.42	1.35
15	c1	414	CLA	C4B-NB	7.91	1.42	1.35
15	a3	421	CLA	C4B-NB	7.90	1.42	1.35
15	b5	414	CLA	C4B-NB	7.89	1.42	1.35
15	b3	421	CLA	C4B-NB	7.88	1.42	1.35
15	a1	422	CLA	C4B-NB	7.87	1.42	1.35
15	a1	413	CLA	C4B-NB	7.85	1.42	1.35
15	a5	414	CLA	C4B-NB	7.85	1.42	1.35
15	c3	421	CLA	C4B-NB	7.83	1.42	1.35
15	cA	841	CLA	C4B-NB	7.81	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	841	CLA	C4B-NB	7.81	1.42	1.35
15	c2	415	CLA	C4B-NB	7.79	1.42	1.35
15	bA	841	CLA	C4B-NB	7.79	1.42	1.35
15	b3	414	CLA	C4B-NB	7.78	1.42	1.35
15	c5	414	CLA	C4B-NB	7.77	1.42	1.35
15	c4	414	CLA	C4B-NB	7.77	1.42	1.35
15	b2	415	CLA	C4B-NB	7.76	1.42	1.35
15	a4	414	CLA	C4B-NB	7.74	1.42	1.35
15	a2	415	CLA	C4B-NB	7.73	1.42	1.35
15	c3	414	CLA	C4B-NB	7.73	1.42	1.35
15	b4	414	CLA	C4B-NB	7.73	1.42	1.35
15	c2	422	CLA	C4B-NB	7.68	1.42	1.35
15	a2	422	CLA	C4B-NB	7.62	1.42	1.35
15	bB	842	CLA	C4B-NB	7.59	1.42	1.35
15	b2	422	CLA	C4B-NB	7.55	1.41	1.35
15	aB	842	CLA	C4B-NB	7.54	1.41	1.35
15	c6	405	CLA	C4B-NB	7.53	1.41	1.35
15	a6	405	CLA	C4B-NB	7.53	1.41	1.35
15	cB	842	CLA	C4B-NB	7.49	1.41	1.35
15	b6	405	CLA	C4B-NB	7.49	1.41	1.35
15	c6	416	CLA	C4B-NB	7.46	1.41	1.35
15	a6	416	CLA	C4B-NB	7.42	1.41	1.35
15	b1	413	CLA	C4B-NB	7.42	1.41	1.35
15	b2	404	CLA	C4B-NB	7.41	1.41	1.35
15	b6	416	CLA	C4B-NB	7.38	1.41	1.35
15	c1	406	CLA	C4B-NB	7.37	1.41	1.35
15	cB	833	CLA	C4B-NB	7.37	1.41	1.35
15	c1	409	CLA	C4B-NB	7.37	1.41	1.35
15	b4	406	CLA	C4B-NB	7.37	1.41	1.35
15	c1	413	CLA	C4B-NB	7.36	1.41	1.35
15	bB	841	CLA	C4B-NB	7.36	1.41	1.35
15	b5	402	CLA	C4B-NB	7.36	1.41	1.35
15	a1	408	CLA	C4B-NB	7.35	1.41	1.35
15	a2	404	CLA	C4B-NB	7.35	1.41	1.35
15	c4	406	CLA	C4B-NB	7.34	1.41	1.35
15	a1	412	CLA	C4B-NB	7.34	1.41	1.35
15	a5	402	CLA	C4B-NB	7.34	1.41	1.35
15	aB	833	CLA	C4B-NB	7.34	1.41	1.35
15	b5	406	CLA	C4B-NB	7.34	1.41	1.35
15	a4	406	CLA	C4B-NB	7.33	1.41	1.35
15	cB	841	CLA	C4B-NB	7.33	1.41	1.35
15	b3	406	CLA	C4B-NB	7.32	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	403	CLA	C4B-NB	7.30	1.41	1.35
15	c5	402	CLA	C4B-NB	7.29	1.41	1.35
15	c5	406	CLA	C4B-NB	7.29	1.41	1.35
15	c1	404	CLA	C4B-NB	7.28	1.41	1.35
15	a3	406	CLA	C4B-NB	7.28	1.41	1.35
15	c5	409	CLA	C4B-NB	7.28	1.41	1.35
15	b1	406	CLA	C4B-NB	7.28	1.41	1.35
15	b3	404	CLA	C4B-NB	7.28	1.41	1.35
15	bB	833	CLA	C4B-NB	7.28	1.41	1.35
15	a5	406	CLA	C4B-NB	7.27	1.41	1.35
15	a3	404	CLA	C4B-NB	7.26	1.41	1.35
15	b1	409	CLA	C4B-NB	7.26	1.41	1.35
15	a1	405	CLA	C4B-NB	7.26	1.41	1.35
15	c3	404	CLA	C4B-NB	7.25	1.41	1.35
15	aB	841	CLA	C4B-NB	7.24	1.41	1.35
15	c2	404	CLA	C4B-NB	7.24	1.41	1.35
15	b1	404	CLA	C4B-NB	7.24	1.41	1.35
15	bX	102	CLA	C4B-NB	7.22	1.41	1.35
15	c2	412	CLA	C4B-NB	7.22	1.41	1.35
15	b5	409	CLA	C4B-NB	7.22	1.41	1.35
15	bA	837	CLA	C4B-NB	7.22	1.41	1.35
15	c3	406	CLA	C4B-NB	7.21	1.41	1.35
15	aB	808	CLA	C4B-NB	7.21	1.41	1.35
15	cA	837	CLA	C4B-NB	7.21	1.41	1.35
15	bB	808	CLA	C4B-NB	7.21	1.41	1.35
15	a5	409	CLA	C4B-NB	7.20	1.41	1.35
15	b2	412	CLA	C4B-NB	7.20	1.41	1.35
15	cB	808	CLA	C4B-NB	7.20	1.41	1.35
15	c6	410	CLA	C4B-NB	7.19	1.41	1.35
15	a4	413	CLA	C4B-NB	7.19	1.41	1.35
15	b4	411	CLA	C4B-NB	7.19	1.41	1.35
15	c5	404	CLA	C4B-NB	7.18	1.41	1.35
15	aA	837	CLA	C4B-NB	7.18	1.41	1.35
15	a5	404	CLA	C4B-NB	7.16	1.41	1.35
15	b6	414	CLA	C4B-NB	7.16	1.41	1.35
15	aB	813	CLA	C4B-NB	7.15	1.41	1.35
15	c6	414	CLA	C4B-NB	7.15	1.41	1.35
15	a2	412	CLA	C4B-NB	7.15	1.41	1.35
15	aX	102	CLA	C4B-NB	7.14	1.41	1.35
15	bA	843	CLA	C4B-NB	7.14	1.41	1.35
15	c4	413	CLA	C4B-NB	7.13	1.41	1.35
15	c4	404	CLA	C4B-NB	7.12	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	407	CLA	C4B-NB	7.12	1.41	1.35
15	cX	102	CLA	C4B-NB	7.12	1.41	1.35
15	b2	407	CLA	C4B-NB	7.12	1.41	1.35
15	b5	404	CLA	C4B-NB	7.12	1.41	1.35
15	a2	407	CLA	C4B-NB	7.11	1.41	1.35
15	a1	410	CLA	C4B-NB	7.11	1.41	1.35
15	b2	402	CLA	C4B-NB	7.11	1.41	1.35
15	b6	410	CLA	C4B-NB	7.11	1.41	1.35
15	b4	413	CLA	C4B-NB	7.10	1.41	1.35
15	c1	411	CLA	C4B-NB	7.10	1.41	1.35
15	bB	813	CLA	C4B-NB	7.09	1.41	1.35
15	cB	813	CLA	C4B-NB	7.08	1.41	1.35
15	a2	402	CLA	C4B-NB	7.08	1.41	1.35
15	cB	815	CLA	C4B-NB	7.06	1.41	1.35
15	a6	410	CLA	C4B-NB	7.06	1.41	1.35
15	b2	405	CLA	C4B-NB	7.06	1.41	1.35
15	a4	411	CLA	C4B-NB	7.06	1.41	1.35
15	cA	842	CLA	C4B-NB	7.05	1.41	1.35
15	a4	404	CLA	C4B-NB	7.05	1.41	1.35
15	aA	843	CLA	C4B-NB	7.05	1.41	1.35
15	a2	414	CLA	C4B-NB	7.04	1.41	1.35
15	b6	407	CLA	C4B-NB	7.04	1.41	1.35
15	a5	413	CLA	C4B-NB	7.03	1.41	1.35
15	b2	414	CLA	C4B-NB	7.03	1.41	1.35
15	a6	407	CLA	C4B-NB	7.03	1.41	1.35
15	aB	815	CLA	C4B-NB	7.02	1.41	1.35
15	a2	408	CLA	C4B-NB	7.02	1.41	1.35
15	b4	404	CLA	C4B-NB	7.02	1.41	1.35
15	a2	405	CLA	C4B-NB	7.00	1.41	1.35
15	c5	413	CLA	C4B-NB	7.00	1.41	1.35
15	c2	405	CLA	C4B-NB	6.98	1.41	1.35
15	a6	414	CLA	C4B-NB	6.98	1.41	1.35
15	c2	408	CLA	C4B-NB	6.98	1.41	1.35
15	c6	407	CLA	C4B-NB	6.97	1.41	1.35
15	b2	413	CLA	C4B-NB	6.97	1.41	1.35
15	c4	402	CLA	C4B-NB	6.97	1.41	1.35
15	c2	414	CLA	C4B-NB	6.96	1.41	1.35
15	c5	407	CLA	C4B-NB	6.96	1.41	1.35
15	b6	413	CLA	C4B-NB	6.96	1.41	1.35
15	a4	409	CLA	C4B-NB	6.96	1.41	1.35
15	c4	411	CLA	C4B-NB	6.96	1.41	1.35
15	bB	815	CLA	C4B-NB	6.96	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	409	CLA	C4B-NB	6.96	1.41	1.35
15	c5	415	CLA	C4B-NB	6.96	1.41	1.35
15	c4	409	CLA	C4B-NB	6.95	1.41	1.35
15	c2	410	CLA	C4B-NB	6.95	1.41	1.35
15	b1	411	CLA	C4B-NB	6.94	1.41	1.35
15	b5	413	CLA	C4B-NB	6.94	1.41	1.35
15	c2	413	CLA	C4B-NB	6.93	1.41	1.35
15	c5	411	CLA	C4B-NB	6.93	1.41	1.35
15	c6	408	CLA	C4B-NB	6.93	1.41	1.35
15	b5	411	CLA	C4B-NB	6.93	1.41	1.35
15	c2	402	CLA	C4B-NB	6.93	1.41	1.35
16	aA	846	PQN	C3-C2	6.92	1.47	1.35
15	a6	403	CLA	C4B-NB	6.92	1.41	1.35
15	bA	817	CLA	C4B-NB	6.92	1.41	1.35
15	a3	413	CLA	C4B-NB	6.91	1.41	1.35
15	c6	413	CLA	C4B-NB	6.91	1.41	1.35
15	a3	409	CLA	C4B-NB	6.91	1.41	1.35
15	b3	412	CLA	C4B-NB	6.90	1.41	1.35
15	c3	413	CLA	C4B-NB	6.90	1.41	1.35
15	c5	403	CLA	C4B-NB	6.90	1.41	1.35
15	a6	408	CLA	C4B-NB	6.90	1.41	1.35
15	aJ	203	CLA	C4B-NB	6.88	1.41	1.35
15	b2	410	CLA	C4B-NB	6.88	1.41	1.35
15	b2	403	CLA	C4B-NB	6.88	1.41	1.35
15	bB	821	CLA	C4B-NB	6.88	1.41	1.35
16	bA	846	PQN	C3-C2	6.88	1.47	1.35
15	bB	824	CLA	C4B-NB	6.87	1.41	1.35
15	cB	821	CLA	C4B-NB	6.87	1.41	1.35
15	cJ	102	CLA	C4B-NB	6.87	1.41	1.35
15	a1	401	CLA	C4B-NB	6.87	1.41	1.35
15	cB	801	CLA	C4B-NB	6.87	1.41	1.35
15	b6	406	CLA	C4B-NB	6.87	1.41	1.35
15	a6	413	CLA	C4B-NB	6.86	1.41	1.35
15	aA	828	CLA	C4B-NB	6.86	1.41	1.35
15	b4	409	CLA	C4B-NB	6.86	1.41	1.35
15	cA	817	CLA	C4B-NB	6.86	1.41	1.35
16	cA	845	PQN	C3-C2	6.86	1.47	1.35
15	a5	407	CLA	C4B-NB	6.86	1.41	1.35
15	a2	410	CLA	C4B-NB	6.86	1.41	1.35
15	aA	811	CLA	C4B-NB	6.86	1.41	1.35
15	a6	406	CLA	C4B-NB	6.85	1.41	1.35
15	b3	409	CLA	C4B-NB	6.85	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	406	CLA	C4B-NB	6.85	1.41	1.35
15	b2	408	CLA	C4B-NB	6.85	1.41	1.35
15	aA	817	CLA	C4B-NB	6.84	1.41	1.35
15	a4	402	CLA	C4B-NB	6.84	1.41	1.35
15	cA	804	CLA	C4B-NB	6.84	1.41	1.35
15	b3	413	CLA	C4B-NB	6.84	1.41	1.35
15	b5	415	CLA	C4B-NB	6.84	1.41	1.35
15	b6	408	CLA	C4B-NB	6.83	1.41	1.35
15	b4	402	CLA	C4B-NB	6.83	1.41	1.35
15	bA	811	CLA	C4B-NB	6.83	1.41	1.35
15	bJ	102	CLA	C4B-NB	6.83	1.41	1.35
15	c1	402	CLA	C4B-NB	6.83	1.41	1.35
15	b3	402	CLA	C4B-NB	6.82	1.41	1.35
15	cA	811	CLA	C4B-NB	6.82	1.41	1.35
15	b1	403	CLA	C4B-NB	6.82	1.41	1.35
15	a2	413	CLA	C4B-NB	6.82	1.41	1.35
15	b5	403	CLA	C4B-NB	6.82	1.41	1.35
15	b5	407	CLA	C4B-NB	6.82	1.41	1.35
15	a5	403	CLA	C4B-NB	6.81	1.41	1.35
15	a5	411	CLA	C4B-NB	6.81	1.41	1.35
15	aB	821	CLA	C4B-NB	6.81	1.41	1.35
15	c5	412	CLA	C4B-NB	6.81	1.41	1.35
15	b6	403	CLA	C4B-NB	6.80	1.41	1.35
15	c6	403	CLA	C4B-NB	6.80	1.41	1.35
15	b3	411	CLA	C4B-NB	6.80	1.41	1.35
15	b1	402	CLA	C4B-NB	6.79	1.41	1.35
15	c3	402	CLA	C4B-NB	6.79	1.41	1.35
15	c3	403	CLA	C4B-NB	6.79	1.41	1.35
15	aB	801	CLA	C4B-NB	6.79	1.41	1.35
15	bB	801	CLA	C4B-NB	6.79	1.41	1.35
15	a1	414	CLA	C4B-NB	6.78	1.41	1.35
15	c3	412	CLA	C4B-NB	6.78	1.41	1.35
15	c1	403	CLA	C4B-NB	6.78	1.41	1.35
15	c2	403	CLA	C4B-NB	6.78	1.41	1.35
16	cB	843	PQN	C3-C2	6.78	1.47	1.35
16	aB	843	PQN	C3-C2	6.78	1.47	1.35
15	a3	402	CLA	C4B-NB	6.77	1.41	1.35
15	aB	824	CLA	C4B-NB	6.77	1.41	1.35
15	a3	403	CLA	C4B-NB	6.77	1.41	1.35
15	b6	412	CLA	C4B-NB	6.77	1.41	1.35
16	bB	843	PQN	C3-C2	6.77	1.47	1.35
15	c1	415	CLA	C4B-NB	6.77	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	403	CLA	C4B-NB	6.76	1.41	1.35
15	a6	409	CLA	C4B-NB	6.76	1.41	1.35
15	b4	403	CLA	C4B-NB	6.76	1.41	1.35
15	b6	409	CLA	C4B-NB	6.76	1.41	1.35
15	aA	804	CLA	C4B-NB	6.76	1.41	1.35
15	a5	415	CLA	C4B-NB	6.76	1.41	1.35
15	a3	411	CLA	C4B-NB	6.76	1.41	1.35
15	b1	415	CLA	C4B-NB	6.76	1.41	1.35
15	b1	410	CLA	C4B-NB	6.75	1.41	1.35
15	bA	828	CLA	C4B-NB	6.75	1.41	1.35
15	b2	416	CLA	C4B-NB	6.75	1.41	1.35
15	aA	842	CLA	C4B-NB	6.74	1.41	1.35
15	bA	804	CLA	C4B-NB	6.74	1.41	1.35
15	c2	416	CLA	C4B-NB	6.74	1.41	1.35
15	cB	822	CLA	C4B-NB	6.73	1.41	1.35
15	a2	416	CLA	C4B-NB	6.72	1.41	1.35
15	bA	842	CLA	C4B-NB	6.72	1.41	1.35
15	bJ	101	CLA	C4B-NB	6.72	1.41	1.35
15	a6	404	CLA	C4B-NB	6.72	1.41	1.35
15	a1	402	CLA	C4B-NB	6.72	1.41	1.35
15	b1	405	CLA	C4B-NB	6.72	1.41	1.35
15	aA	835	CLA	C4B-NB	6.72	1.41	1.35
15	b1	408	CLA	C4B-NB	6.72	1.41	1.35
15	b4	412	CLA	C4B-NB	6.71	1.41	1.35
15	cA	813	CLA	C4B-NB	6.71	1.41	1.35
15	c6	409	CLA	C4B-NB	6.71	1.41	1.35
15	aA	821	CLA	C4B-NB	6.71	1.41	1.35
15	c3	411	CLA	C4B-NB	6.71	1.41	1.35
15	c1	405	CLA	C4B-NB	6.71	1.41	1.35
15	a4	412	CLA	C4B-NB	6.71	1.41	1.35
15	aA	808	CLA	C4B-NB	6.70	1.41	1.35
15	bA	835	CLA	C4B-NB	6.70	1.41	1.35
15	cA	818	CLA	C4B-NB	6.70	1.41	1.35
15	a5	412	CLA	C4B-NB	6.70	1.41	1.35
15	aB	812	CLA	C4B-NB	6.70	1.41	1.35
15	cF	201	CLA	C4B-NB	6.69	1.41	1.35
15	a6	411	CLA	C4B-NB	6.69	1.41	1.35
15	bA	818	CLA	C4B-NB	6.69	1.41	1.35
15	bB	812	CLA	C4B-NB	6.69	1.41	1.35
15	a1	406	CLA	C4B-NB	6.69	1.41	1.35
15	b5	412	CLA	C4B-NB	6.69	1.41	1.35
15	c4	403	CLA	C4B-NB	6.69	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	813	CLA	C4B-NB	6.69	1.41	1.35
15	a3	412	CLA	C4B-NB	6.68	1.41	1.35
15	cB	834	CLA	C4B-NB	6.68	1.41	1.35
15	a1	404	CLA	C4B-NB	6.68	1.41	1.35
15	b4	410	CLA	C4B-NB	6.68	1.41	1.35
15	bB	834	CLA	C4B-NB	6.67	1.41	1.35
15	c5	405	CLA	C4B-NB	6.67	1.41	1.35
15	c6	404	CLA	C4B-NB	6.67	1.41	1.35
15	bA	808	CLA	C4B-NB	6.67	1.41	1.35
15	bB	822	CLA	C4B-NB	6.67	1.41	1.35
15	cA	808	CLA	C4B-NB	6.67	1.41	1.35
15	cA	828	CLA	C4B-NB	6.67	1.41	1.35
15	aA	825	CLA	C4B-NB	6.67	1.41	1.35
15	cB	824	CLA	C4B-NB	6.66	1.41	1.35
15	a5	405	CLA	C4B-NB	6.66	1.41	1.35
15	c6	412	CLA	C4B-NB	6.66	1.41	1.35
15	b5	405	CLA	C4B-NB	6.66	1.41	1.35
15	cA	835	CLA	C4B-NB	6.66	1.41	1.35
15	aA	818	CLA	C4B-NB	6.66	1.41	1.35
15	a4	403	CLA	C4B-NB	6.66	1.41	1.35
15	c4	412	CLA	C4B-NB	6.66	1.41	1.35
15	a6	412	CLA	C4B-NB	6.65	1.41	1.35
15	bA	813	CLA	C4B-NB	6.65	1.41	1.35
15	cA	825	CLA	C4B-NB	6.65	1.41	1.35
15	b6	404	CLA	C4B-NB	6.65	1.41	1.35
15	cB	812	CLA	C4B-NB	6.64	1.41	1.35
15	aB	834	CLA	C4B-NB	6.64	1.41	1.35
15	aJ	202	CLA	C4B-NB	6.63	1.41	1.35
15	aA	815	CLA	C4B-NB	6.62	1.41	1.35
15	c4	410	CLA	C4B-NB	6.62	1.41	1.35
15	b3	403	CLA	C4B-NB	6.62	1.41	1.35
15	cJ	101	CLA	C4B-NB	6.62	1.41	1.35
15	c1	410	CLA	C4B-NB	6.62	1.41	1.35
15	bA	825	CLA	C4B-NB	6.61	1.41	1.35
15	aB	822	CLA	C4B-NB	6.60	1.41	1.35
15	c1	407	CLA	C4B-NB	6.59	1.41	1.35
15	bA	815	CLA	C4B-NB	6.59	1.41	1.35
15	c2	411	CLA	C4B-NB	6.59	1.41	1.35
15	a1	409	CLA	C4B-NB	6.59	1.41	1.35
15	cA	821	CLA	C4B-NB	6.59	1.41	1.35
15	b1	412	CLA	C4B-NB	6.58	1.41	1.35
15	b6	411	CLA	C4B-NB	6.57	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	405	CLA	C4B-NB	6.57	1.41	1.35
15	cA	844	CLA	C4B-NB	6.57	1.41	1.35
15	c4	415	CLA	C4B-NB	6.57	1.41	1.35
15	c4	408	CLA	C4B-NB	6.57	1.41	1.35
15	b1	407	CLA	C4B-NB	6.57	1.41	1.35
15	bA	816	CLA	C4B-NB	6.56	1.41	1.35
15	a4	410	CLA	C4B-NB	6.56	1.41	1.35
15	c6	411	CLA	C4B-NB	6.55	1.41	1.35
15	cA	815	CLA	C4B-NB	6.55	1.41	1.35
15	a1	407	CLA	C4B-NB	6.55	1.41	1.35
15	bA	821	CLA	C4B-NB	6.55	1.41	1.35
15	a4	415	CLA	C4B-NB	6.54	1.41	1.35
15	a1	411	CLA	C4B-NB	6.54	1.41	1.35
15	bA	845	CLA	C4B-NB	6.54	1.41	1.35
15	c5	408	CLA	C4B-NB	6.54	1.41	1.35
15	a5	408	CLA	C4B-NB	6.54	1.41	1.35
15	b5	408	CLA	C4B-NB	6.53	1.41	1.35
15	aA	845	CLA	C4B-NB	6.53	1.41	1.35
15	c1	412	CLA	C4B-NB	6.53	1.41	1.35
15	b4	408	CLA	C4B-NB	6.52	1.41	1.35
15	b3	415	CLA	C4B-NB	6.51	1.41	1.35
15	aA	816	CLA	C4B-NB	6.51	1.41	1.35
15	cA	843	CLA	C4B-NB	6.50	1.41	1.35
15	c3	415	CLA	C4B-NB	6.50	1.41	1.35
15	a3	407	CLA	C4B-NB	6.50	1.41	1.35
15	cA	816	CLA	C4B-NB	6.50	1.41	1.35
15	c1	408	CLA	C4B-NB	6.50	1.41	1.35
15	c4	405	CLA	C4B-NB	6.48	1.41	1.35
15	b4	407	CLA	C4B-NB	6.47	1.41	1.35
15	c5	410	CLA	C4B-NB	6.46	1.41	1.35
15	a4	407	CLA	C4B-NB	6.46	1.41	1.35
15	c3	407	CLA	C4B-NB	6.46	1.41	1.35
15	b4	415	CLA	C4B-NB	6.46	1.41	1.35
15	aB	820	CLA	C4B-NB	6.45	1.41	1.35
15	c2	409	CLA	C4B-NB	6.45	1.41	1.35
15	b3	408	CLA	C4B-NB	6.45	1.41	1.35
15	bA	844	CLA	C4B-NB	6.45	1.41	1.35
15	aA	824	CLA	C4B-NB	6.45	1.41	1.35
15	a3	408	CLA	C4B-NB	6.44	1.41	1.35
15	a3	415	CLA	C4B-NB	6.44	1.41	1.35
15	a4	408	CLA	C4B-NB	6.44	1.40	1.35
15	a2	411	CLA	C4B-NB	6.43	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	820	CLA	C4B-NB	6.43	1.40	1.35
15	bA	824	CLA	C4B-NB	6.43	1.40	1.35
15	a2	409	CLA	C4B-NB	6.43	1.40	1.35
15	b5	410	CLA	C4B-NB	6.43	1.40	1.35
15	a4	405	CLA	C4B-NB	6.42	1.40	1.35
15	c4	407	CLA	C4B-NB	6.42	1.40	1.35
15	aA	844	CLA	C4B-NB	6.41	1.40	1.35
15	b2	409	CLA	C4B-NB	6.41	1.40	1.35
15	aA	812	CLA	C4B-NB	6.41	1.40	1.35
15	cA	824	CLA	C4B-NB	6.41	1.40	1.35
15	bB	820	CLA	C4B-NB	6.41	1.40	1.35
15	aA	823	CLA	C4B-NB	6.40	1.40	1.35
15	bB	835	CLA	C4B-NB	6.40	1.40	1.35
15	cB	835	CLA	C4B-NB	6.40	1.40	1.35
15	bA	823	CLA	C4B-NB	6.40	1.40	1.35
15	cA	819	CLA	C4B-NB	6.39	1.40	1.35
15	bA	819	CLA	C4B-NB	6.39	1.40	1.35
15	c3	408	CLA	C4B-NB	6.39	1.40	1.35
15	aA	819	CLA	C4B-NB	6.39	1.40	1.35
15	a5	410	CLA	C4B-NB	6.38	1.40	1.35
15	b3	405	CLA	C4B-NB	6.38	1.40	1.35
15	cA	820	CLA	C4B-NB	6.38	1.40	1.35
15	bB	840	CLA	C4B-NB	6.38	1.40	1.35
15	cA	812	CLA	C4B-NB	6.37	1.40	1.35
15	cA	823	CLA	C4B-NB	6.37	1.40	1.35
15	aB	835	CLA	C4B-NB	6.35	1.40	1.35
15	a3	405	CLA	C4B-NB	6.34	1.40	1.35
15	c3	410	CLA	C4B-NB	6.33	1.40	1.35
15	b3	410	CLA	C4B-NB	6.33	1.40	1.35
15	bA	812	CLA	C4B-NB	6.32	1.40	1.35
15	c3	405	CLA	C4B-NB	6.32	1.40	1.35
15	cB	840	CLA	C4B-NB	6.32	1.40	1.35
15	a3	410	CLA	C4B-NB	6.32	1.40	1.35
15	b3	407	CLA	C4B-NB	6.31	1.40	1.35
15	aB	840	CLA	C4B-NB	6.29	1.40	1.35
15	aB	805	CLA	C4B-NB	6.28	1.40	1.35
15	b2	411	CLA	C4B-NB	6.28	1.40	1.35
15	cA	836	CLA	C4B-NB	6.27	1.40	1.35
15	aA	836	CLA	C4B-NB	6.27	1.40	1.35
15	bA	836	CLA	C4B-NB	6.26	1.40	1.35
15	aA	810	CLA	C4B-NB	6.26	1.40	1.35
15	bA	820	CLA	C4B-NB	6.25	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	810	CLA	C4B-NB	6.24	1.40	1.35
15	aA	820	CLA	C4B-NB	6.24	1.40	1.35
15	cB	805	CLA	C4B-NB	6.22	1.40	1.35
15	bA	810	CLA	C4B-NB	6.22	1.40	1.35
15	bB	823	CLA	C4B-NB	6.21	1.40	1.35
15	cB	823	CLA	C4B-NB	6.18	1.40	1.35
15	bB	805	CLA	C4B-NB	6.16	1.40	1.35
15	aB	823	CLA	C4B-NB	6.12	1.40	1.35
15	bK	101	CLA	C4B-NB	6.08	1.40	1.35
15	cB	816	CLA	C4B-NB	6.08	1.40	1.35
15	bA	809	CLA	C4B-NB	6.07	1.40	1.35
15	cB	831	CLA	C4B-NB	6.06	1.40	1.35
15	aB	831	CLA	C4B-NB	6.06	1.40	1.35
15	aJ	201	CLA	C4B-NB	6.06	1.40	1.35
15	cA	805	CLA	C4B-NB	6.04	1.40	1.35
15	aA	809	CLA	C4B-NB	6.04	1.40	1.35
15	aA	832	CLA	C4B-NB	6.04	1.40	1.35
15	aL	201	CLA	C4B-NB	6.03	1.40	1.35
15	aK	102	CLA	C4B-NB	6.03	1.40	1.35
15	bF	201	CLA	C4B-NB	6.03	1.40	1.35
15	bB	831	CLA	C4B-NB	6.03	1.40	1.35
15	bB	809	CLA	C4B-NB	6.02	1.40	1.35
15	bL	202	CLA	C4B-NB	6.02	1.40	1.35
15	bA	832	CLA	C4B-NB	6.01	1.40	1.35
15	cF	203	CLA	C4B-NB	5.99	1.40	1.35
15	cA	809	CLA	C4B-NB	5.99	1.40	1.35
15	cA	832	CLA	C4B-NB	5.99	1.40	1.35
15	cB	839	CLA	C4B-NB	5.99	1.40	1.35
15	aB	839	CLA	C4B-NB	5.99	1.40	1.35
15	aB	816	CLA	C4B-NB	5.97	1.40	1.35
15	aA	805	CLA	C4B-NB	5.97	1.40	1.35
15	bB	839	CLA	C4B-NB	5.97	1.40	1.35
15	bB	816	CLA	C4B-NB	5.96	1.40	1.35
15	cK	102	CLA	C4B-NB	5.95	1.40	1.35
15	cB	809	CLA	C4B-NB	5.95	1.40	1.35
15	cL	201	CLA	C4B-NB	5.94	1.40	1.35
15	cA	802	CLA	C4B-NB	5.94	1.40	1.35
15	bA	802	CLA	C4B-NB	5.93	1.40	1.35
15	bA	805	CLA	C4B-NB	5.93	1.40	1.35
15	aB	809	CLA	C4B-NB	5.92	1.40	1.35
15	aA	802	CLA	C4B-NB	5.91	1.40	1.35
15	aA	831	CLA	C4B-NB	5.87	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	807	CLA	C4B-NB	5.86	1.40	1.35
15	cA	822	CLA	C4B-NB	5.86	1.40	1.35
15	aA	803	CLA	C4B-NB	5.84	1.40	1.35
15	bB	804	CLA	C4B-NB	5.84	1.40	1.35
15	aB	804	CLA	C4B-NB	5.83	1.40	1.35
15	bA	807	CLA	C4B-NB	5.83	1.40	1.35
15	aA	807	CLA	C4B-NB	5.82	1.40	1.35
15	aB	838	CLA	C4B-NB	5.82	1.40	1.35
15	cB	837	CLA	C4B-NB	5.80	1.40	1.35
15	bB	838	CLA	C4B-NB	5.78	1.40	1.35
15	cA	803	CLA	C4B-NB	5.78	1.40	1.35
15	bA	822	CLA	C4B-NB	5.77	1.40	1.35
15	bL	203	CLA	C4B-NB	5.77	1.40	1.35
15	cL	202	CLA	C4B-NB	5.77	1.40	1.35
15	cB	838	CLA	C4B-NB	5.76	1.40	1.35
15	bA	803	CLA	C4B-NB	5.76	1.40	1.35
15	aB	814	CLA	C4B-NB	5.74	1.40	1.35
15	cB	830	CLA	C4B-NB	5.73	1.40	1.35
15	cB	804	CLA	C4B-NB	5.73	1.40	1.35
15	bB	837	CLA	C4B-NB	5.72	1.40	1.35
15	aB	837	CLA	C4B-NB	5.71	1.40	1.35
15	bA	831	CLA	C4B-NB	5.71	1.40	1.35
15	aA	822	CLA	C4B-NB	5.71	1.40	1.35
15	cB	836	CLA	C4B-NB	5.71	1.40	1.35
15	aB	830	CLA	C4B-NB	5.69	1.40	1.35
15	aA	814	CLA	C4B-NB	5.69	1.40	1.35
15	aL	202	CLA	C4B-NB	5.69	1.40	1.35
15	cB	814	CLA	C4B-NB	5.69	1.40	1.35
15	cA	831	CLA	C4B-NB	5.68	1.40	1.35
15	bB	814	CLA	C4B-NB	5.68	1.40	1.35
15	bB	830	CLA	C4B-NB	5.68	1.40	1.35
15	bB	827	CLA	C4B-NB	5.66	1.40	1.35
15	aB	826	CLA	C4B-NB	5.65	1.40	1.35
15	bB	826	CLA	C4B-NB	5.65	1.40	1.35
15	cA	814	CLA	C4B-NB	5.63	1.40	1.35
15	aB	829	CLA	C4B-NB	5.62	1.40	1.35
15	aB	836	CLA	C4B-NB	5.61	1.40	1.35
15	bA	814	CLA	C4B-NB	5.61	1.40	1.35
15	cB	826	CLA	C4B-NB	5.61	1.40	1.35
15	bB	836	CLA	C4B-NB	5.60	1.40	1.35
15	aB	827	CLA	C4B-NB	5.58	1.40	1.35
15	aA	806	CLA	C4B-NB	5.57	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	830	CLA	C4B-NB	5.56	1.40	1.35
15	cA	806	CLA	C4B-NB	5.55	1.40	1.35
15	cB	827	CLA	C4B-NB	5.54	1.40	1.35
15	bA	806	CLA	C4B-NB	5.53	1.40	1.35
15	cB	829	CLA	C4B-NB	5.53	1.40	1.35
15	bB	819	CLA	C4B-NB	5.52	1.40	1.35
15	cB	817	CLA	C4B-NB	5.52	1.40	1.35
15	bA	830	CLA	C4B-NB	5.52	1.40	1.35
15	bA	839	CLA	C4B-NB	5.51	1.40	1.35
15	bB	829	CLA	C4B-NB	5.50	1.40	1.35
15	aA	830	CLA	C4B-NB	5.50	1.40	1.35
15	cA	839	CLA	C4B-NB	5.48	1.40	1.35
15	aB	819	CLA	C4B-NB	5.48	1.40	1.35
15	aB	817	CLA	C4B-NB	5.48	1.40	1.35
15	cB	807	CLA	C4B-NB	5.46	1.40	1.35
15	cB	819	CLA	C4B-NB	5.45	1.40	1.35
15	bB	817	CLA	C4B-NB	5.43	1.40	1.35
15	cA	827	CLA	C4B-NB	5.42	1.40	1.35
15	bB	807	CLA	C4B-NB	5.42	1.40	1.35
15	aB	806	CLA	C4B-NB	5.41	1.40	1.35
15	cA	829	CLA	C4B-NB	5.39	1.40	1.35
15	bA	826	CLA	C4B-NB	5.38	1.40	1.35
15	aA	827	CLA	C4B-NB	5.38	1.40	1.35
15	bA	827	CLA	C4B-NB	5.37	1.40	1.35
15	bA	829	CLA	C4B-NB	5.36	1.40	1.35
15	aA	839	CLA	C4B-NB	5.36	1.40	1.35
15	aA	829	CLA	C4B-NB	5.36	1.40	1.35
15	aB	807	CLA	C4B-NB	5.36	1.40	1.35
15	aA	826	CLA	C4B-NB	5.35	1.40	1.35
15	cA	826	CLA	C4B-NB	5.34	1.40	1.35
15	cB	806	CLA	C4B-NB	5.34	1.40	1.35
15	cB	832	CLA	C4B-NB	5.33	1.40	1.35
15	bB	832	CLA	C4B-NB	5.32	1.40	1.35
15	bB	806	CLA	C4B-NB	5.30	1.39	1.35
15	cA	834	CLA	C4B-NB	5.30	1.39	1.35
15	cB	825	CLA	C4B-NB	5.28	1.39	1.35
15	bA	834	CLA	C4B-NB	5.27	1.39	1.35
15	aB	802	CLA	C4B-NB	5.25	1.39	1.35
15	aA	834	CLA	C4B-NB	5.25	1.39	1.35
15	bL	204	CLA	C4B-NB	5.24	1.39	1.35
15	aB	832	CLA	C4B-NB	5.24	1.39	1.35
15	cB	802	CLA	C4B-NB	5.24	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	825	CLA	C4B-NB	5.22	1.39	1.35
15	bB	802	CLA	C4B-NB	5.22	1.39	1.35
15	bB	825	CLA	C4B-NB	5.20	1.39	1.35
15	cL	203	CLA	C4B-NB	5.17	1.39	1.35
15	aL	203	CLA	C4B-NB	5.16	1.39	1.35
15	cB	803	CLA	C4B-NB	5.12	1.39	1.35
15	cB	818	CLA	C4B-NB	5.11	1.39	1.35
15	aB	810	CLA	C4B-NB	5.08	1.39	1.35
15	bB	803	CLA	C4B-NB	5.07	1.39	1.35
15	cB	810	CLA	C4B-NB	5.05	1.39	1.35
15	aB	818	CLA	C4B-NB	5.04	1.39	1.35
15	bB	818	CLA	C4B-NB	5.02	1.39	1.35
14	cA	801	CL0	C3B-C2B	5.02	1.47	1.40
15	aB	803	CLA	C4B-NB	5.01	1.39	1.35
15	bB	810	CLA	C4B-NB	4.98	1.39	1.35
14	aA	801	CL0	C3B-C2B	4.97	1.47	1.40
15	b2	418	CLA	C1D-ND	4.97	1.43	1.37
14	bA	801	CL0	C3B-C2B	4.96	1.47	1.40
15	c6	418	CLA	C1D-ND	4.93	1.43	1.37
15	b6	418	CLA	C1D-ND	4.91	1.43	1.37
15	bB	811	CLA	C4B-NB	4.90	1.39	1.35
15	a3	416	CLA	C4B-NB	4.88	1.39	1.35
15	a6	418	CLA	C1D-ND	4.86	1.43	1.37
15	a2	418	CLA	C1D-ND	4.83	1.43	1.37
15	cB	811	CLA	C4B-NB	4.81	1.39	1.35
15	b3	416	CLA	C4B-NB	4.80	1.39	1.35
15	c3	416	CLA	C4B-NB	4.78	1.39	1.35
15	cA	831	CLA	CMB-C2B	-4.78	1.41	1.51
15	bA	831	CLA	CMB-C2B	-4.78	1.41	1.51
15	aA	831	CLA	CMB-C2B	-4.78	1.41	1.51
15	bA	833	CLA	C4B-NB	4.74	1.39	1.35
15	c1	417	CLA	C1D-ND	4.74	1.43	1.37
15	c2	418	CLA	C1D-ND	4.72	1.43	1.37
15	a1	416	CLA	C1D-ND	4.71	1.43	1.37
15	aB	811	CLA	C4B-NB	4.71	1.39	1.35
15	cA	833	CLA	C4B-NB	4.70	1.39	1.35
15	b1	417	CLA	C1D-ND	4.69	1.43	1.37
15	cA	840	CLA	C4B-NB	4.69	1.39	1.35
14	aA	801	CL0	O2D-CGD	4.68	1.44	1.33
14	cA	801	CL0	O2D-CGD	4.68	1.44	1.33
14	bA	801	CL0	O2D-CGD	4.67	1.44	1.33
15	aA	833	CLA	C4B-NB	4.67	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	840	CLA	C4B-NB	4.67	1.39	1.35
15	a3	417	CLA	C1D-ND	4.63	1.43	1.37
15	c4	416	CLA	C4B-NB	4.63	1.39	1.35
15	aA	806	CLA	C4D-ND	-4.63	1.31	1.37
15	aB	830	CLA	CMB-C2B	-4.61	1.42	1.51
15	cA	806	CLA	C4D-ND	-4.61	1.31	1.37
15	bA	806	CLA	C4D-ND	-4.61	1.31	1.37
15	aA	840	CLA	C4B-NB	4.61	1.39	1.35
14	bA	801	CL0	C3C-C2C	4.61	1.46	1.36
15	b3	417	CLA	C1D-ND	4.60	1.43	1.37
14	cA	801	CL0	C3C-C2C	4.59	1.46	1.36
14	aA	801	CL0	C3C-C2C	4.59	1.46	1.36
15	cB	830	CLA	CMB-C2B	-4.59	1.42	1.51
15	b6	417	CLA	C4B-NB	4.58	1.39	1.35
15	c6	417	CLA	C4B-NB	4.56	1.39	1.35
15	bB	830	CLA	CMB-C2B	-4.56	1.42	1.51
15	c3	417	CLA	C1D-ND	4.54	1.43	1.37
15	a6	417	CLA	C4B-NB	4.50	1.39	1.35
15	c2	405	CLA	C1D-ND	4.49	1.43	1.37
15	bB	802	CLA	C4D-ND	-4.49	1.31	1.37
15	b4	416	CLA	C4B-NB	4.48	1.39	1.35
15	c5	417	CLA	C1D-ND	4.47	1.43	1.37
15	b2	405	CLA	C1D-ND	4.46	1.43	1.37
15	a2	405	CLA	C1D-ND	4.46	1.43	1.37
15	b5	417	CLA	C1D-ND	4.45	1.43	1.37
15	a5	417	CLA	C1D-ND	4.45	1.43	1.37
15	cB	802	CLA	C4D-ND	-4.44	1.31	1.37
15	aB	802	CLA	C4D-ND	-4.43	1.31	1.37
15	a4	416	CLA	C4B-NB	4.43	1.39	1.35
15	b6	406	CLA	C1D-ND	4.42	1.43	1.37
15	b1	416	CLA	C4B-NB	4.41	1.39	1.35
15	c6	418	CLA	CHC-C1C	4.40	1.46	1.35
15	cA	840	CLA	C4D-ND	-4.40	1.31	1.37
15	a6	406	CLA	C1D-ND	4.39	1.43	1.37
15	b2	417	CLA	C4B-NB	4.39	1.39	1.35
15	aB	828	CLA	C4B-NB	4.38	1.39	1.35
15	bA	840	CLA	C4D-ND	-4.37	1.31	1.37
15	aA	840	CLA	C4D-ND	-4.37	1.31	1.37
15	c4	417	CLA	C1D-ND	4.36	1.43	1.37
15	c6	406	CLA	C1D-ND	4.36	1.43	1.37
15	a5	417	CLA	CHC-C1C	4.36	1.46	1.35
15	cB	828	CLA	C4B-NB	4.35	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	418	CLA	CHC-C1C	4.35	1.46	1.35
15	b6	418	CLA	CHC-C1C	4.35	1.46	1.35
15	c5	416	CLA	C4B-NB	4.35	1.39	1.35
15	bA	834	CLA	C4D-ND	-4.34	1.31	1.37
15	aL	203	CLA	C4D-ND	-4.34	1.31	1.37
15	cA	802	CLA	C4D-ND	-4.34	1.31	1.37
15	cB	806	CLA	C4D-ND	-4.34	1.31	1.37
15	b5	416	CLA	C4B-NB	4.34	1.39	1.35
15	c1	416	CLA	C4B-NB	4.34	1.39	1.35
15	aA	834	CLA	C4D-ND	-4.34	1.31	1.37
15	a4	417	CLA	CHC-C1C	4.34	1.46	1.35
15	bB	804	CLA	C4D-ND	-4.33	1.31	1.37
15	aL	202	CLA	C4D-ND	-4.33	1.31	1.37
14	aA	801	CL0	CHC-C1C	4.33	1.46	1.35
15	aB	807	CLA	C4D-ND	-4.32	1.31	1.37
15	c4	417	CLA	CHC-C1C	4.32	1.46	1.35
14	bA	801	CL0	CHC-C1C	4.32	1.46	1.35
15	bL	204	CLA	C4D-ND	-4.32	1.31	1.37
15	b4	417	CLA	CHC-C1C	4.32	1.46	1.35
15	b5	417	CLA	CHC-C1C	4.31	1.46	1.35
15	a4	417	CLA	C1D-ND	4.31	1.43	1.37
15	a5	416	CLA	C4B-NB	4.31	1.39	1.35
15	cB	828	CLA	C4D-ND	-4.31	1.31	1.37
15	c5	417	CLA	CHC-C1C	4.31	1.46	1.35
15	aB	804	CLA	C4D-ND	-4.31	1.31	1.37
14	cA	801	CL0	CHC-C1C	4.30	1.46	1.35
15	bL	203	CLA	C4D-ND	-4.30	1.31	1.37
15	b4	417	CLA	C1D-ND	4.30	1.43	1.37
15	bB	806	CLA	C4D-ND	-4.30	1.31	1.37
15	aA	843	CLA	C4D-ND	-4.30	1.31	1.37
15	cB	807	CLA	C4D-ND	-4.30	1.31	1.37
15	cA	834	CLA	C4D-ND	-4.29	1.31	1.37
15	a3	417	CLA	CHC-C1C	4.29	1.46	1.35
15	cL	202	CLA	C4D-ND	-4.29	1.31	1.37
15	cL	203	CLA	C4D-ND	-4.29	1.31	1.37
15	c3	417	CLA	CHC-C1C	4.29	1.46	1.35
15	bA	843	CLA	C4D-ND	-4.29	1.31	1.37
15	cB	804	CLA	C4D-ND	-4.29	1.31	1.37
15	aB	828	CLA	C4D-ND	-4.29	1.31	1.37
15	aB	806	CLA	C4D-ND	-4.28	1.31	1.37
15	aA	802	CLA	C4D-ND	-4.28	1.31	1.37
15	bB	828	CLA	C4D-ND	-4.28	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	417	CLA	CHC-C1C	4.27	1.45	1.35
15	c1	417	CLA	CHC-C1C	4.27	1.45	1.35
15	bB	807	CLA	C4D-ND	-4.26	1.31	1.37
15	b1	417	CLA	CHC-C1C	4.26	1.45	1.35
15	c2	417	CLA	C4B-NB	4.26	1.39	1.35
15	a2	418	CLA	CHC-C1C	4.25	1.45	1.35
15	cA	839	CLA	C4D-ND	-4.25	1.31	1.37
15	bA	802	CLA	C4D-ND	-4.24	1.31	1.37
15	cA	842	CLA	C4D-ND	-4.24	1.31	1.37
15	a2	417	CLA	C4B-NB	4.24	1.39	1.35
15	c2	417	CLA	C4D-ND	-4.23	1.31	1.37
15	aA	839	CLA	C4D-ND	-4.23	1.31	1.37
15	b2	417	CLA	C4D-ND	-4.23	1.31	1.37
15	c2	418	CLA	CHC-C1C	4.23	1.45	1.35
15	bA	839	CLA	C4D-ND	-4.23	1.31	1.37
15	bB	828	CLA	C4B-NB	4.22	1.39	1.35
15	b2	418	CLA	CHC-C1C	4.22	1.45	1.35
15	a3	405	CLA	C1D-ND	4.21	1.43	1.37
15	a1	415	CLA	C4B-NB	4.21	1.39	1.35
15	bA	833	CLA	C4D-ND	-4.21	1.31	1.37
15	a1	416	CLA	CHC-C1C	4.20	1.45	1.35
15	cA	807	CLA	C4D-ND	-4.20	1.31	1.37
15	bB	803	CLA	C4D-ND	-4.20	1.31	1.37
15	a2	417	CLA	C4D-ND	-4.19	1.31	1.37
15	aA	838	CLA	C4B-NB	4.19	1.38	1.35
15	aA	814	CLA	C4D-ND	-4.19	1.31	1.37
15	aA	833	CLA	C4D-ND	-4.18	1.32	1.37
15	cB	836	CLA	C4D-ND	-4.18	1.32	1.37
15	cB	837	CLA	C4D-ND	-4.17	1.32	1.37
15	aA	845	CLA	C4D-ND	-4.17	1.32	1.37
15	aA	813	CLA	C4D-ND	-4.17	1.32	1.37
15	aB	837	CLA	C4D-ND	-4.16	1.32	1.37
15	bL	202	CLA	C4D-ND	-4.16	1.32	1.37
15	c3	405	CLA	C1D-ND	4.16	1.42	1.37
15	bB	837	CLA	C4D-ND	-4.16	1.32	1.37
15	bA	807	CLA	C4D-ND	-4.16	1.32	1.37
15	aB	803	CLA	C4D-ND	-4.16	1.32	1.37
15	bB	819	CLA	C4D-ND	-4.16	1.32	1.37
15	aB	838	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	833	CLA	C4D-ND	-4.15	1.32	1.37
15	aL	201	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	827	CLA	C4D-ND	-4.15	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	803	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	802	CLA	CMB-C2B	-4.15	1.43	1.51
15	bA	838	CLA	C4B-NB	4.15	1.38	1.35
15	a4	405	CLA	C1D-ND	4.15	1.42	1.37
15	bA	845	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	844	CLA	C4D-ND	-4.15	1.32	1.37
15	b3	405	CLA	C1D-ND	4.15	1.42	1.37
15	bB	836	CLA	C4D-ND	-4.14	1.32	1.37
15	cB	838	CLA	C4D-ND	-4.14	1.32	1.37
15	aA	807	CLA	C4D-ND	-4.14	1.32	1.37
15	bA	838	CLA	C4D-ND	-4.14	1.32	1.37
15	cA	838	CLA	C4B-NB	4.14	1.38	1.35
15	b4	405	CLA	C1D-ND	4.14	1.42	1.37
15	aA	802	CLA	CMB-C2B	-4.13	1.43	1.51
15	cA	814	CLA	C4D-ND	-4.13	1.32	1.37
15	cB	819	CLA	C4D-ND	-4.13	1.32	1.37
15	bA	814	CLA	C4D-ND	-4.13	1.32	1.37
15	b1	405	CLA	C1D-ND	4.13	1.42	1.37
15	bA	827	CLA	C4D-ND	-4.13	1.32	1.37
15	aB	836	CLA	C4D-ND	-4.12	1.32	1.37
15	bA	802	CLA	CMB-C2B	-4.12	1.43	1.51
15	bA	813	CLA	C4D-ND	-4.12	1.32	1.37
15	b5	405	CLA	C1D-ND	4.12	1.42	1.37
15	c1	405	CLA	C1D-ND	4.12	1.42	1.37
15	bB	838	CLA	C4D-ND	-4.11	1.32	1.37
15	c4	405	CLA	C1D-ND	4.11	1.42	1.37
15	a5	405	CLA	C1D-ND	4.11	1.42	1.37
15	cA	813	CLA	C4D-ND	-4.11	1.32	1.37
15	cL	201	CLA	C4D-ND	-4.11	1.32	1.37
18	bB	850	BCR	C30-C25	-4.10	1.48	1.53
15	aB	819	CLA	C4D-ND	-4.10	1.32	1.37
15	cA	838	CLA	C4D-ND	-4.10	1.32	1.37
15	b4	416	CLA	C4D-ND	-4.10	1.32	1.37
15	c3	416	CLA	C4D-ND	-4.09	1.32	1.37
18	cB	849	BCR	C30-C25	-4.09	1.48	1.53
19	aA	853	LHG	O7-C5	-4.09	1.36	1.46
15	a3	416	CLA	C4D-ND	-4.08	1.32	1.37
15	aA	827	CLA	C4D-ND	-4.08	1.32	1.37
15	aA	838	CLA	C4D-ND	-4.07	1.32	1.37
15	a1	404	CLA	C1D-ND	4.07	1.42	1.37
15	c5	405	CLA	C1D-ND	4.07	1.42	1.37
19	cA	852	LHG	O7-C5	-4.06	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	416	CLA	C4D-ND	-4.06	1.32	1.37
19	bA	854	LHG	O7-C5	-4.06	1.36	1.46
15	aB	813	CLA	C4D-ND	-4.06	1.32	1.37
15	a4	416	CLA	C4D-ND	-4.05	1.32	1.37
15	cB	832	CLA	C4D-ND	-4.05	1.32	1.37
15	c4	416	CLA	C4D-ND	-4.05	1.32	1.37
15	aB	832	CLA	C4D-ND	-4.05	1.32	1.37
15	cB	813	CLA	C4D-ND	-4.05	1.32	1.37
15	bB	832	CLA	C4D-ND	-4.04	1.32	1.37
18	aB	849	BCR	C30-C25	-4.04	1.48	1.53
15	aB	827	CLA	C4D-ND	-4.04	1.32	1.37
16	bA	846	PQN	C10-C5	4.04	1.47	1.40
15	cB	833	CLA	C4D-ND	-4.03	1.32	1.37
15	bB	833	CLA	C4D-ND	-4.03	1.32	1.37
15	bB	840	CLA	C4D-ND	-4.03	1.32	1.37
15	cB	827	CLA	C4D-ND	-4.01	1.32	1.37
15	bB	827	CLA	C4D-ND	-4.01	1.32	1.37
15	aB	810	CLA	C4D-ND	-4.00	1.32	1.37
15	bB	810	CLA	C4D-ND	-4.00	1.32	1.37
15	bB	813	CLA	C4D-ND	-4.00	1.32	1.37
15	cB	840	CLA	C4D-ND	-3.99	1.32	1.37
15	b5	416	CLA	C4D-ND	-3.98	1.32	1.37
18	b4	418	BCR	C30-C25	-3.98	1.48	1.53
15	cA	829	CLA	C4D-ND	-3.98	1.32	1.37
18	cB	848	BCR	C30-C25	-3.98	1.48	1.53
15	a5	416	CLA	C4D-ND	-3.98	1.32	1.37
18	a4	418	BCR	C30-C25	-3.98	1.48	1.53
16	aA	846	PQN	C10-C5	3.97	1.47	1.40
16	cA	845	PQN	C10-C5	3.96	1.47	1.40
15	aA	828	CLA	C4D-ND	-3.96	1.32	1.37
15	aB	833	CLA	C4D-ND	-3.95	1.32	1.37
15	aB	840	CLA	C4D-ND	-3.95	1.32	1.37
15	bA	831	CLA	C4D-ND	-3.95	1.32	1.37
15	bB	810	CLA	CMB-C2B	-3.94	1.43	1.51
15	bA	828	CLA	C4D-ND	-3.94	1.32	1.37
15	cB	810	CLA	C4D-ND	-3.94	1.32	1.37
15	aB	811	CLA	C4D-ND	-3.94	1.32	1.37
15	aA	819	CLA	C4D-ND	-3.93	1.32	1.37
15	cA	819	CLA	C4D-ND	-3.93	1.32	1.37
14	aA	801	CL0	C1B-NB	-3.93	1.31	1.35
15	aB	810	CLA	CMB-C2B	-3.93	1.43	1.51
15	cB	810	CLA	CMB-C2B	-3.93	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	829	CLA	C4D-ND	-3.92	1.32	1.37
15	cA	828	CLA	C4D-ND	-3.92	1.32	1.37
18	aB	848	BCR	C30-C25	-3.91	1.48	1.53
18	c4	418	BCR	C30-C25	-3.91	1.48	1.53
18	c2	419	BCR	C30-C25	-3.91	1.48	1.53
15	c5	416	CLA	C4D-ND	-3.91	1.32	1.37
15	bB	811	CLA	C4D-ND	-3.91	1.32	1.37
15	a6	416	CLA	C1D-ND	3.91	1.42	1.37
15	cA	831	CLA	C4D-ND	-3.90	1.32	1.37
15	c6	417	CLA	C4D-ND	-3.90	1.32	1.37
15	aA	829	CLA	C4D-ND	-3.90	1.32	1.37
15	bA	803	CLA	C4D-ND	-3.90	1.32	1.37
15	cA	803	CLA	C4D-ND	-3.90	1.32	1.37
18	bB	848	BCR	C30-C25	-3.90	1.48	1.53
15	c1	412	CLA	C1D-ND	3.90	1.42	1.37
15	aA	830	CLA	C4D-ND	-3.90	1.32	1.37
15	cB	811	CLA	C4D-ND	-3.90	1.32	1.37
14	bA	801	CL0	C1B-NB	-3.89	1.31	1.35
15	b6	416	CLA	C1D-ND	3.89	1.42	1.37
15	a6	417	CLA	C4D-ND	-3.89	1.32	1.37
15	b6	414	CLA	C1D-ND	3.89	1.42	1.37
18	b1	418	BCR	C30-C25	-3.89	1.48	1.53
15	bA	830	CLA	C4D-ND	-3.88	1.32	1.37
18	a3	418	BCR	C30-C25	-3.88	1.48	1.53
15	bA	819	CLA	C4D-ND	-3.88	1.32	1.37
15	c1	416	CLA	C4D-ND	-3.88	1.32	1.37
15	aA	826	CLA	C4D-ND	-3.88	1.32	1.37
15	a1	415	CLA	C4D-ND	-3.88	1.32	1.37
15	b6	417	CLA	C4D-ND	-3.88	1.32	1.37
15	cB	839	CLA	C4D-ND	-3.88	1.32	1.37
15	a1	411	CLA	C1D-ND	3.88	1.42	1.37
15	c6	416	CLA	C1D-ND	3.87	1.42	1.37
15	bA	823	CLA	C4D-ND	-3.87	1.32	1.37
15	bB	818	CLA	C4D-ND	-3.87	1.32	1.37
15	cA	830	CLA	C4D-ND	-3.87	1.32	1.37
15	bB	839	CLA	C4D-ND	-3.87	1.32	1.37
15	aA	831	CLA	C4D-ND	-3.87	1.32	1.37
18	c3	418	BCR	C30-C25	-3.87	1.48	1.53
18	c1	418	BCR	C30-C25	-3.87	1.48	1.53
14	cA	801	CL0	O2A-CGA	3.87	1.44	1.33
15	aA	803	CLA	C4D-ND	-3.87	1.32	1.37
15	aB	821	CLA	C4D-ND	-3.86	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a2	419	BCR	C30-C25	-3.86	1.48	1.53
15	cB	814	CLA	C4D-ND	-3.86	1.32	1.37
15	b1	412	CLA	C1D-ND	3.86	1.42	1.37
14	aA	801	CL0	O2A-CGA	3.86	1.44	1.33
15	cB	821	CLA	C4D-ND	-3.86	1.32	1.37
15	bA	826	CLA	C4D-ND	-3.86	1.32	1.37
15	b1	416	CLA	C4D-ND	-3.85	1.32	1.37
14	bA	801	CL0	O2A-CGA	3.85	1.44	1.33
18	a1	417	BCR	C30-C25	-3.85	1.48	1.53
14	cA	801	CL0	C1B-NB	-3.85	1.31	1.35
15	aA	823	CLA	C4D-ND	-3.85	1.32	1.37
15	cK	102	CLA	C4D-ND	-3.84	1.32	1.37
15	c6	414	CLA	C1D-ND	3.84	1.42	1.37
15	aB	814	CLA	C4D-ND	-3.84	1.32	1.37
15	cA	812	CLA	C4D-ND	-3.84	1.32	1.37
15	aB	839	CLA	C4D-ND	-3.83	1.32	1.37
15	cA	823	CLA	C4D-ND	-3.83	1.32	1.37
15	a6	413	CLA	C1D-ND	3.83	1.42	1.37
18	b3	418	BCR	C30-C25	-3.83	1.48	1.53
15	cB	818	CLA	C4D-ND	-3.82	1.32	1.37
18	b2	419	BCR	C30-C25	-3.82	1.48	1.53
15	cA	826	CLA	C4D-ND	-3.82	1.32	1.37
15	bB	814	CLA	C4D-ND	-3.82	1.32	1.37
18	a6	419	BCR	C30-C25	-3.82	1.48	1.53
15	c2	413	CLA	C1D-ND	3.81	1.42	1.37
15	aA	812	CLA	C4D-ND	-3.81	1.32	1.37
15	aB	818	CLA	C4D-ND	-3.81	1.32	1.37
15	cA	820	CLA	C4D-ND	-3.80	1.32	1.37
15	bK	101	CLA	C4D-ND	-3.80	1.32	1.37
15	aK	102	CLA	C4D-ND	-3.80	1.32	1.37
16	aB	843	PQN	C10-C5	3.80	1.47	1.40
15	bB	821	CLA	C4D-ND	-3.80	1.32	1.37
15	b6	413	CLA	C1D-ND	3.80	1.42	1.37
18	b6	419	BCR	C30-C25	-3.79	1.48	1.53
15	cB	825	CLA	C4D-ND	-3.78	1.32	1.37
15	bB	825	CLA	C4D-ND	-3.78	1.32	1.37
15	bA	812	CLA	C4D-ND	-3.78	1.32	1.37
15	bA	820	CLA	C4D-ND	-3.78	1.32	1.37
16	bB	843	PQN	C10-C5	3.78	1.46	1.40
15	aA	820	CLA	C4D-ND	-3.76	1.32	1.37
15	c1	407	CLA	C1D-ND	3.76	1.42	1.37
15	cA	822	CLA	C4D-ND	-3.76	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	cI	102	BCR	C30-C25	-3.75	1.48	1.53
15	c4	412	CLA	C1D-ND	3.75	1.42	1.37
18	a5	418	BCR	C30-C25	-3.75	1.48	1.53
16	cB	843	PQN	C10-C5	3.74	1.46	1.40
15	bX	102	CLA	C4D-ND	-3.74	1.32	1.37
18	c6	419	BCR	C30-C25	-3.74	1.48	1.53
15	b3	415	CLA	C1D-ND	3.74	1.42	1.37
18	c5	418	BCR	C30-C25	-3.73	1.48	1.53
15	aX	102	CLA	C4D-ND	-3.73	1.32	1.37
15	c6	413	CLA	C1D-ND	3.73	1.42	1.37
15	aA	822	CLA	C4D-ND	-3.73	1.32	1.37
18	b5	418	BCR	C30-C25	-3.73	1.48	1.53
18	bI	102	BCR	C30-C25	-3.73	1.48	1.53
15	bA	822	CLA	C4D-ND	-3.72	1.32	1.37
15	bB	830	CLA	C4D-ND	-3.72	1.32	1.37
15	b2	413	CLA	C1D-ND	3.72	1.42	1.37
15	cX	102	CLA	C4D-ND	-3.72	1.32	1.37
18	aI	102	BCR	C30-C25	-3.71	1.48	1.53
18	bA	852	BCR	C30-C25	-3.71	1.48	1.53
15	a2	413	CLA	C1D-ND	3.70	1.42	1.37
15	cB	829	CLA	C4D-ND	-3.69	1.32	1.37
15	cB	830	CLA	C4D-ND	-3.69	1.32	1.37
15	a5	415	CLA	C1D-ND	3.69	1.42	1.37
15	c5	415	CLA	C1D-ND	3.69	1.42	1.37
15	c2	416	CLA	C1D-ND	3.69	1.42	1.37
15	bB	842	CLA	C1D-ND	3.69	1.42	1.37
15	cB	840	CLA	C3B-C2B	-3.68	1.35	1.40
15	aB	825	CLA	C4D-ND	-3.68	1.32	1.37
15	b6	405	CLA	C1D-ND	3.68	1.42	1.37
15	a6	405	CLA	C1D-ND	3.68	1.42	1.37
15	bB	840	CLA	C3B-C2B	-3.68	1.35	1.40
15	aB	840	CLA	C3B-C2B	-3.68	1.35	1.40
15	a2	422	CLA	C4D-ND	-3.67	1.32	1.37
18	cJ	103	BCR	C1-C6	-3.67	1.48	1.53
15	b4	412	CLA	C1D-ND	3.67	1.42	1.37
15	a2	416	CLA	C1D-ND	3.67	1.42	1.37
15	a1	406	CLA	C1D-ND	3.67	1.42	1.37
15	b1	407	CLA	C1D-ND	3.67	1.42	1.37
15	bB	829	CLA	C4D-ND	-3.67	1.32	1.37
18	cA	850	BCR	C30-C25	-3.67	1.48	1.53
15	b2	416	CLA	C1D-ND	3.67	1.42	1.37
15	a4	415	CLA	C4D-ND	-3.66	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	804	CLA	C4D-ND	-3.66	1.32	1.37
15	aB	829	CLA	C4D-ND	-3.66	1.32	1.37
15	a3	415	CLA	C1D-ND	3.66	1.42	1.37
18	bJ	103	BCR	C1-C6	-3.66	1.48	1.53
18	aA	851	BCR	C30-C25	-3.65	1.48	1.53
15	bA	808	CLA	C4D-ND	-3.65	1.32	1.37
15	cA	805	CLA	C4D-ND	-3.65	1.32	1.37
15	aA	805	CLA	C4D-ND	-3.65	1.32	1.37
15	a5	407	CLA	C1D-ND	3.65	1.42	1.37
15	bB	840	CLA	CMB-C2B	-3.65	1.44	1.51
15	c6	415	CLA	C1D-ND	3.65	1.42	1.37
15	bA	809	CLA	C4D-ND	-3.65	1.32	1.37
15	cB	842	CLA	C1D-ND	3.64	1.42	1.37
15	b2	422	CLA	C4D-ND	-3.64	1.32	1.37
15	bA	821	CLA	C4D-ND	-3.64	1.32	1.37
15	bB	824	CLA	C1D-ND	3.64	1.42	1.37
15	aA	804	CLA	C4D-ND	-3.64	1.32	1.37
15	cB	801	CLA	C4D-ND	-3.64	1.32	1.37
15	bA	805	CLA	C4D-ND	-3.64	1.32	1.37
15	cA	808	CLA	C4D-ND	-3.64	1.32	1.37
15	b6	415	CLA	C1D-ND	3.64	1.42	1.37
15	aB	842	CLA	C1D-ND	3.64	1.42	1.37
15	b5	415	CLA	C1D-ND	3.64	1.42	1.37
15	c6	408	CLA	C1D-ND	3.63	1.42	1.37
15	aB	830	CLA	C4D-ND	-3.63	1.32	1.37
15	cA	809	CLA	C4D-ND	-3.63	1.32	1.37
15	cB	840	CLA	CMB-C2B	-3.63	1.44	1.51
18	bL	205	BCR	C30-C25	-3.63	1.48	1.53
15	b5	414	CLA	C1D-ND	3.63	1.42	1.37
15	bB	801	CLA	C4D-ND	-3.63	1.32	1.37
14	cA	801	CL0	CHD-C1D	3.63	1.45	1.38
14	bA	801	CL0	CHD-C1D	3.62	1.45	1.38
15	aB	840	CLA	CMB-C2B	-3.62	1.44	1.51
15	aA	821	CLA	C4D-ND	-3.62	1.32	1.37
18	aJ	204	BCR	C1-C6	-3.62	1.48	1.53
15	aB	801	CLA	C4D-ND	-3.62	1.32	1.37
15	aA	836	CLA	C4D-ND	-3.62	1.32	1.37
15	c5	407	CLA	C1D-ND	3.61	1.42	1.37
15	cA	821	CLA	C4D-ND	-3.61	1.32	1.37
15	aA	808	CLA	C4D-ND	-3.61	1.32	1.37
15	cA	836	CLA	C4D-ND	-3.61	1.32	1.37
15	c2	408	CLA	C1D-ND	3.61	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b1	404	CLA	C1D-ND	3.61	1.42	1.37
15	c5	412	CLA	C1D-ND	3.61	1.42	1.37
15	a6	415	CLA	C1D-ND	3.61	1.42	1.37
15	c4	415	CLA	C1D-ND	3.61	1.42	1.37
15	bB	820	CLA	C4D-ND	-3.61	1.32	1.37
18	bJ	104	BCR	C1-C6	-3.61	1.48	1.53
15	bA	825	CLA	C4D-ND	-3.61	1.32	1.37
14	aA	801	CL0	CHD-C1D	3.61	1.45	1.38
15	a4	412	CLA	C1D-ND	3.60	1.42	1.37
15	c2	422	CLA	C4D-ND	-3.60	1.32	1.37
15	b1	414	CLA	C1D-ND	3.60	1.42	1.37
15	cA	804	CLA	C4D-ND	-3.60	1.32	1.37
15	c5	414	CLA	C1D-ND	3.60	1.42	1.37
15	a6	408	CLA	C1D-ND	3.60	1.42	1.37
15	bB	818	CLA	C1D-ND	3.60	1.42	1.37
15	b5	407	CLA	C1D-ND	3.60	1.42	1.37
15	aB	804	CLA	CMC-C2C	-3.60	1.43	1.50
15	c3	415	CLA	C1D-ND	3.60	1.42	1.37
15	aA	825	CLA	C4D-ND	-3.60	1.32	1.37
15	aB	831	CLA	C4D-ND	-3.60	1.32	1.37
15	b6	408	CLA	C1D-ND	3.60	1.42	1.37
15	b3	407	CLA	C4D-ND	-3.59	1.32	1.37
15	aA	809	CLA	C4D-ND	-3.59	1.32	1.37
18	cJ	104	BCR	C1-C6	-3.59	1.48	1.53
15	a3	409	CLA	C4D-ND	-3.59	1.32	1.37
15	bB	817	CLA	C4D-ND	-3.59	1.32	1.37
15	b4	415	CLA	C1D-ND	3.59	1.42	1.37
15	aB	805	CLA	C4D-ND	-3.59	1.32	1.37
15	cB	824	CLA	C1D-ND	3.59	1.42	1.37
15	aA	818	CLA	C4D-ND	-3.59	1.32	1.37
15	bB	804	CLA	CMC-C2C	-3.59	1.43	1.50
15	aB	820	CLA	C4D-ND	-3.59	1.32	1.37
15	b4	415	CLA	C4D-ND	-3.58	1.32	1.37
15	a3	411	CLA	C4D-ND	-3.58	1.32	1.37
15	a3	407	CLA	C4D-ND	-3.58	1.32	1.37
15	cB	804	CLA	CMC-C2C	-3.58	1.43	1.50
15	aB	824	CLA	C1D-ND	3.58	1.42	1.37
15	cA	811	CLA	C4D-ND	-3.58	1.32	1.37
15	cA	825	CLA	C4D-ND	-3.58	1.32	1.37
18	aJ	205	BCR	C1-C6	-3.58	1.48	1.53
15	bB	805	CLA	C4D-ND	-3.57	1.32	1.37
15	cB	817	CLA	C4D-ND	-3.57	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	831	CLA	C4D-ND	-3.57	1.32	1.37
15	aB	818	CLA	C1D-ND	3.57	1.42	1.37
18	aK	101	BCR	C1-C6	-3.57	1.48	1.53
15	a6	422	CLA	C2A-C1A	3.57	1.60	1.52
15	aJ	201	CLA	C4D-ND	-3.57	1.32	1.37
15	b5	412	CLA	C1D-ND	3.56	1.42	1.37
15	c1	414	CLA	C1D-ND	3.56	1.42	1.37
15	b2	408	CLA	C1D-ND	3.56	1.42	1.37
18	cK	101	BCR	C1-C6	-3.56	1.48	1.53
18	bA	848	BCR	C1-C6	-3.56	1.48	1.53
15	aA	811	CLA	C4D-ND	-3.56	1.32	1.37
15	aB	808	CLA	C4D-ND	-3.56	1.32	1.37
15	aB	809	CLA	C4D-ND	-3.56	1.32	1.37
15	c3	407	CLA	C4D-ND	-3.56	1.32	1.37
15	a2	408	CLA	C1D-ND	3.56	1.42	1.37
15	c6	405	CLA	C1D-ND	3.56	1.42	1.37
15	cB	812	CLA	C4D-ND	-3.56	1.32	1.37
20	cB	850	LMG	O1-C7	-3.55	1.37	1.43
18	aI	103	BCR	C30-C25	-3.55	1.48	1.53
18	bJ	104	BCR	C30-C25	-3.55	1.48	1.53
18	cL	204	BCR	C30-C25	-3.55	1.48	1.53
15	c1	404	CLA	C1D-ND	3.55	1.42	1.37
15	bA	841	CLA	C4D-ND	-3.55	1.32	1.37
15	a1	413	CLA	C1D-ND	3.54	1.42	1.37
20	aB	850	LMG	O1-C7	-3.54	1.37	1.43
15	cB	805	CLA	C4D-ND	-3.54	1.32	1.37
15	bA	811	CLA	C4D-ND	-3.54	1.32	1.37
15	cB	824	CLA	C4D-ND	-3.54	1.32	1.37
18	aJ	205	BCR	C30-C25	-3.54	1.48	1.53
15	cB	820	CLA	C4D-ND	-3.54	1.32	1.37
15	cF	203	CLA	C4D-ND	-3.54	1.32	1.37
15	c3	415	CLA	C4D-ND	-3.53	1.32	1.37
15	bA	836	CLA	C4D-ND	-3.53	1.32	1.37
15	aA	824	CLA	C4D-ND	-3.53	1.32	1.37
15	aB	817	CLA	C4D-ND	-3.53	1.32	1.37
15	bB	812	CLA	C4D-ND	-3.53	1.32	1.37
15	c4	414	CLA	C1D-ND	3.53	1.42	1.37
15	b5	411	CLA	C4D-ND	-3.53	1.32	1.37
15	bB	831	CLA	C4D-ND	-3.53	1.32	1.37
15	c3	411	CLA	C4D-ND	-3.53	1.32	1.37
15	c2	415	CLA	C1D-ND	3.52	1.42	1.37
15	b2	402	CLA	C1D-ND	3.52	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	402	CLA	C1D-ND	3.52	1.42	1.37
15	a1	403	CLA	C1D-ND	3.52	1.42	1.37
15	a4	415	CLA	C1D-ND	3.52	1.42	1.37
15	aB	822	CLA	C4D-ND	-3.52	1.32	1.37
15	aB	824	CLA	C4D-ND	-3.52	1.32	1.37
15	a1	405	CLA	C1D-ND	3.52	1.42	1.37
15	a5	414	CLA	C1D-ND	3.52	1.42	1.37
15	a3	412	CLA	C1D-ND	3.52	1.42	1.37
15	cB	809	CLA	C4D-ND	-3.52	1.32	1.37
20	bB	851	LMG	O1-C7	-3.52	1.37	1.43
15	a3	415	CLA	C4D-ND	-3.52	1.32	1.37
15	b4	404	CLA	C4D-ND	-3.52	1.32	1.37
15	c4	415	CLA	C4D-ND	-3.51	1.32	1.37
15	b6	403	CLA	C1D-ND	3.51	1.42	1.37
15	bB	822	CLA	C4D-ND	-3.51	1.32	1.37
15	b3	411	CLA	C4D-ND	-3.51	1.32	1.37
15	a5	411	CLA	C4D-ND	-3.51	1.32	1.37
15	a2	404	CLA	C1D-ND	3.51	1.42	1.37
18	cJ	104	BCR	C30-C25	-3.51	1.48	1.53
15	bB	809	CLA	C4D-ND	-3.51	1.32	1.37
15	cB	818	CLA	C1D-ND	3.51	1.42	1.37
15	bB	801	CLA	CMB-C2B	-3.51	1.44	1.51
15	b3	409	CLA	C4D-ND	-3.51	1.32	1.37
15	c4	413	CLA	C1D-ND	3.51	1.42	1.37
15	bF	201	CLA	C4D-ND	-3.51	1.32	1.37
15	aB	822	CLA	C1D-ND	3.51	1.42	1.37
15	b2	407	CLA	C1D-ND	3.50	1.42	1.37
15	cA	827	CLA	CMD-C2D	-3.50	1.43	1.50
15	cB	822	CLA	C4D-ND	-3.50	1.32	1.37
15	a2	415	CLA	C1D-ND	3.50	1.42	1.37
15	cB	822	CLA	C1D-ND	3.50	1.42	1.37
15	bB	808	CLA	C4D-ND	-3.50	1.32	1.37
15	aB	812	CLA	C4D-ND	-3.50	1.32	1.37
15	cB	808	CLA	C4D-ND	-3.50	1.32	1.37
15	cA	841	CLA	C4D-ND	-3.49	1.32	1.37
15	bA	818	CLA	C4D-ND	-3.49	1.32	1.37
15	b5	402	CLA	C1D-ND	3.49	1.42	1.37
15	c5	411	CLA	C4D-ND	-3.49	1.32	1.37
15	b4	414	CLA	C1D-ND	3.49	1.42	1.37
15	cA	824	CLA	C4D-ND	-3.49	1.32	1.37
15	bA	824	CLA	C4D-ND	-3.49	1.32	1.37
15	b6	407	CLA	C1D-ND	3.49	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a3	418	BCR	C1-C6	-3.49	1.49	1.53
15	cA	818	CLA	C4D-ND	-3.49	1.32	1.37
15	c3	409	CLA	C4D-ND	-3.49	1.32	1.37
15	aB	801	CLA	CMB-C2B	-3.49	1.44	1.51
15	bB	816	CLA	C1D-ND	3.48	1.42	1.37
15	aA	827	CLA	CMD-C2D	-3.48	1.43	1.50
15	a5	402	CLA	C1D-ND	3.48	1.42	1.37
15	c1	415	CLA	C1D-ND	3.48	1.42	1.37
15	aA	816	CLA	C4D-ND	-3.48	1.32	1.37
15	c4	404	CLA	C4D-ND	-3.48	1.32	1.37
15	bB	822	CLA	C1D-ND	3.48	1.42	1.37
15	bA	810	CLA	C4D-ND	-3.48	1.32	1.37
15	b1	415	CLA	C1D-ND	3.48	1.42	1.37
15	a6	403	CLA	C1D-ND	3.48	1.42	1.37
15	cB	801	CLA	CMB-C2B	-3.48	1.44	1.51
18	c3	418	BCR	C1-C6	-3.47	1.49	1.53
15	bA	827	CLA	CMD-C2D	-3.47	1.43	1.50
15	a3	412	CLA	C4D-ND	-3.47	1.32	1.37
15	b2	404	CLA	C1D-ND	3.47	1.42	1.37
15	c1	406	CLA	C1D-ND	3.47	1.42	1.37
15	aB	816	CLA	C1D-ND	3.47	1.42	1.37
15	b1	402	CLA	C1D-ND	3.47	1.42	1.37
15	b2	415	CLA	C1D-ND	3.47	1.42	1.37
15	a5	406	CLA	C1D-ND	3.47	1.42	1.37
15	a5	412	CLA	C1D-ND	3.47	1.42	1.37
15	c4	404	CLA	C1D-ND	3.47	1.42	1.37
15	c2	407	CLA	C1D-ND	3.47	1.42	1.37
15	b3	412	CLA	C4D-ND	-3.47	1.32	1.37
15	cA	810	CLA	C4D-ND	-3.47	1.32	1.37
15	aB	841	CLA	C4D-ND	-3.47	1.32	1.37
15	c5	402	CLA	C1D-ND	3.47	1.42	1.37
15	aB	826	CLA	C4D-ND	-3.46	1.32	1.37
15	a6	422	CLA	C1D-ND	3.46	1.42	1.37
15	c2	404	CLA	C1D-ND	3.46	1.42	1.37
15	cA	822	CLA	CMB-C2B	-3.46	1.44	1.51
15	aA	817	CLA	C1D-ND	3.46	1.42	1.37
15	bA	822	CLA	CMB-C2B	-3.46	1.44	1.51
15	a4	414	CLA	C1D-ND	3.46	1.42	1.37
15	c2	402	CLA	C1D-ND	3.46	1.42	1.37
15	bA	816	CLA	C4D-ND	-3.46	1.32	1.37
15	a5	415	CLA	C4D-ND	-3.45	1.32	1.37
15	bA	832	CLA	C4D-ND	-3.45	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	824	CLA	C4D-ND	-3.45	1.32	1.37
15	cB	816	CLA	C1D-ND	3.45	1.42	1.37
15	b3	415	CLA	C4D-ND	-3.45	1.33	1.37
15	cA	816	CLA	C4D-ND	-3.45	1.33	1.37
15	a1	401	CLA	C1D-ND	3.45	1.42	1.37
15	b5	415	CLA	C4D-ND	-3.45	1.33	1.37
15	bA	836	CLA	CMB-C2B	-3.45	1.44	1.51
15	a4	404	CLA	C4D-ND	-3.45	1.33	1.37
15	cJ	101	CLA	C1D-ND	3.45	1.42	1.37
15	a4	409	CLA	C4D-ND	-3.45	1.33	1.37
15	b5	406	CLA	C1D-ND	3.45	1.42	1.37
15	b3	421	CLA	C4D-ND	-3.45	1.33	1.37
15	bJ	101	CLA	C1D-ND	3.44	1.42	1.37
15	aA	832	CLA	C4D-ND	-3.44	1.33	1.37
15	a4	407	CLA	C4D-ND	-3.44	1.33	1.37
15	c6	403	CLA	C1D-ND	3.44	1.42	1.37
15	b3	413	CLA	C1D-ND	3.44	1.42	1.37
18	b3	418	BCR	C1-C6	-3.44	1.49	1.53
15	b2	413	CLA	C4D-ND	-3.44	1.33	1.37
15	c6	407	CLA	C1D-ND	3.44	1.42	1.37
15	aA	822	CLA	CMB-C2B	-3.44	1.44	1.51
15	b6	422	CLA	C1D-ND	3.44	1.42	1.37
15	c4	407	CLA	C4D-ND	-3.44	1.33	1.37
15	bB	826	CLA	C4D-ND	-3.44	1.33	1.37
15	cA	815	CLA	C4D-ND	-3.44	1.33	1.37
15	b2	408	CLA	C4D-ND	-3.44	1.33	1.37
15	b3	412	CLA	C1D-ND	3.43	1.42	1.37
15	cA	816	CLA	C1D-ND	3.43	1.42	1.37
15	bB	841	CLA	C4D-ND	-3.43	1.33	1.37
15	b3	404	CLA	C1D-ND	3.43	1.42	1.37
15	aJ	202	CLA	C1D-ND	3.43	1.42	1.37
15	c3	412	CLA	C1D-ND	3.43	1.42	1.37
15	c4	411	CLA	C1D-ND	3.43	1.42	1.37
15	a1	414	CLA	C1D-ND	3.43	1.42	1.37
15	c6	411	CLA	C1D-ND	3.43	1.42	1.37
15	c3	412	CLA	C4D-ND	-3.43	1.33	1.37
15	aA	841	CLA	C4D-ND	-3.42	1.33	1.37
15	cA	832	CLA	C4D-ND	-3.42	1.33	1.37
18	aF	201	BCR	C30-C25	-3.42	1.49	1.53
15	b1	406	CLA	C1D-ND	3.42	1.42	1.37
15	c2	413	CLA	C4D-ND	-3.42	1.33	1.37
15	c5	415	CLA	C4D-ND	-3.42	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	407	CLA	C1D-ND	3.42	1.42	1.37
15	cA	836	CLA	CMB-C2B	-3.42	1.44	1.51
15	a2	402	CLA	C1D-ND	3.42	1.42	1.37
15	cA	817	CLA	C1D-ND	3.42	1.42	1.37
15	bA	815	CLA	C4D-ND	-3.42	1.33	1.37
15	aA	815	CLA	C4D-ND	-3.42	1.33	1.37
15	a6	413	CLA	C4D-ND	-3.42	1.33	1.37
15	b4	411	CLA	C1D-ND	3.42	1.42	1.37
15	a2	407	CLA	C1D-ND	3.42	1.42	1.37
15	c3	414	CLA	C1D-ND	3.41	1.42	1.37
15	b4	407	CLA	C4D-ND	-3.41	1.33	1.37
15	cB	841	CLA	C4D-ND	-3.41	1.33	1.37
15	b1	411	CLA	C1D-ND	3.41	1.42	1.37
15	aA	836	CLA	CMB-C2B	-3.41	1.44	1.51
15	b4	410	CLA	C1D-ND	3.41	1.42	1.37
15	b3	407	CLA	C1D-ND	3.41	1.42	1.37
15	b6	411	CLA	C1D-ND	3.41	1.42	1.37
15	b1	410	CLA	C1D-ND	3.41	1.42	1.37
15	b3	414	CLA	C1D-ND	3.41	1.42	1.37
15	b4	409	CLA	C4D-ND	-3.41	1.33	1.37
15	c4	411	CLA	C4D-ND	-3.41	1.33	1.37
15	c2	410	CLA	C4D-ND	-3.41	1.33	1.37
15	a6	411	CLA	C1D-ND	3.41	1.42	1.37
15	b4	413	CLA	C1D-ND	3.41	1.42	1.37
15	b3	409	CLA	C1D-ND	3.40	1.42	1.37
18	cF	202	BCR	C30-C25	-3.40	1.49	1.53
15	c4	409	CLA	C1D-ND	3.40	1.42	1.37
15	b4	411	CLA	C4D-ND	-3.40	1.33	1.37
15	c3	409	CLA	C1D-ND	3.40	1.42	1.37
15	b4	407	CLA	C1D-ND	3.40	1.42	1.37
15	cB	826	CLA	C4D-ND	-3.40	1.33	1.37
15	a4	409	CLA	C1D-ND	3.40	1.42	1.37
15	a2	410	CLA	C4D-ND	-3.40	1.33	1.37
15	a4	410	CLA	C1D-ND	3.39	1.42	1.37
15	bA	816	CLA	C1D-ND	3.39	1.42	1.37
15	a4	411	CLA	C4D-ND	-3.39	1.33	1.37
15	c4	409	CLA	C4D-ND	-3.39	1.33	1.37
15	aA	810	CLA	C4D-ND	-3.39	1.33	1.37
15	b6	413	CLA	C4D-ND	-3.39	1.33	1.37
18	aB	844	BCR	C1-C6	-3.39	1.49	1.53
15	b2	404	CLA	C4D-ND	-3.39	1.33	1.37
15	b6	410	CLA	C4D-ND	-3.39	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	409	CLA	C1D-ND	3.39	1.42	1.37
15	bA	837	CLA	C1D-ND	3.39	1.42	1.37
15	c6	413	CLA	C4D-ND	-3.39	1.33	1.37
15	a5	410	CLA	C1D-ND	3.39	1.41	1.37
15	c4	410	CLA	C1D-ND	3.39	1.41	1.37
15	a2	413	CLA	C4D-ND	-3.39	1.33	1.37
15	a3	421	CLA	C4D-ND	-3.39	1.33	1.37
15	c2	416	CLA	C4D-ND	-3.38	1.33	1.37
15	b2	412	CLA	C1D-ND	3.38	1.41	1.37
15	c5	406	CLA	C1D-ND	3.38	1.41	1.37
15	a1	410	CLA	C1D-ND	3.38	1.41	1.37
18	cB	844	BCR	C1-C6	-3.38	1.49	1.53
15	b4	404	CLA	C1D-ND	3.38	1.41	1.37
15	cF	203	CLA	CMB-C2B	-3.38	1.44	1.51
15	b4	408	CLA	C4D-ND	-3.38	1.33	1.37
15	a4	404	CLA	C1D-ND	3.38	1.41	1.37
15	a4	413	CLA	C1D-ND	3.38	1.41	1.37
15	aJ	201	CLA	CMB-C2B	-3.37	1.44	1.51
15	cA	835	CLA	C4D-ND	-3.37	1.33	1.37
15	c3	421	CLA	C4D-ND	-3.37	1.33	1.37
15	aA	816	CLA	C1D-ND	3.37	1.41	1.37
15	a2	408	CLA	C4D-ND	-3.37	1.33	1.37
15	aA	835	CLA	C4D-ND	-3.37	1.33	1.37
15	a5	409	CLA	C4D-ND	-3.37	1.33	1.37
15	b6	412	CLA	C4D-ND	-3.37	1.33	1.37
15	bA	815	CLA	C1D-ND	3.37	1.41	1.37
15	bA	817	CLA	C1D-ND	3.37	1.41	1.37
15	b5	404	CLA	C1D-ND	3.37	1.41	1.37
15	a5	403	CLA	C4D-ND	-3.37	1.33	1.37
15	b2	416	CLA	C4D-ND	-3.37	1.33	1.37
15	c5	403	CLA	C4D-ND	-3.37	1.33	1.37
15	cA	837	CLA	C1D-ND	3.37	1.41	1.37
15	c2	408	CLA	C4D-ND	-3.37	1.33	1.37
15	b5	409	CLA	C4D-ND	-3.36	1.33	1.37
15	bF	201	CLA	CMB-C2B	-3.36	1.44	1.51
15	b1	409	CLA	C1D-ND	3.36	1.41	1.37
15	aA	837	CLA	C1D-ND	3.36	1.41	1.37
15	bA	835	CLA	C4D-ND	-3.36	1.33	1.37
15	b5	410	CLA	C1D-ND	3.36	1.41	1.37
15	c6	412	CLA	C4D-ND	-3.36	1.33	1.37
15	a4	411	CLA	C1D-ND	3.36	1.41	1.37
18	bB	849	BCR	C30-C25	-3.36	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	411	CLA	C1D-ND	3.36	1.41	1.37
18	bB	844	BCR	C1-C6	-3.36	1.49	1.53
15	a3	413	CLA	C1D-ND	3.36	1.41	1.37
15	a4	407	CLA	C1D-ND	3.36	1.41	1.37
18	cA	849	BCR	C1-C6	-3.35	1.49	1.53
15	cA	815	CLA	C1D-ND	3.35	1.41	1.37
15	a3	404	CLA	C4D-ND	-3.35	1.33	1.37
15	aA	844	CLA	C4D-ND	-3.35	1.33	1.37
15	a4	408	CLA	C4D-ND	-3.35	1.33	1.37
15	c6	410	CLA	C4D-ND	-3.35	1.33	1.37
15	a3	414	CLA	C1D-ND	3.35	1.41	1.37
15	c2	411	CLA	C1D-ND	3.35	1.41	1.37
15	c3	404	CLA	C4D-ND	-3.35	1.33	1.37
18	b4	418	BCR	C1-C6	-3.35	1.49	1.53
15	aB	835	CLA	C4D-ND	-3.34	1.33	1.37
15	aB	829	CLA	CMD-C2D	-3.34	1.43	1.50
15	a3	407	CLA	C1D-ND	3.34	1.41	1.37
15	c5	409	CLA	C4D-ND	-3.34	1.33	1.37
15	b4	412	CLA	C4D-ND	-3.34	1.33	1.37
15	c2	412	CLA	C1D-ND	3.34	1.41	1.37
15	a4	412	CLA	C4D-ND	-3.34	1.33	1.37
15	cA	843	CLA	C4D-ND	-3.34	1.33	1.37
15	c1	403	CLA	C4D-ND	-3.34	1.33	1.37
14	aA	801	CL0	C4B-NB	-3.34	1.32	1.35
15	a1	422	CLA	C1D-ND	3.34	1.41	1.37
15	b4	409	CLA	C1D-ND	3.34	1.41	1.37
15	c4	407	CLA	C1D-ND	3.34	1.41	1.37
15	b6	410	CLA	C1D-ND	3.34	1.41	1.37
15	a6	410	CLA	C4D-ND	-3.34	1.33	1.37
15	aA	815	CLA	C1D-ND	3.33	1.41	1.37
15	cB	835	CLA	C4D-ND	-3.33	1.33	1.37
15	b2	410	CLA	C1D-ND	3.33	1.41	1.37
15	c6	412	CLA	C1D-ND	3.33	1.41	1.37
15	bA	844	CLA	C4D-ND	-3.33	1.33	1.37
15	a2	404	CLA	C4D-ND	-3.33	1.33	1.37
15	a2	416	CLA	C4D-ND	-3.33	1.33	1.37
15	a1	409	CLA	C1D-ND	3.33	1.41	1.37
15	b5	403	CLA	C4D-ND	-3.33	1.33	1.37
15	b3	402	CLA	C1D-ND	3.33	1.41	1.37
15	a2	414	CLA	C4D-ND	-3.33	1.33	1.37
15	bB	835	CLA	C4D-ND	-3.33	1.33	1.37
15	c3	413	CLA	C1D-ND	3.33	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	404	CLA	C4D-ND	-3.32	1.33	1.37
14	bA	801	CL0	C4B-NB	-3.32	1.32	1.35
15	c4	406	CLA	C1D-ND	3.32	1.41	1.37
15	b3	408	CLA	C4D-ND	-3.32	1.33	1.37
15	cA	817	CLA	C4D-ND	-3.32	1.33	1.37
15	c3	408	CLA	C4D-ND	-3.32	1.33	1.37
15	a1	410	CLA	C4D-ND	-3.32	1.33	1.37
15	c1	410	CLA	C1D-ND	3.32	1.41	1.37
15	c2	410	CLA	C1D-ND	3.32	1.41	1.37
15	c4	412	CLA	C4D-ND	-3.32	1.33	1.37
15	a3	411	CLA	C1D-ND	3.32	1.41	1.37
15	c3	403	CLA	C4D-ND	-3.32	1.33	1.37
15	bB	829	CLA	CMD-C2D	-3.32	1.43	1.50
15	c3	404	CLA	C1D-ND	3.32	1.41	1.37
15	b1	411	CLA	C4D-ND	-3.32	1.33	1.37
15	a2	414	CLA	C1D-ND	3.31	1.41	1.37
15	a6	412	CLA	C4D-ND	-3.31	1.33	1.37
18	b1	419	BCR	C1-C6	-3.31	1.49	1.53
15	a2	410	CLA	C1D-ND	3.31	1.41	1.37
18	bB	850	BCR	C1-C6	-3.31	1.49	1.53
15	c5	410	CLA	C1D-ND	3.31	1.41	1.37
18	aF	201	BCR	C1-C6	-3.31	1.49	1.53
15	a3	403	CLA	C4D-ND	-3.31	1.33	1.37
15	b3	404	CLA	C4D-ND	-3.31	1.33	1.37
15	c2	406	CLA	C4D-ND	-3.31	1.33	1.37
15	a2	411	CLA	C1D-ND	3.31	1.41	1.37
15	a4	406	CLA	C1D-ND	3.31	1.41	1.37
18	aA	850	BCR	C1-C6	-3.31	1.49	1.53
15	aA	837	CLA	C4D-ND	-3.31	1.33	1.37
15	b6	405	CLA	C4D-ND	-3.31	1.33	1.37
15	c5	404	CLA	C4D-ND	-3.30	1.33	1.37
15	a1	408	CLA	C4D-ND	-3.30	1.33	1.37
15	a2	412	CLA	C1D-ND	3.30	1.41	1.37
15	c5	412	CLA	C4D-ND	-3.30	1.33	1.37
15	b3	405	CLA	C4D-ND	-3.30	1.33	1.37
15	c2	414	CLA	C4D-ND	-3.30	1.33	1.37
15	bA	817	CLA	C4D-ND	-3.30	1.33	1.37
15	b6	404	CLA	C4D-ND	-3.30	1.33	1.37
15	b2	414	CLA	C1D-ND	3.30	1.41	1.37
15	b3	406	CLA	C1D-ND	3.30	1.41	1.37
15	c5	404	CLA	C1D-ND	3.30	1.41	1.37
15	cB	817	CLA	CMC-C2C	-3.29	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	412	CLA	C1D-ND	3.29	1.41	1.37
15	a1	402	CLA	C4D-ND	-3.29	1.33	1.37
15	b5	412	CLA	C4D-ND	-3.29	1.33	1.37
18	bA	851	BCR	C1-C6	-3.29	1.49	1.53
15	aA	825	CLA	C1D-ND	3.29	1.41	1.37
15	b1	403	CLA	C1D-ND	3.29	1.41	1.37
15	b6	412	CLA	C1D-ND	3.29	1.41	1.37
15	cB	829	CLA	CMD-C2D	-3.29	1.43	1.50
15	bA	837	CLA	C4D-ND	-3.29	1.33	1.37
15	c3	407	CLA	C1D-ND	3.29	1.41	1.37
15	c6	405	CLA	C4D-ND	-3.29	1.33	1.37
18	c6	420	BCR	C1-C6	-3.29	1.49	1.53
15	c3	402	CLA	C1D-ND	3.29	1.41	1.37
15	aB	834	CLA	C1D-ND	3.29	1.41	1.37
15	b4	406	CLA	C1D-ND	3.29	1.41	1.37
18	a1	418	BCR	C1-C6	-3.29	1.49	1.53
15	a2	406	CLA	C4D-ND	-3.29	1.33	1.37
15	b2	406	CLA	C4D-ND	-3.29	1.33	1.37
15	aA	804	CLA	CMD-C2D	-3.29	1.43	1.50
14	aA	801	CL0	CHD-C4C	3.29	1.46	1.39
15	c3	406	CLA	C4D-ND	-3.29	1.33	1.37
18	c4	418	BCR	C1-C6	-3.29	1.49	1.53
15	bA	842	CLA	C4D-ND	-3.29	1.33	1.37
18	aB	849	BCR	C1-C6	-3.29	1.49	1.53
15	c5	408	CLA	C4D-ND	-3.29	1.33	1.37
15	a6	405	CLA	C4D-ND	-3.28	1.33	1.37
18	cB	846	BCR	C30-C25	-3.28	1.49	1.53
15	b2	410	CLA	C4D-ND	-3.28	1.33	1.37
15	cA	837	CLA	C4D-ND	-3.28	1.33	1.37
15	aA	842	CLA	CMD-C2D	-3.28	1.43	1.50
15	a3	405	CLA	C4D-ND	-3.28	1.33	1.37
15	c1	411	CLA	C4D-ND	-3.28	1.33	1.37
15	c6	410	CLA	C1D-ND	3.28	1.41	1.37
15	a5	412	CLA	C4D-ND	-3.28	1.33	1.37
15	cA	825	CLA	C1D-ND	3.28	1.41	1.37
15	b1	409	CLA	C4D-ND	-3.28	1.33	1.37
15	bB	841	CLA	C1D-ND	3.28	1.41	1.37
15	b2	411	CLA	C1D-ND	3.28	1.41	1.37
15	a3	408	CLA	C4D-ND	-3.28	1.33	1.37
15	cA	809	CLA	CHC-C1C	3.28	1.43	1.35
15	a3	413	CLA	C4D-ND	-3.27	1.33	1.37
14	cA	801	CL0	CHD-C4C	3.27	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	842	CLA	CMD-C2D	-3.27	1.43	1.50
15	c2	414	CLA	C1D-ND	3.27	1.41	1.37
15	a5	404	CLA	C4D-ND	-3.27	1.33	1.37
15	a6	409	CLA	C1D-ND	3.27	1.41	1.37
15	a3	404	CLA	C1D-ND	3.27	1.41	1.37
15	a6	410	CLA	C1D-ND	3.27	1.41	1.37
15	bB	834	CLA	C1D-ND	3.27	1.41	1.37
15	bB	817	CLA	CMC-C2C	-3.27	1.43	1.50
15	c2	404	CLA	C4D-ND	-3.27	1.33	1.37
15	a4	412	CLA	CMB-C2B	-3.27	1.44	1.51
15	bA	804	CLA	CMD-C2D	-3.27	1.43	1.50
15	a5	408	CLA	C4D-ND	-3.27	1.33	1.37
15	c3	413	CLA	C4D-ND	-3.27	1.33	1.37
18	cB	849	BCR	C1-C6	-3.27	1.49	1.53
14	bA	801	CL0	CHD-C4C	3.27	1.46	1.39
15	cF	201	CLA	C4D-ND	-3.27	1.33	1.37
15	a5	413	CLA	C1D-ND	3.27	1.41	1.37
15	b5	408	CLA	C4D-ND	-3.27	1.33	1.37
15	c6	409	CLA	C1D-ND	3.26	1.41	1.37
15	c1	409	CLA	C4D-ND	-3.26	1.33	1.37
15	c4	412	CLA	CMB-C2B	-3.26	1.44	1.51
15	cF	201	CLA	CMD-C2D	-3.26	1.43	1.50
15	a3	402	CLA	C1D-ND	3.26	1.41	1.37
15	aA	835	CLA	C1D-ND	3.26	1.41	1.37
15	bA	825	CLA	C1D-ND	3.26	1.41	1.37
15	cA	804	CLA	CMD-C2D	-3.26	1.43	1.50
15	b4	402	CLA	C1D-ND	3.26	1.41	1.37
15	c4	414	CLA	C4D-ND	-3.26	1.33	1.37
15	bA	809	CLA	CHC-C1C	3.26	1.43	1.35
15	c4	408	CLA	C4D-ND	-3.26	1.33	1.37
18	a4	418	BCR	C1-C6	-3.26	1.49	1.53
15	aB	817	CLA	CMC-C2C	-3.26	1.43	1.50
15	c4	405	CLA	C4D-ND	-3.26	1.33	1.37
15	bA	835	CLA	C1D-ND	3.26	1.41	1.37
15	b2	409	CLA	C1D-ND	3.26	1.41	1.37
18	cF	202	BCR	C1-C6	-3.26	1.49	1.53
15	aA	842	CLA	C4D-ND	-3.26	1.33	1.37
15	c1	412	CLA	C4D-ND	-3.26	1.33	1.37
15	b3	403	CLA	C4D-ND	-3.25	1.33	1.37
15	a3	406	CLA	C1D-ND	3.25	1.41	1.37
15	c3	405	CLA	C4D-ND	-3.25	1.33	1.37
15	c3	406	CLA	C1D-ND	3.25	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	413	CLA	C4D-ND	-3.25	1.33	1.37
14	cA	801	CL0	C4B-NB	-3.25	1.32	1.35
15	b4	412	CLA	CMB-C2B	-3.25	1.44	1.51
15	a4	405	CLA	C4D-ND	-3.25	1.33	1.37
15	b1	403	CLA	C4D-ND	-3.25	1.33	1.37
15	c5	413	CLA	C1D-ND	3.25	1.41	1.37
15	c6	404	CLA	C4D-ND	-3.25	1.33	1.37
15	b3	406	CLA	C4D-ND	-3.25	1.33	1.37
15	b2	414	CLA	C4D-ND	-3.24	1.33	1.37
15	c6	407	CLA	C4D-ND	-3.24	1.33	1.37
15	cB	841	CLA	C1D-ND	3.24	1.41	1.37
18	a3	418	BCR	C38-C26	-3.24	1.45	1.50
15	cJ	102	CLA	C1D-ND	3.24	1.41	1.37
15	a4	403	CLA	C4D-ND	-3.24	1.33	1.37
15	a1	408	CLA	C1D-ND	3.24	1.41	1.37
15	aA	819	CLA	C1D-ND	3.24	1.41	1.37
15	b4	414	CLA	C4D-ND	-3.24	1.33	1.37
15	a4	402	CLA	C1D-ND	3.24	1.41	1.37
15	a2	406	CLA	C1D-ND	3.24	1.41	1.37
15	cA	835	CLA	C1D-ND	3.24	1.41	1.37
15	c3	411	CLA	C1D-ND	3.24	1.41	1.37
15	a1	407	CLA	C1D-ND	3.24	1.41	1.37
15	aA	809	CLA	CHC-C1C	3.24	1.43	1.35
15	a1	402	CLA	C1D-ND	3.23	1.41	1.37
15	aB	834	CLA	C4D-ND	-3.23	1.33	1.37
15	bK	101	CLA	C1D-ND	3.23	1.41	1.37
15	a5	404	CLA	C1D-ND	3.23	1.41	1.37
15	aJ	203	CLA	C1D-ND	3.23	1.41	1.37
15	a1	411	CLA	C4D-ND	-3.23	1.33	1.37
15	b6	409	CLA	C1D-ND	3.23	1.41	1.37
15	a1	414	CLA	C4D-ND	-3.23	1.33	1.37
18	c1	419	BCR	C1-C6	-3.23	1.49	1.53
18	c4	418	BCR	C38-C26	-3.23	1.45	1.50
15	a6	407	CLA	C4D-ND	-3.23	1.33	1.37
18	bB	846	BCR	C30-C25	-3.23	1.49	1.53
18	bM	101	BCR	C1-C6	-3.23	1.49	1.53
15	aB	841	CLA	C1D-ND	3.23	1.41	1.37
18	bB	849	BCR	C1-C6	-3.22	1.49	1.53
15	a5	406	CLA	C4D-ND	-3.22	1.33	1.37
15	c1	403	CLA	C1D-ND	3.22	1.41	1.37
15	c1	409	CLA	C1D-ND	3.22	1.41	1.37
15	c1	415	CLA	C4D-ND	-3.22	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b6	420	BCR	C1-C6	-3.22	1.49	1.53
15	bJ	102	CLA	C1D-ND	3.22	1.41	1.37
15	b5	409	CLA	C1D-ND	3.22	1.41	1.37
15	bB	834	CLA	C4D-ND	-3.22	1.33	1.37
15	cB	834	CLA	C1D-ND	3.22	1.41	1.37
15	c4	402	CLA	C1D-ND	3.22	1.41	1.37
18	aM	101	BCR	C1-C6	-3.22	1.49	1.53
15	aA	817	CLA	C4D-ND	-3.22	1.33	1.37
15	c5	409	CLA	C1D-ND	3.22	1.41	1.37
15	b2	413	CLA	CMB-C2B	-3.22	1.45	1.51
15	b4	405	CLA	C4D-ND	-3.21	1.33	1.37
18	a4	418	BCR	C38-C26	-3.21	1.45	1.50
15	b5	413	CLA	C1D-ND	3.21	1.41	1.37
15	a2	409	CLA	C1D-ND	3.21	1.41	1.37
18	aB	846	BCR	C30-C25	-3.21	1.49	1.53
18	b4	418	BCR	C38-C26	-3.21	1.45	1.50
15	a1	412	CLA	C4D-ND	-3.21	1.33	1.37
15	a4	414	CLA	C4D-ND	-3.21	1.33	1.37
18	a6	420	BCR	C1-C6	-3.21	1.49	1.53
15	cB	809	CLA	CMB-C2B	-3.21	1.45	1.51
15	a3	406	CLA	C4D-ND	-3.21	1.33	1.37
15	c3	402	CLA	C4D-ND	-3.21	1.33	1.37
15	aB	814	CLA	CHC-C1C	3.21	1.43	1.35
15	cB	814	CLA	CHC-C1C	3.21	1.43	1.35
18	aB	846	BCR	C1-C6	-3.21	1.49	1.53
15	b6	407	CLA	C4D-ND	-3.20	1.33	1.37
15	c1	407	CLA	C4D-ND	-3.20	1.33	1.37
15	c3	410	CLA	C1D-ND	3.20	1.41	1.37
15	c1	404	CLA	C4D-ND	-3.20	1.33	1.37
18	cM	101	BCR	C1-C6	-3.20	1.49	1.53
15	bB	811	CLA	C1D-ND	3.20	1.41	1.37
15	c1	408	CLA	C1D-ND	3.20	1.41	1.37
15	a5	408	CLA	C1D-ND	3.20	1.41	1.37
15	a5	411	CLA	C1D-ND	3.20	1.41	1.37
15	c4	403	CLA	C4D-ND	-3.20	1.33	1.37
15	b2	406	CLA	C1D-ND	3.20	1.41	1.37
15	aA	840	CLA	CMB-C2B	-3.20	1.45	1.51
15	c2	413	CLA	CMB-C2B	-3.20	1.45	1.51
15	a6	404	CLA	C4D-ND	-3.20	1.33	1.37
15	a3	412	CLA	CMB-C2B	-3.20	1.45	1.51
15	a5	409	CLA	C1D-ND	3.20	1.41	1.37
15	cK	102	CLA	C1D-ND	3.20	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	836	CLA	CMB-C2B	-3.19	1.45	1.51
15	c2	412	CLA	C4D-ND	-3.19	1.33	1.37
15	bB	814	CLA	CHC-C1C	3.19	1.43	1.35
15	c2	409	CLA	C1D-ND	3.19	1.41	1.37
15	b1	415	CLA	C4D-ND	-3.19	1.33	1.37
15	c2	403	CLA	C4D-ND	-3.19	1.33	1.37
15	c2	406	CLA	C1D-ND	3.19	1.41	1.37
15	b4	413	CLA	C4D-ND	-3.19	1.33	1.37
18	b3	418	BCR	C38-C26	-3.19	1.45	1.50
15	cA	820	CLA	CMB-C2B	-3.19	1.45	1.51
15	b1	412	CLA	C4D-ND	-3.19	1.33	1.37
15	aB	811	CLA	C1D-ND	3.19	1.41	1.37
15	c1	413	CLA	CMB-C2B	-3.19	1.45	1.51
18	bB	846	BCR	C1-C6	-3.19	1.49	1.53
15	a4	413	CLA	C4D-ND	-3.19	1.33	1.37
18	cA	850	BCR	C1-C6	-3.19	1.49	1.53
15	b5	411	CLA	C1D-ND	3.19	1.41	1.37
15	bB	809	CLA	CMB-C2B	-3.19	1.45	1.51
15	aA	831	CLA	C3B-C2B	-3.19	1.35	1.40
15	a6	414	CLA	CMB-C2B	-3.18	1.45	1.51
15	bA	829	CLA	C1D-ND	3.18	1.41	1.37
15	b1	408	CLA	C1D-ND	3.18	1.41	1.37
15	c5	408	CLA	C1D-ND	3.18	1.41	1.37
15	bA	844	CLA	C1D-ND	3.18	1.41	1.37
20	bB	851	LMG	O8-C9	-3.18	1.37	1.45
18	aA	851	BCR	C1-C6	-3.18	1.49	1.53
15	bL	202	CLA	C3B-C2B	-3.18	1.36	1.40
15	c2	403	CLA	C1D-ND	3.18	1.41	1.37
15	a4	406	CLA	C4D-ND	-3.18	1.33	1.37
15	cB	834	CLA	C4D-ND	-3.18	1.33	1.37
15	cB	836	CLA	CMB-C2B	-3.18	1.45	1.51
15	cL	201	CLA	CMB-C2B	-3.18	1.45	1.51
15	bB	836	CLA	CMB-C2B	-3.18	1.45	1.51
15	a2	412	CLA	C4D-ND	-3.18	1.33	1.37
15	b1	405	CLA	C4D-ND	-3.18	1.33	1.37
15	b2	409	CLA	C4D-ND	-3.18	1.33	1.37
15	cA	843	CLA	C1D-ND	3.18	1.41	1.37
15	aA	836	CLA	C3B-C2B	-3.18	1.36	1.40
18	aA	852	BCR	C30-C25	-3.18	1.49	1.53
18	cF	204	BCR	C1-C6	-3.18	1.49	1.53
15	bB	842	CLA	C4D-ND	-3.18	1.33	1.37
15	cA	836	CLA	C3B-C2B	-3.18	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	809	CLA	CMB-C2B	-3.18	1.45	1.51
15	aK	102	CLA	C1D-ND	3.18	1.41	1.37
15	a2	409	CLA	C4D-ND	-3.18	1.33	1.37
15	b3	411	CLA	C1D-ND	3.18	1.41	1.37
15	c5	411	CLA	C1D-ND	3.18	1.41	1.37
15	b4	403	CLA	C4D-ND	-3.18	1.33	1.37
15	a2	413	CLA	CMB-C2B	-3.18	1.45	1.51
15	bA	831	CLA	C3B-C2B	-3.18	1.36	1.40
15	b4	406	CLA	C4D-ND	-3.17	1.33	1.37
18	bA	853	BCR	C30-C25	-3.17	1.49	1.53
18	b3	420	BCR	C1-C6	-3.17	1.49	1.53
15	a5	407	CLA	C4D-ND	-3.17	1.33	1.37
15	a5	413	CLA	C4D-ND	-3.17	1.33	1.37
15	cB	816	CLA	C4D-ND	-3.17	1.33	1.37
15	c5	413	CLA	C4D-ND	-3.17	1.33	1.37
18	b1	420	BCR	C1-C6	-3.17	1.49	1.53
15	bA	819	CLA	C1D-ND	3.17	1.41	1.37
15	bA	840	CLA	CMB-C2B	-3.17	1.45	1.51
15	b1	413	CLA	C4D-ND	-3.17	1.33	1.37
15	aB	841	CLA	CHC-C1C	3.17	1.43	1.35
15	bB	841	CLA	CHC-C1C	3.17	1.43	1.35
15	a1	408	CLA	CHC-C1C	3.17	1.43	1.35
20	cB	850	LMG	O8-C9	-3.17	1.37	1.45
15	c3	412	CLA	CMB-C2B	-3.17	1.45	1.51
15	bB	816	CLA	C4D-ND	-3.17	1.33	1.37
18	bA	852	BCR	C1-C6	-3.17	1.49	1.53
15	a6	422	CLA	C4D-ND	-3.17	1.33	1.37
15	b5	408	CLA	C1D-ND	3.17	1.41	1.37
18	b6	419	BCR	C1-C6	-3.17	1.49	1.53
20	aB	850	LMG	O8-C9	-3.17	1.37	1.45
15	c4	413	CLA	C4D-ND	-3.16	1.33	1.37
15	aA	839	CLA	CMB-C2B	-3.16	1.45	1.51
15	a1	406	CLA	C4D-ND	-3.16	1.33	1.37
15	b2	410	CLA	CHC-C1C	3.16	1.43	1.35
15	b5	406	CLA	C4D-ND	-3.16	1.33	1.37
15	cB	841	CLA	CHC-C1C	3.16	1.43	1.35
15	aA	844	CLA	C1D-ND	3.16	1.41	1.37
15	c2	414	CLA	CMB-C2B	-3.16	1.45	1.51
18	c3	418	BCR	C38-C26	-3.16	1.45	1.50
18	cA	847	BCR	C1-C6	-3.16	1.49	1.53
15	cB	842	CLA	C4D-ND	-3.16	1.33	1.37
15	b2	414	CLA	CMB-C2B	-3.16	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	415	CLA	C4D-ND	-3.16	1.33	1.37
15	aL	201	CLA	C3B-C2B	-3.16	1.36	1.40
18	cB	846	BCR	C1-C6	-3.16	1.49	1.53
15	cA	808	CLA	C1D-ND	3.16	1.41	1.37
15	aA	820	CLA	CMB-C2B	-3.16	1.45	1.51
15	aB	815	CLA	C1D-ND	3.16	1.41	1.37
15	b3	402	CLA	C4D-ND	-3.16	1.33	1.37
15	c5	405	CLA	C4D-ND	-3.16	1.33	1.37
15	bA	820	CLA	CMB-C2B	-3.16	1.45	1.51
15	cB	841	CLA	CMB-C2B	-3.16	1.45	1.51
15	cA	831	CLA	C3B-C2B	-3.16	1.36	1.40
15	cA	802	CLA	C3B-C2B	-3.16	1.36	1.40
15	cA	819	CLA	C1D-ND	3.16	1.41	1.37
18	c5	418	BCR	C38-C26	-3.15	1.45	1.50
15	cA	840	CLA	CMB-C2B	-3.15	1.45	1.51
18	aA	848	BCR	C1-C6	-3.15	1.49	1.53
15	cB	801	CLA	C1D-ND	3.15	1.41	1.37
18	b5	418	BCR	C38-C26	-3.15	1.45	1.50
15	bB	841	CLA	CMB-C2B	-3.15	1.45	1.51
18	bA	849	BCR	C1-C6	-3.15	1.49	1.53
15	a2	417	CLA	MG-ND	-3.15	1.99	2.05
15	b2	403	CLA	C4D-ND	-3.15	1.33	1.37
15	b5	405	CLA	C4D-ND	-3.15	1.33	1.37
15	bB	815	CLA	C1D-ND	3.15	1.41	1.37
15	aB	841	CLA	CMB-C2B	-3.15	1.45	1.51
15	cA	839	CLA	CMB-C2B	-3.15	1.45	1.51
15	aA	835	CLA	C3B-C2B	-3.15	1.36	1.40
15	cA	805	CLA	CMB-C2B	-3.15	1.45	1.51
15	b1	407	CLA	C4D-ND	-3.15	1.33	1.37
15	bA	802	CLA	C3B-C2B	-3.15	1.36	1.40
15	b3	412	CLA	CMB-C2B	-3.15	1.45	1.51
15	a5	409	CLA	CHC-C1C	3.15	1.43	1.35
15	c1	413	CLA	C4D-ND	-3.15	1.33	1.37
18	c1	420	BCR	C1-C6	-3.14	1.49	1.53
15	a3	402	CLA	C4D-ND	-3.14	1.33	1.37
15	c2	409	CLA	C4D-ND	-3.14	1.33	1.37
18	aI	103	BCR	C1-C6	-3.14	1.49	1.53
15	cA	829	CLA	C1D-ND	3.14	1.41	1.37
15	a3	410	CLA	C1D-ND	3.14	1.41	1.37
15	bA	839	CLA	CMB-C2B	-3.14	1.45	1.51
15	a6	411	CLA	C4D-ND	-3.14	1.33	1.37
14	aA	801	CL0	C1D-ND	3.14	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	409	CLA	CHC-C1C	3.14	1.43	1.35
15	a1	403	CLA	C4D-ND	-3.14	1.33	1.37
15	a2	403	CLA	C4D-ND	-3.14	1.33	1.37
15	b2	412	CLA	C4D-ND	-3.14	1.33	1.37
15	b5	407	CLA	C4D-ND	-3.14	1.33	1.37
15	cB	811	CLA	C1D-ND	3.14	1.41	1.37
15	aA	805	CLA	CMB-C2B	-3.14	1.45	1.51
15	c6	409	CLA	C4D-ND	-3.14	1.33	1.37
15	c6	413	CLA	CMB-C2B	-3.14	1.45	1.51
15	aA	808	CLA	C1D-ND	3.14	1.41	1.37
15	c2	417	CLA	MG-ND	-3.14	1.99	2.05
15	a6	408	CLA	C4D-ND	-3.13	1.33	1.37
15	c4	406	CLA	C4D-ND	-3.13	1.33	1.37
15	bB	813	CLA	CHC-C1C	3.13	1.43	1.35
15	aB	801	CLA	C1D-ND	3.13	1.41	1.37
15	b6	408	CLA	C4D-ND	-3.13	1.33	1.37
15	bA	836	CLA	C3B-C2B	-3.13	1.36	1.40
15	aA	802	CLA	C3B-C2B	-3.13	1.36	1.40
15	aB	813	CLA	CHC-C1C	3.13	1.43	1.35
15	bA	842	CLA	C1D-ND	3.13	1.41	1.37
15	bA	835	CLA	C3B-C2B	-3.13	1.36	1.40
15	a6	410	CLA	CHC-C1C	3.13	1.43	1.35
15	b6	411	CLA	C4D-ND	-3.13	1.33	1.37
15	b5	402	CLA	C4D-ND	-3.13	1.33	1.37
15	bA	805	CLA	CMB-C2B	-3.13	1.45	1.51
18	a6	419	BCR	C1-C6	-3.13	1.49	1.53
18	bF	202	BCR	C1-C6	-3.13	1.49	1.53
15	aB	823	CLA	C4D-ND	-3.13	1.33	1.37
18	a5	418	BCR	C38-C26	-3.13	1.45	1.50
15	b5	413	CLA	C4D-ND	-3.13	1.33	1.37
15	c1	412	CLA	CMB-C2B	-3.13	1.45	1.51
18	a1	419	BCR	C1-C6	-3.13	1.49	1.53
15	c2	410	CLA	CHC-C1C	3.12	1.43	1.35
15	c5	412	CLA	CMB-C2B	-3.12	1.45	1.51
15	cF	201	CLA	C1D-ND	3.12	1.41	1.37
15	a5	405	CLA	C4D-ND	-3.12	1.33	1.37
15	b6	406	CLA	C4D-ND	-3.12	1.33	1.37
15	c5	406	CLA	C4D-ND	-3.12	1.33	1.37
15	b6	416	CLA	C4D-ND	-3.12	1.33	1.37
15	cA	835	CLA	C3B-C2B	-3.12	1.36	1.40
15	aA	842	CLA	C1D-ND	3.12	1.41	1.37
15	b1	409	CLA	CHC-C1C	3.12	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	842	CLA	C4D-ND	-3.12	1.33	1.37
15	aL	201	CLA	CMB-C2B	-3.12	1.45	1.51
14	bA	801	CL0	C1D-ND	3.12	1.41	1.37
14	cA	801	CL0	C1D-ND	3.12	1.41	1.37
15	bA	808	CLA	C1D-ND	3.12	1.41	1.37
15	bB	823	CLA	C4D-ND	-3.12	1.33	1.37
15	b5	420	CLA	C1D-ND	3.12	1.41	1.37
15	cB	823	CLA	C4D-ND	-3.12	1.33	1.37
15	a6	416	CLA	C4D-ND	-3.12	1.33	1.37
18	c2	419	BCR	C38-C26	-3.12	1.45	1.50
15	b6	404	CLA	C1D-ND	3.12	1.41	1.37
15	a4	409	CLA	CHC-C1C	3.12	1.43	1.35
15	a1	411	CLA	CMB-C2B	-3.12	1.45	1.51
15	c6	416	CLA	C4D-ND	-3.11	1.33	1.37
18	aF	202	BCR	C1-C6	-3.11	1.49	1.53
14	cA	801	CL0	C3D-C4D	-3.11	1.37	1.44
15	c5	402	CLA	C4D-ND	-3.11	1.33	1.37
15	bB	801	CLA	C1D-ND	3.11	1.41	1.37
15	b4	409	CLA	CHC-C1C	3.11	1.42	1.35
15	c5	409	CLA	CHC-C1C	3.11	1.42	1.35
18	a2	419	BCR	C38-C26	-3.11	1.45	1.50
15	b2	406	CLA	CHC-C1C	3.11	1.42	1.35
15	aA	814	CLA	C1D-ND	3.11	1.41	1.37
15	c6	410	CLA	CHC-C1C	3.11	1.42	1.35
15	a2	410	CLA	CHC-C1C	3.11	1.42	1.35
15	a2	403	CLA	C1D-ND	3.11	1.41	1.37
15	c5	407	CLA	C4D-ND	-3.11	1.33	1.37
15	bB	809	CLA	C3B-C2B	-3.11	1.36	1.40
15	aB	816	CLA	C4D-ND	-3.11	1.33	1.37
18	aI	101	BCR	C1-C6	-3.11	1.49	1.53
15	a1	412	CLA	CMB-C2B	-3.11	1.45	1.51
15	b5	409	CLA	CHC-C1C	3.11	1.42	1.35
15	c2	406	CLA	CHC-C1C	3.11	1.42	1.35
15	c3	414	CLA	C4D-ND	-3.11	1.33	1.37
18	a5	418	BCR	C1-C6	-3.11	1.49	1.53
15	aB	809	CLA	C3B-C2B	-3.10	1.36	1.40
15	b6	414	CLA	CMB-C2B	-3.10	1.45	1.51
15	bA	814	CLA	C1D-ND	3.10	1.41	1.37
15	c6	404	CLA	C1D-ND	3.10	1.41	1.37
18	cI	101	BCR	C1-C6	-3.10	1.49	1.53
15	a1	401	CLA	C4D-ND	-3.10	1.33	1.37
15	bA	845	CLA	CHC-C1C	3.10	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	841	CLA	C1D-ND	3.10	1.41	1.37
15	a2	411	CLA	C4D-ND	-3.10	1.33	1.37
15	bB	833	CLA	C3B-C2B	-3.10	1.36	1.40
15	bA	828	CLA	CMC-C2C	-3.10	1.44	1.50
15	a2	414	CLA	CMB-C2B	-3.10	1.45	1.51
15	b6	410	CLA	CHC-C1C	3.10	1.42	1.35
18	a3	420	BCR	C1-C6	-3.10	1.49	1.53
15	b3	410	CLA	C4D-ND	-3.10	1.33	1.37
15	a4	403	CLA	C1D-ND	3.10	1.41	1.37
15	b5	413	CLA	CMB-C2B	-3.10	1.45	1.51
15	c3	413	CLA	CMB-C2B	-3.10	1.45	1.51
15	bL	202	CLA	CMB-C2B	-3.10	1.45	1.51
15	b1	404	CLA	C4D-ND	-3.10	1.33	1.37
15	cB	809	CLA	C3B-C2B	-3.10	1.36	1.40
15	b2	403	CLA	C1D-ND	3.10	1.41	1.37
15	cA	828	CLA	CMC-C2C	-3.10	1.44	1.50
15	aB	833	CLA	C3B-C2B	-3.10	1.36	1.40
15	b3	410	CLA	C1D-ND	3.10	1.41	1.37
15	b1	406	CLA	C4D-ND	-3.10	1.33	1.37
18	c6	419	BCR	C1-C6	-3.10	1.49	1.53
15	b3	413	CLA	CMB-C2B	-3.10	1.45	1.51
15	cA	828	CLA	CHC-C1C	3.09	1.42	1.35
18	a2	419	BCR	C1-C6	-3.09	1.49	1.53
15	cA	844	CLA	CHC-C1C	3.09	1.42	1.35
15	b1	413	CLA	CMB-C2B	-3.09	1.45	1.51
18	c2	419	BCR	C1-C6	-3.09	1.49	1.53
15	cB	813	CLA	CHC-C1C	3.09	1.42	1.35
15	cA	839	CLA	C3B-C2B	-3.09	1.36	1.40
15	aA	828	CLA	CHC-C1C	3.09	1.42	1.35
15	a3	414	CLA	C4D-ND	-3.09	1.33	1.37
18	c5	418	BCR	C1-C6	-3.09	1.49	1.53
15	a5	420	CLA	C1D-ND	3.09	1.41	1.37
15	a5	413	CLA	CMB-C2B	-3.09	1.45	1.51
15	b2	415	CLA	C4D-ND	-3.09	1.33	1.37
15	a3	416	CLA	CMD-C2D	-3.09	1.44	1.50
18	bI	101	BCR	C1-C6	-3.09	1.49	1.53
15	b3	411	CLA	CMB-C2B	-3.09	1.45	1.51
15	a2	407	CLA	C4D-ND	-3.09	1.33	1.37
18	c3	420	BCR	C1-C6	-3.08	1.49	1.53
15	aA	824	CLA	C1D-ND	3.08	1.41	1.37
15	b6	414	CLA	C4D-ND	-3.08	1.33	1.37
20	aB	850	LMG	O7-C8	-3.08	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cL	201	CLA	C3B-C2B	-3.08	1.36	1.40
18	b2	419	BCR	C38-C26	-3.08	1.45	1.50
18	a1	417	BCR	C1-C6	-3.08	1.49	1.53
15	a4	416	CLA	MG-ND	-3.08	1.99	2.05
15	c3	414	CLA	CHC-C1C	3.08	1.42	1.35
15	cB	823	CLA	C1D-ND	3.08	1.41	1.37
15	b4	402	CLA	C4D-ND	-3.08	1.33	1.37
15	c6	406	CLA	C4D-ND	-3.08	1.33	1.37
15	c4	416	CLA	MG-ND	-3.08	1.99	2.05
15	bA	843	CLA	C3B-C2B	-3.08	1.36	1.40
15	b2	407	CLA	C4D-ND	-3.08	1.33	1.37
15	a6	413	CLA	CMB-C2B	-3.08	1.45	1.51
18	bA	850	BCR	C30-C25	-3.08	1.49	1.53
18	cA	851	BCR	C30-C25	-3.08	1.49	1.53
15	cB	815	CLA	C1D-ND	3.08	1.41	1.37
15	aA	815	CLA	CHC-C1C	3.08	1.42	1.35
15	cA	841	CLA	C1D-ND	3.08	1.41	1.37
15	cA	835	CLA	CMB-C2B	-3.08	1.45	1.51
15	c1	405	CLA	C4D-ND	-3.07	1.33	1.37
18	bL	205	BCR	C1-C6	-3.07	1.49	1.53
14	bA	801	CL0	C3D-C4D	-3.07	1.37	1.44
15	bB	831	CLA	C1D-ND	3.07	1.41	1.37
15	b4	416	CLA	MG-ND	-3.07	1.99	2.05
15	c4	409	CLA	CHC-C1C	3.07	1.42	1.35
15	aB	802	CLA	C3B-C2B	-3.07	1.36	1.40
15	a1	404	CLA	C4D-ND	-3.07	1.33	1.37
18	b5	419	BCR	C1-C6	-3.07	1.49	1.53
18	c6	419	BCR	C38-C26	-3.07	1.45	1.50
15	a6	409	CLA	C4D-ND	-3.07	1.33	1.37
15	b3	414	CLA	C4D-ND	-3.07	1.33	1.37
20	cB	850	LMG	O7-C8	-3.07	1.38	1.46
15	a4	411	CLA	CHC-C1C	3.07	1.42	1.35
15	c4	413	CLA	CMB-C2B	-3.07	1.45	1.51
15	a2	415	CLA	C4D-ND	-3.07	1.33	1.37
18	c5	419	BCR	C1-C6	-3.07	1.49	1.53
15	bA	835	CLA	CMB-C2B	-3.07	1.45	1.51
15	c6	408	CLA	C4D-ND	-3.07	1.33	1.37
15	c6	411	CLA	C4D-ND	-3.07	1.33	1.37
15	c3	411	CLA	CMB-C2B	-3.07	1.45	1.51
15	aB	831	CLA	C1D-ND	3.07	1.41	1.37
15	a6	406	CLA	C4D-ND	-3.07	1.33	1.37
15	b5	412	CLA	CMB-C2B	-3.07	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	402	CLA	C4D-ND	-3.07	1.33	1.37
15	c4	402	CLA	C4D-ND	-3.07	1.33	1.37
15	b4	411	CLA	CHC-C1C	3.07	1.42	1.35
15	b6	413	CLA	CMB-C2B	-3.07	1.45	1.51
18	a6	419	BCR	C38-C26	-3.07	1.45	1.50
15	aA	829	CLA	C1D-ND	3.06	1.41	1.37
18	aA	849	BCR	C30-C25	-3.06	1.49	1.53
15	bA	828	CLA	CHC-C1C	3.06	1.42	1.35
15	b6	415	CLA	CHC-C1C	3.06	1.42	1.35
15	a4	413	CLA	CMB-C2B	-3.06	1.45	1.51
15	c2	411	CLA	C4D-ND	-3.06	1.33	1.37
15	b3	416	CLA	CMD-C2D	-3.06	1.44	1.50
15	cJ	101	CLA	C4D-ND	-3.06	1.33	1.37
15	c2	407	CLA	C4D-ND	-3.06	1.33	1.37
15	aB	820	CLA	CMB-C2B	-3.06	1.45	1.51
15	a6	414	CLA	C1D-ND	3.06	1.41	1.37
15	cA	824	CLA	C1D-ND	3.06	1.41	1.37
15	b6	409	CLA	C4D-ND	-3.06	1.33	1.37
14	aA	801	CL0	C3D-C4D	-3.06	1.37	1.44
15	a3	413	CLA	CMB-C2B	-3.06	1.45	1.51
15	aA	828	CLA	CMC-C2C	-3.06	1.44	1.50
15	a2	406	CLA	CHC-C1C	3.06	1.42	1.35
15	aJ	202	CLA	C4D-ND	-3.06	1.33	1.37
15	c5	413	CLA	CMB-C2B	-3.06	1.45	1.51
15	c5	416	CLA	MG-ND	-3.06	1.99	2.05
15	aA	845	CLA	CHC-C1C	3.06	1.42	1.35
15	bB	815	CLA	CHC-C1C	3.06	1.42	1.35
15	cB	825	CLA	C1D-ND	3.06	1.41	1.37
15	c6	414	CLA	C4D-ND	-3.06	1.33	1.37
18	b3	401	BCR	C1-C6	-3.06	1.49	1.53
18	cL	204	BCR	C1-C6	-3.06	1.49	1.53
15	c3	416	CLA	CMD-C2D	-3.06	1.44	1.50
15	bA	815	CLA	CHC-C1C	3.05	1.42	1.35
18	cF	205	BCR	C30-C25	-3.05	1.49	1.53
15	b3	414	CLA	CHC-C1C	3.05	1.42	1.35
15	a3	411	CLA	CMB-C2B	-3.05	1.45	1.51
18	a1	418	BCR	C34-C9	-3.05	1.44	1.50
15	b1	412	CLA	CMB-C2B	-3.05	1.45	1.51
15	cA	815	CLA	CHC-C1C	3.05	1.42	1.35
20	bB	851	LMG	O7-C8	-3.05	1.39	1.46
15	bA	824	CLA	C1D-ND	3.05	1.41	1.37
15	b2	417	CLA	MG-ND	-3.05	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	833	CLA	CHC-C1C	3.05	1.42	1.35
15	b4	421	CLA	C1D-ND	3.05	1.41	1.37
15	aB	815	CLA	CHC-C1C	3.05	1.42	1.35
15	bB	802	CLA	CMC-C2C	-3.05	1.44	1.50
15	bJ	101	CLA	C4D-ND	-3.05	1.33	1.37
15	a5	412	CLA	CMB-C2B	-3.05	1.45	1.51
15	b4	413	CLA	CMB-C2B	-3.05	1.45	1.51
15	aA	835	CLA	CMB-C2B	-3.05	1.45	1.51
15	b5	420	CLA	CHC-C1C	3.05	1.42	1.35
15	cB	833	CLA	C3B-C2B	-3.05	1.36	1.40
15	a1	405	CLA	C4D-ND	-3.04	1.33	1.37
15	bB	830	CLA	CMD-C2D	-3.04	1.44	1.50
18	b6	419	BCR	C38-C26	-3.04	1.45	1.50
15	cB	820	CLA	CMB-C2B	-3.04	1.45	1.51
15	c5	420	CLA	CHC-C1C	3.04	1.42	1.35
18	a5	419	BCR	C1-C6	-3.04	1.49	1.53
18	cA	848	BCR	C30-C25	-3.04	1.49	1.53
15	aB	830	CLA	CMD-C2D	-3.04	1.44	1.50
15	c4	411	CLA	CHC-C1C	3.04	1.42	1.35
15	cB	830	CLA	CMD-C2D	-3.04	1.44	1.50
15	c1	406	CLA	C4D-ND	-3.04	1.33	1.37
15	cB	815	CLA	CHC-C1C	3.04	1.42	1.35
15	c4	403	CLA	C1D-ND	3.04	1.41	1.37
15	a1	410	CLA	CHC-C1C	3.04	1.42	1.35
15	a5	420	CLA	CHC-C1C	3.04	1.42	1.35
18	aF	203	BCR	C30-C25	-3.04	1.49	1.53
15	aB	802	CLA	CMC-C2C	-3.04	1.44	1.50
15	a6	404	CLA	C1D-ND	3.03	1.41	1.37
15	aA	803	CLA	CMB-C2B	-3.03	1.45	1.51
15	c6	414	CLA	CMB-C2B	-3.03	1.45	1.51
15	bB	820	CLA	CMB-C2B	-3.03	1.45	1.51
15	a3	410	CLA	C4D-ND	-3.03	1.33	1.37
15	cB	831	CLA	C1D-ND	3.03	1.41	1.37
15	cB	833	CLA	CHC-C1C	3.03	1.42	1.35
18	bJ	103	BCR	C30-C25	-3.03	1.49	1.53
18	aJ	204	BCR	C30-C25	-3.03	1.49	1.53
15	cB	802	CLA	C3B-C2B	-3.03	1.36	1.40
15	a1	415	CLA	MG-ND	-3.03	1.99	2.05
15	a5	414	CLA	CHC-C1C	3.03	1.42	1.35
15	cA	842	CLA	CMB-C2B	-3.03	1.45	1.51
15	b1	416	CLA	CMD-C2D	-3.03	1.44	1.50
15	a4	421	CLA	C1D-ND	3.03	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	833	CLA	CHC-C1C	3.03	1.42	1.35
18	cB	848	BCR	C1-C6	-3.03	1.49	1.53
15	bA	839	CLA	C3B-C2B	-3.03	1.36	1.40
15	c5	414	CLA	CHC-C1C	3.03	1.42	1.35
15	b2	411	CLA	C4D-ND	-3.03	1.33	1.37
15	aB	811	CLA	CMB-C2B	-3.03	1.45	1.51
15	aB	825	CLA	C1D-ND	3.03	1.41	1.37
15	bA	838	CLA	CMD-C2D	-3.03	1.44	1.50
15	c2	417	CLA	CMD-C2D	-3.03	1.44	1.50
15	aA	838	CLA	CMD-C2D	-3.03	1.44	1.50
15	bB	825	CLA	C1D-ND	3.03	1.41	1.37
15	cA	814	CLA	C1D-ND	3.03	1.41	1.37
15	bA	803	CLA	CMB-C2B	-3.02	1.45	1.51
15	c6	415	CLA	CHC-C1C	3.02	1.42	1.35
15	c2	403	CLA	CHC-C1C	3.02	1.42	1.35
15	b4	403	CLA	C1D-ND	3.02	1.41	1.37
14	cA	801	CL0	C3D-C2D	3.02	1.47	1.39
18	bB	848	BCR	C1-C6	-3.02	1.49	1.53
15	aA	810	CLA	CMB-C2B	-3.02	1.45	1.51
15	aB	823	CLA	C1D-ND	3.02	1.41	1.37
15	c1	408	CLA	C4D-ND	-3.02	1.33	1.37
15	a5	416	CLA	MG-ND	-3.02	1.99	2.05
18	b5	418	BCR	C1-C6	-3.02	1.49	1.53
15	b6	417	CLA	CMD-C2D	-3.02	1.44	1.50
15	a1	413	CLA	CHC-C1C	3.02	1.42	1.35
18	b1	419	BCR	C34-C9	-3.02	1.44	1.50
15	b2	403	CLA	CHC-C1C	3.02	1.42	1.35
18	b2	419	BCR	C1-C6	-3.02	1.49	1.53
15	aA	832	CLA	CMB-C2B	-3.02	1.45	1.51
18	b1	418	BCR	C1-C6	-3.02	1.49	1.53
18	cJ	103	BCR	C30-C25	-3.02	1.49	1.53
15	a1	415	CLA	CMD-C2D	-3.02	1.44	1.50
15	b1	416	CLA	MG-ND	-3.02	1.99	2.05
15	a4	402	CLA	C4D-ND	-3.02	1.33	1.37
15	cA	803	CLA	CMB-C2B	-3.02	1.45	1.51
15	c1	411	CLA	CHC-C1C	3.02	1.42	1.35
15	cB	802	CLA	CMC-C2C	-3.02	1.44	1.50
15	cA	832	CLA	CMB-C2B	-3.01	1.45	1.51
15	c5	420	CLA	C1D-ND	3.01	1.41	1.37
15	a5	420	CLA	C4D-ND	-3.01	1.33	1.37
15	a3	414	CLA	CHC-C1C	3.01	1.42	1.35
15	c3	421	CLA	C1D-ND	3.01	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	417	CLA	MG-ND	-3.01	1.99	2.05
15	c5	420	CLA	C4D-ND	-3.01	1.33	1.37
15	cA	841	CLA	CHC-C1C	3.01	1.42	1.35
18	a3	401	BCR	C33-C5	-3.01	1.46	1.50
15	a5	402	CLA	C4D-ND	-3.01	1.33	1.37
15	aB	812	CLA	CHC-C1C	3.01	1.42	1.35
15	c1	416	CLA	MG-ND	-3.01	1.99	2.05
15	c3	410	CLA	C4D-ND	-3.01	1.33	1.37
15	a6	415	CLA	CHC-C1C	3.01	1.42	1.35
15	c1	416	CLA	CMD-C2D	-3.01	1.44	1.50
14	aA	801	CL0	C3D-C2D	3.01	1.47	1.39
18	c2	401	BCR	C1-C6	-3.01	1.49	1.53
15	c2	402	CLA	C4D-ND	-3.01	1.33	1.37
15	a1	422	CLA	CHC-C1C	3.01	1.42	1.35
15	a2	403	CLA	CHC-C1C	3.01	1.42	1.35
18	b1	418	BCR	C38-C26	-3.01	1.46	1.50
18	c3	401	BCR	C33-C5	-3.01	1.46	1.50
15	aA	841	CLA	CHC-C1C	3.01	1.42	1.35
18	a1	417	BCR	C38-C26	-3.01	1.46	1.50
18	c1	418	BCR	C1-C6	-3.01	1.49	1.53
15	b5	416	CLA	MG-ND	-3.01	1.99	2.05
15	a6	414	CLA	C4D-ND	-3.01	1.33	1.37
15	aA	843	CLA	CMB-C2B	-3.01	1.45	1.51
18	bJ	105	BCR	C30-C25	-3.00	1.49	1.53
15	b3	409	CLA	CHC-C1C	3.00	1.42	1.35
15	cB	812	CLA	CHC-C1C	3.00	1.42	1.35
15	c4	404	CLA	CHC-C1C	3.00	1.42	1.35
18	c3	401	BCR	C1-C6	-3.00	1.49	1.53
15	aA	843	CLA	C3B-C2B	-3.00	1.36	1.40
15	bA	832	CLA	CMB-C2B	-3.00	1.45	1.51
15	b1	402	CLA	C4D-ND	-3.00	1.33	1.37
15	cB	811	CLA	CMB-C2B	-3.00	1.45	1.51
15	cB	813	CLA	CMB-C2B	-3.00	1.45	1.51
18	a3	401	BCR	C1-C6	-3.00	1.49	1.53
18	b2	420	BCR	C1-C6	-3.00	1.49	1.53
15	a6	417	CLA	CMD-C2D	-3.00	1.44	1.50
15	aA	841	CLA	C1D-ND	3.00	1.41	1.37
15	a3	409	CLA	CHC-C1C	3.00	1.42	1.35
15	b4	404	CLA	CHC-C1C	3.00	1.42	1.35
15	a6	415	CLA	C4D-ND	-3.00	1.33	1.37
15	cA	809	CLA	C1D-ND	2.99	1.41	1.37
15	cB	826	CLA	CHC-C1C	2.99	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	839	CLA	C3B-C2B	-2.99	1.36	1.40
15	b6	422	CLA	CHC-C1C	2.99	1.42	1.35
15	cA	810	CLA	CMB-C2B	-2.99	1.45	1.51
15	bB	815	CLA	C4D-ND	-2.99	1.33	1.37
15	bB	839	CLA	CHC-C1C	2.99	1.42	1.35
15	aL	203	CLA	CMB-C2B	-2.99	1.45	1.51
18	c1	419	BCR	C34-C9	-2.99	1.44	1.50
15	bB	811	CLA	CMB-C2B	-2.99	1.45	1.51
15	aB	826	CLA	CHC-C1C	2.99	1.42	1.35
15	bB	802	CLA	C3B-C2B	-2.99	1.36	1.40
15	b1	414	CLA	CHC-C1C	2.99	1.42	1.35
15	a5	403	CLA	CHC-C1C	2.99	1.42	1.35
15	c1	414	CLA	CHC-C1C	2.99	1.42	1.35
18	b3	401	BCR	C33-C5	-2.99	1.46	1.50
15	c3	409	CLA	CHC-C1C	2.99	1.42	1.35
15	b6	411	CLA	CHC-C1C	2.99	1.42	1.35
18	a2	401	BCR	C1-C6	-2.99	1.49	1.53
18	c4	420	BCR	C1-C6	-2.99	1.49	1.53
15	bA	841	CLA	CHC-C1C	2.98	1.42	1.35
15	a6	403	CLA	C4D-ND	-2.98	1.33	1.37
15	a5	411	CLA	CMB-C2B	-2.98	1.45	1.51
15	b2	412	CLA	CHC-C1C	2.98	1.42	1.35
15	cA	838	CLA	CMD-C2D	-2.98	1.44	1.50
15	c6	417	CLA	MG-ND	-2.98	1.99	2.05
15	a4	410	CLA	C4D-ND	-2.98	1.33	1.37
15	b4	410	CLA	C4D-ND	-2.98	1.33	1.37
15	b5	414	CLA	CHC-C1C	2.98	1.42	1.35
18	aB	848	BCR	C1-C6	-2.98	1.49	1.53
15	bB	813	CLA	CMB-C2B	-2.98	1.45	1.51
15	aB	839	CLA	CHC-C1C	2.98	1.42	1.35
15	cB	839	CLA	CHC-C1C	2.98	1.42	1.35
15	a6	422	CLA	CMB-C2B	-2.98	1.45	1.51
15	bB	823	CLA	C1D-ND	2.98	1.41	1.37
15	cL	203	CLA	CMB-C2B	-2.98	1.45	1.51
15	bA	843	CLA	CMB-C2B	-2.98	1.45	1.51
18	c1	418	BCR	C38-C26	-2.98	1.46	1.50
15	bB	812	CLA	CHC-C1C	2.98	1.42	1.35
15	a4	404	CLA	CHC-C1C	2.98	1.42	1.35
15	a6	404	CLA	CHC-C1C	2.98	1.42	1.35
15	bB	826	CLA	CHC-C1C	2.98	1.42	1.35
15	a1	407	CLA	C4D-ND	-2.97	1.33	1.37
14	bA	801	CL0	C3D-C2D	2.97	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	422	CLA	C4D-ND	-2.97	1.33	1.37
15	b2	402	CLA	C4D-ND	-2.97	1.33	1.37
15	bA	810	CLA	CMB-C2B	-2.97	1.45	1.51
15	c6	404	CLA	CHC-C1C	2.97	1.42	1.35
15	c3	411	CLA	CHC-C1C	2.97	1.42	1.35
15	bB	828	CLA	CMB-C2B	-2.97	1.45	1.51
15	a3	421	CLA	MG-ND	-2.97	1.99	2.05
15	b1	408	CLA	C4D-ND	-2.97	1.33	1.37
15	a1	415	CLA	CMB-C2B	-2.97	1.45	1.51
18	a4	420	BCR	C1-C6	-2.97	1.49	1.53
15	bL	204	CLA	CMB-C2B	-2.97	1.45	1.51
15	aB	813	CLA	CMB-C2B	-2.97	1.45	1.51
15	a2	417	CLA	CMD-C2D	-2.97	1.44	1.50
15	bB	837	CLA	CHC-C1C	2.97	1.42	1.35
15	b5	411	CLA	CMB-C2B	-2.97	1.45	1.51
15	cB	833	CLA	CMB-C2B	-2.97	1.45	1.51
15	a1	422	CLA	C2A-C1A	2.97	1.58	1.52
18	b4	420	BCR	C1-C6	-2.96	1.49	1.53
18	aB	847	BCR	C30-C25	-2.96	1.49	1.53
15	aA	821	CLA	C1D-ND	2.96	1.41	1.37
15	b3	421	CLA	C1D-ND	2.96	1.41	1.37
15	a2	402	CLA	C4D-ND	-2.96	1.33	1.37
15	c5	403	CLA	C1D-ND	2.96	1.41	1.37
15	c6	417	CLA	CMD-C2D	-2.96	1.44	1.50
15	aB	815	CLA	C4D-ND	-2.96	1.33	1.37
15	c4	421	CLA	C1D-ND	2.96	1.41	1.37
15	b1	411	CLA	CHC-C1C	2.96	1.42	1.35
15	b2	404	CLA	CHC-C1C	2.96	1.42	1.35
15	c3	408	CLA	C1D-ND	2.96	1.41	1.37
15	cA	842	CLA	C3B-C2B	-2.96	1.36	1.40
18	c2	421	BCR	C1-C6	-2.96	1.49	1.53
15	c6	415	CLA	C4D-ND	-2.96	1.33	1.37
18	a2	420	BCR	C1-C6	-2.96	1.49	1.53
15	cA	834	CLA	MG-ND	-2.96	1.99	2.05
15	aL	203	CLA	C1D-ND	2.96	1.41	1.37
18	c6	402	BCR	C33-C5	-2.96	1.46	1.50
15	bA	834	CLA	MG-ND	-2.96	1.99	2.05
18	aI	101	BCR	C30-C25	-2.96	1.49	1.53
15	aB	807	CLA	CMD-C2D	-2.96	1.44	1.50
18	aL	205	BCR	C1-C6	-2.96	1.49	1.53
18	a6	402	BCR	C33-C5	-2.96	1.46	1.50
15	a6	411	CLA	CHC-C1C	2.96	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	839	CLA	C1D-ND	2.96	1.41	1.37
15	c6	403	CLA	C4D-ND	-2.96	1.33	1.37
15	b6	404	CLA	CHC-C1C	2.95	1.42	1.35
15	bA	817	CLA	CMB-C2B	-2.95	1.45	1.51
15	b6	403	CLA	C4D-ND	-2.95	1.33	1.37
15	c3	416	CLA	MG-ND	-2.95	1.99	2.05
15	b6	405	CLA	CHC-C1C	2.95	1.42	1.35
15	cB	837	CLA	CHC-C1C	2.95	1.42	1.35
15	bB	833	CLA	CMB-C2B	-2.95	1.45	1.51
15	bA	809	CLA	C1D-ND	2.95	1.41	1.37
15	bB	838	CLA	CMB-C2B	-2.95	1.45	1.51
18	b2	401	BCR	C1-C6	-2.95	1.49	1.53
15	cB	828	CLA	CMB-C2B	-2.95	1.45	1.51
15	c4	410	CLA	C4D-ND	-2.95	1.33	1.37
15	b6	417	CLA	MG-ND	-2.95	1.99	2.05
15	cB	803	CLA	MG-ND	-2.95	1.99	2.05
15	cB	838	CLA	CMB-C2B	-2.95	1.45	1.51
15	aB	837	CLA	CHC-C1C	2.95	1.42	1.35
15	b3	411	CLA	CHC-C1C	2.95	1.42	1.35
15	a2	412	CLA	CHC-C1C	2.95	1.42	1.35
18	bI	101	BCR	C30-C25	-2.95	1.49	1.53
15	a3	421	CLA	C1D-ND	2.95	1.41	1.37
15	c1	416	CLA	CMB-C2B	-2.95	1.45	1.51
15	c2	412	CLA	CHC-C1C	2.95	1.42	1.35
18	a2	421	BCR	C1-C6	-2.94	1.49	1.53
15	c5	411	CLA	CMB-C2B	-2.94	1.45	1.51
15	aA	802	CLA	MG-ND	-2.94	2.00	2.05
15	a6	405	CLA	CHC-C1C	2.94	1.42	1.35
15	b1	416	CLA	CMB-C2B	-2.94	1.45	1.51
18	c2	420	BCR	C1-C6	-2.94	1.49	1.53
15	b4	408	CLA	C1D-ND	2.94	1.41	1.37
15	b2	417	CLA	CMD-C2D	-2.94	1.44	1.50
15	b4	416	CLA	CMB-C2B	-2.94	1.45	1.51
15	aA	809	CLA	C1D-ND	2.94	1.41	1.37
15	cB	815	CLA	C4D-ND	-2.94	1.33	1.37
15	c4	416	CLA	CMB-C2B	-2.94	1.45	1.51
15	aB	803	CLA	MG-ND	-2.94	2.00	2.05
15	c2	404	CLA	CHC-C1C	2.94	1.42	1.35
15	b5	420	CLA	C4D-ND	-2.94	1.33	1.37
15	bB	803	CLA	MG-ND	-2.94	2.00	2.05
15	b5	403	CLA	CHC-C1C	2.94	1.42	1.35
18	a1	419	BCR	C30-C25	-2.94	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	805	CLA	C1D-ND	2.93	1.41	1.37
15	c3	403	CLA	CHC-C1C	2.93	1.42	1.35
15	cB	807	CLA	CMD-C2D	-2.93	1.44	1.50
15	b3	416	CLA	MG-ND	-2.93	2.00	2.05
15	c6	403	CLA	CHC-C1C	2.93	1.42	1.35
15	cA	802	CLA	MG-ND	-2.93	2.00	2.05
15	a3	416	CLA	CMB-C2B	-2.93	1.45	1.51
15	bB	836	CLA	C3B-C2B	-2.93	1.36	1.40
15	cB	836	CLA	C3B-C2B	-2.93	1.36	1.40
15	a3	411	CLA	CHC-C1C	2.93	1.42	1.35
15	a2	416	CLA	CMB-C2B	-2.93	1.45	1.51
15	c6	411	CLA	CHC-C1C	2.93	1.42	1.35
15	a4	403	CLA	CHC-C1C	2.93	1.42	1.35
15	aB	824	CLA	CHC-C1C	2.93	1.42	1.35
15	c2	405	CLA	C4D-ND	-2.93	1.33	1.37
15	bB	839	CLA	C1D-ND	2.93	1.41	1.37
15	c2	416	CLA	CMB-C2B	-2.93	1.45	1.51
15	c3	416	CLA	CMB-C2B	-2.93	1.45	1.51
15	bB	807	CLA	CMD-C2D	-2.93	1.44	1.50
15	c5	415	CLA	CMD-C2D	-2.93	1.44	1.50
15	aB	833	CLA	CMB-C2B	-2.93	1.45	1.51
15	aB	828	CLA	CMB-C2B	-2.93	1.45	1.51
15	a4	416	CLA	CMB-C2B	-2.93	1.45	1.51
15	cB	824	CLA	CHC-C1C	2.92	1.42	1.35
15	a5	403	CLA	C1D-ND	2.92	1.41	1.37
15	c3	404	CLA	CHC-C1C	2.92	1.42	1.35
15	c5	403	CLA	CHC-C1C	2.92	1.42	1.35
18	c1	420	BCR	C30-C25	-2.92	1.49	1.53
15	bA	802	CLA	MG-ND	-2.92	2.00	2.05
15	a2	404	CLA	CHC-C1C	2.92	1.42	1.35
15	aA	834	CLA	MG-ND	-2.92	2.00	2.05
15	aA	842	CLA	CHC-C1C	2.92	1.42	1.35
15	bA	817	CLA	CHC-C1C	2.92	1.42	1.35
15	c4	403	CLA	CHC-C1C	2.92	1.42	1.35
15	aB	838	CLA	CMB-C2B	-2.92	1.45	1.51
15	c3	403	CLA	C1D-ND	2.92	1.41	1.37
15	bB	835	CLA	CMB-C2B	-2.92	1.45	1.51
15	a1	414	CLA	CMB-C2B	-2.91	1.45	1.51
15	cA	817	CLA	CMB-C2B	-2.91	1.45	1.51
15	a2	405	CLA	C4D-ND	-2.91	1.33	1.37
15	b5	414	CLA	C4D-ND	-2.91	1.33	1.37
15	b6	415	CLA	C4D-ND	-2.91	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b1	404	CLA	CHC-C1C	2.91	1.42	1.35
15	b2	416	CLA	CMB-C2B	-2.91	1.45	1.51
18	bB	847	BCR	C30-C25	-2.91	1.49	1.53
15	b4	411	CLA	CMB-C2B	-2.91	1.45	1.51
15	b3	421	CLA	MG-ND	-2.91	2.00	2.05
18	cB	847	BCR	C30-C25	-2.91	1.49	1.53
15	aB	835	CLA	CMB-C2B	-2.91	1.45	1.51
15	c6	405	CLA	CHC-C1C	2.91	1.42	1.35
15	c5	414	CLA	C4D-ND	-2.91	1.33	1.37
15	aA	817	CLA	CHC-C1C	2.91	1.42	1.35
15	bA	842	CLA	CHC-C1C	2.91	1.42	1.35
15	b3	404	CLA	CHC-C1C	2.91	1.42	1.35
18	bL	201	BCR	C1-C6	-2.91	1.49	1.53
15	b6	406	CLA	CHC-C1C	2.91	1.42	1.35
15	a6	417	CLA	CMB-C2B	-2.91	1.45	1.51
15	b6	403	CLA	CHC-C1C	2.91	1.42	1.35
18	cI	101	BCR	C30-C25	-2.91	1.49	1.53
18	b4	418	BCR	C40-C30	-2.91	1.48	1.53
15	aA	817	CLA	CMB-C2B	-2.91	1.45	1.51
15	bB	823	CLA	CHC-C1C	2.91	1.42	1.35
15	b5	411	CLA	CHC-C1C	2.91	1.42	1.35
18	a4	418	BCR	C40-C30	-2.91	1.48	1.53
15	cA	812	CLA	C1D-ND	2.91	1.41	1.37
15	c1	404	CLA	CHC-C1C	2.91	1.42	1.35
15	a6	412	CLA	CHC-C1C	2.91	1.42	1.35
15	c4	415	CLA	CMD-C2D	-2.91	1.44	1.50
18	b2	421	BCR	C1-C6	-2.91	1.49	1.53
15	a2	422	CLA	C1D-ND	2.91	1.41	1.37
18	a2	421	BCR	C30-C25	-2.91	1.49	1.53
15	c2	407	CLA	CHC-C1C	2.91	1.42	1.35
15	cF	201	CLA	CHC-C1C	2.91	1.42	1.35
15	cB	802	CLA	CMB-C2B	-2.91	1.45	1.51
15	b6	422	CLA	C4D-ND	-2.91	1.33	1.37
15	bB	828	CLA	CMD-C2D	-2.90	1.44	1.50
15	cA	836	CLA	C1D-ND	2.90	1.41	1.37
15	bB	824	CLA	CHC-C1C	2.90	1.42	1.35
15	a3	416	CLA	MG-ND	-2.90	2.00	2.05
15	aB	836	CLA	C3B-C2B	-2.90	1.36	1.40
15	a1	402	CLA	CHC-C1C	2.90	1.42	1.35
15	c2	412	CLA	CMB-C2B	-2.90	1.45	1.51
15	bA	807	CLA	MG-ND	-2.90	2.00	2.05
15	bB	805	CLA	CHC-C1C	2.90	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	405	CLA	C4D-ND	-2.90	1.33	1.37
15	bA	828	CLA	CMB-C2B	-2.90	1.45	1.51
15	bB	827	CLA	CMB-C2B	-2.90	1.45	1.51
15	c1	415	CLA	CMB-C2B	-2.90	1.45	1.51
15	c3	421	CLA	MG-ND	-2.90	2.00	2.05
15	aB	805	CLA	CHC-C1C	2.90	1.42	1.35
15	b5	410	CLA	C4D-ND	-2.90	1.33	1.37
15	bA	812	CLA	C1D-ND	2.90	1.41	1.37
15	a4	414	CLA	CHC-C1C	2.90	1.42	1.35
15	b4	403	CLA	CHC-C1C	2.90	1.42	1.35
15	bL	204	CLA	C1D-ND	2.90	1.41	1.37
15	aX	102	CLA	CMB-C2B	-2.90	1.45	1.51
15	b1	415	CLA	CMB-C2B	-2.90	1.45	1.51
15	bA	804	CLA	CHC-C1C	2.90	1.42	1.35
15	c1	403	CLA	CHC-C1C	2.90	1.42	1.35
18	b6	402	BCR	C33-C5	-2.90	1.46	1.50
15	b2	407	CLA	CHC-C1C	2.90	1.42	1.35
15	a6	406	CLA	CHC-C1C	2.90	1.42	1.35
15	b5	402	CLA	CHC-C1C	2.90	1.42	1.35
15	cB	835	CLA	CMB-C2B	-2.90	1.45	1.51
15	cB	805	CLA	C1D-ND	2.90	1.41	1.37
15	a5	404	CLA	CHC-C1C	2.90	1.42	1.35
15	b1	413	CLA	C1D-ND	2.90	1.41	1.37
15	c4	408	CLA	C1D-ND	2.90	1.41	1.37
15	cA	828	CLA	CMB-C2B	-2.90	1.45	1.51
15	b4	416	CLA	CMD-C2D	-2.90	1.44	1.50
15	a5	402	CLA	CHC-C1C	2.89	1.42	1.35
15	a6	422	CLA	CHC-C1C	2.89	1.42	1.35
15	c6	409	CLA	CHC-C1C	2.89	1.42	1.35
15	cA	811	CLA	CHC-C1C	2.89	1.42	1.35
15	cA	817	CLA	CHC-C1C	2.89	1.42	1.35
15	aB	839	CLA	C1D-ND	2.89	1.41	1.37
15	c5	402	CLA	CHC-C1C	2.89	1.42	1.35
15	cA	821	CLA	C1D-ND	2.89	1.41	1.37
15	b3	415	CLA	CMB-C2B	-2.89	1.45	1.51
15	a2	402	CLA	CHC-C1C	2.89	1.42	1.35
15	a3	404	CLA	CHC-C1C	2.89	1.42	1.35
15	c6	406	CLA	CHC-C1C	2.89	1.42	1.35
15	c6	417	CLA	CMB-C2B	-2.89	1.45	1.51
18	bL	206	BCR	C1-C6	-2.89	1.49	1.53
15	bA	838	CLA	CMB-C2B	-2.89	1.45	1.51
15	bA	806	CLA	CMB-C2B	-2.89	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	416	CLA	CMB-C2B	-2.89	1.45	1.51
18	c2	421	BCR	C30-C25	-2.89	1.49	1.53
15	a5	416	CLA	CMD-C2D	-2.89	1.44	1.50
15	cA	806	CLA	CMB-C2B	-2.89	1.45	1.51
15	a5	415	CLA	CMD-C2D	-2.89	1.44	1.50
15	cB	828	CLA	CMD-C2D	-2.89	1.44	1.50
18	c6	401	BCR	C1-C6	-2.89	1.49	1.53
15	aB	812	CLA	C1D-ND	2.89	1.41	1.37
15	b5	416	CLA	CMD-C2D	-2.89	1.44	1.50
15	b6	417	CLA	CMB-C2B	-2.89	1.45	1.51
18	b1	420	BCR	C30-C25	-2.89	1.49	1.53
15	cB	805	CLA	CHC-C1C	2.89	1.42	1.35
15	aB	802	CLA	CMB-C2B	-2.89	1.45	1.51
15	b5	404	CLA	CHC-C1C	2.89	1.42	1.35
15	aA	806	CLA	CMB-C2B	-2.89	1.45	1.51
15	a3	410	CLA	CMB-C2B	-2.89	1.45	1.51
15	a2	405	CLA	CHC-C1C	2.89	1.42	1.35
15	c5	404	CLA	CHC-C1C	2.88	1.42	1.35
15	b3	408	CLA	C1D-ND	2.88	1.41	1.37
15	b2	417	CLA	CMB-C2B	-2.88	1.45	1.51
15	b3	403	CLA	CHC-C1C	2.88	1.42	1.35
15	cL	203	CLA	C1D-ND	2.88	1.41	1.37
15	aB	823	CLA	CHC-C1C	2.88	1.42	1.35
15	aA	813	CLA	CMB-C2B	-2.88	1.45	1.51
15	bX	102	CLA	CMB-C2B	-2.88	1.45	1.51
15	aA	807	CLA	CMD-C2D	-2.88	1.44	1.50
18	b3	420	BCR	C30-C25	-2.88	1.49	1.53
15	aA	828	CLA	CMB-C2B	-2.88	1.45	1.51
15	c2	422	CLA	C1D-ND	2.88	1.41	1.37
15	a2	407	CLA	CHC-C1C	2.88	1.42	1.35
15	b6	412	CLA	CHC-C1C	2.88	1.42	1.35
15	a2	412	CLA	CMB-C2B	-2.88	1.45	1.51
15	bA	821	CLA	C1D-ND	2.88	1.41	1.37
15	c2	415	CLA	CHC-C1C	2.88	1.42	1.35
15	a3	408	CLA	C1D-ND	2.88	1.41	1.37
15	a6	403	CLA	CHC-C1C	2.88	1.42	1.35
15	c5	411	CLA	CHC-C1C	2.88	1.42	1.35
15	a4	415	CLA	CMD-C2D	-2.88	1.44	1.50
15	aA	804	CLA	CHC-C1C	2.88	1.42	1.35
15	aA	811	CLA	CHC-C1C	2.88	1.42	1.35
15	b2	422	CLA	MG-ND	-2.88	2.00	2.05
15	cA	807	CLA	MG-ND	-2.88	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c5	419	BCR	C30-C25	-2.88	1.49	1.53
15	bB	802	CLA	CMB-C2B	-2.88	1.45	1.51
15	cA	834	CLA	CMB-C2B	-2.88	1.45	1.51
15	c5	416	CLA	CMD-C2D	-2.88	1.44	1.50
15	a4	408	CLA	C1D-ND	2.88	1.41	1.37
15	cA	809	CLA	CMB-C2B	-2.88	1.45	1.51
15	cB	827	CLA	CMB-C2B	-2.88	1.45	1.51
15	cA	804	CLA	CHC-C1C	2.87	1.42	1.35
15	b4	414	CLA	CHC-C1C	2.87	1.42	1.35
15	a1	409	CLA	C4D-ND	-2.87	1.33	1.37
15	aA	838	CLA	CMB-C2B	-2.87	1.45	1.51
15	b5	415	CLA	CMD-C2D	-2.87	1.44	1.50
15	c2	402	CLA	CHC-C1C	2.87	1.42	1.35
15	a4	421	CLA	C4D-ND	-2.87	1.33	1.37
15	b3	402	CLA	CHC-C1C	2.87	1.42	1.35
15	b1	410	CLA	CHC-C1C	2.87	1.42	1.35
15	cB	804	CLA	CHC-C1C	2.87	1.42	1.35
15	cB	823	CLA	CHC-C1C	2.87	1.42	1.35
15	c6	416	CLA	CMB-C2B	-2.87	1.45	1.51
15	a1	403	CLA	CHC-C1C	2.87	1.42	1.35
15	aB	834	CLA	CMB-C2B	-2.87	1.45	1.51
15	bA	834	CLA	CMB-C2B	-2.87	1.45	1.51
15	b4	415	CLA	CMD-C2D	-2.87	1.44	1.50
15	cA	804	CLA	CMB-C2B	-2.87	1.45	1.51
15	c3	410	CLA	CMB-C2B	-2.87	1.45	1.51
15	c4	411	CLA	CMB-C2B	-2.87	1.45	1.51
15	bB	804	CLA	CHC-C1C	2.87	1.42	1.35
15	b1	403	CLA	CHC-C1C	2.87	1.42	1.35
15	cA	838	CLA	CMB-C2B	-2.87	1.45	1.51
15	aB	803	CLA	CHC-C1C	2.87	1.42	1.35
15	b1	413	CLA	CHC-C1C	2.87	1.42	1.35
15	c2	417	CLA	CMB-C2B	-2.87	1.45	1.51
15	b2	415	CLA	CHC-C1C	2.87	1.42	1.35
15	aA	829	CLA	CHC-C1C	2.87	1.42	1.35
15	bB	821	CLA	CHC-C1C	2.87	1.42	1.35
15	a5	410	CLA	C4D-ND	-2.87	1.33	1.37
15	aB	821	CLA	CHC-C1C	2.87	1.42	1.35
15	c6	412	CLA	CHC-C1C	2.87	1.42	1.35
15	a6	416	CLA	CMB-C2B	-2.87	1.45	1.51
18	a5	419	BCR	C30-C25	-2.87	1.49	1.53
15	b3	410	CLA	CMB-C2B	-2.87	1.45	1.51
15	a5	411	CLA	CHC-C1C	2.87	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	807	CLA	MG-ND	-2.87	2.00	2.05
15	aB	806	CLA	MG-ND	-2.87	2.00	2.05
15	bA	829	CLA	CHC-C1C	2.87	1.42	1.35
15	a2	417	CLA	CMB-C2B	-2.87	1.45	1.51
15	c5	410	CLA	CHC-C1C	2.87	1.42	1.35
15	b2	412	CLA	CMB-C2B	-2.87	1.45	1.51
15	b6	416	CLA	CMB-C2B	-2.87	1.45	1.51
15	a1	405	CLA	CHC-C1C	2.86	1.42	1.35
15	aA	833	CLA	CMB-C2B	-2.86	1.45	1.51
15	a5	414	CLA	C4D-ND	-2.86	1.33	1.37
15	a4	411	CLA	CMB-C2B	-2.86	1.45	1.51
15	a4	421	CLA	CHC-C1C	2.86	1.42	1.35
15	c2	405	CLA	CHC-C1C	2.86	1.42	1.35
15	b2	422	CLA	C1D-ND	2.86	1.41	1.37
15	c1	413	CLA	C1D-ND	2.86	1.41	1.37
15	b5	405	CLA	CHC-C1C	2.86	1.42	1.35
15	a2	415	CLA	CHC-C1C	2.86	1.42	1.35
15	b1	406	CLA	CHC-C1C	2.86	1.42	1.35
15	c3	415	CLA	CMB-C2B	-2.86	1.45	1.51
15	b6	422	CLA	C2A-C1A	2.86	1.58	1.52
15	bA	808	CLA	CMB-C2B	-2.86	1.45	1.51
15	cA	806	CLA	CMC-C2C	-2.86	1.44	1.50
15	a5	410	CLA	CHC-C1C	2.86	1.42	1.35
18	a6	401	BCR	C1-C6	-2.86	1.49	1.53
15	c1	406	CLA	CHC-C1C	2.86	1.42	1.35
15	cJ	102	CLA	C4D-ND	-2.86	1.33	1.37
15	cA	829	CLA	CHC-C1C	2.86	1.42	1.35
15	cB	821	CLA	CHC-C1C	2.86	1.42	1.35
15	cB	817	CLA	CHC-C1C	2.86	1.42	1.35
15	a3	408	CLA	CMD-C2D	-2.86	1.44	1.50
18	aB	845	BCR	C1-C6	-2.86	1.49	1.53
15	b5	403	CLA	C1D-ND	2.86	1.41	1.37
15	bA	813	CLA	CMB-C2B	-2.86	1.45	1.51
15	b4	421	CLA	CHC-C1C	2.86	1.42	1.35
15	aB	827	CLA	CMB-C2B	-2.85	1.45	1.51
15	aJ	203	CLA	C4D-ND	-2.85	1.33	1.37
18	c4	418	BCR	C40-C30	-2.85	1.48	1.53
15	a3	403	CLA	CHC-C1C	2.85	1.42	1.35
15	bB	817	CLA	CHC-C1C	2.85	1.42	1.35
15	b5	410	CLA	CHC-C1C	2.85	1.42	1.35
15	c5	410	CLA	C4D-ND	-2.85	1.33	1.37
15	aA	828	CLA	C3B-C2B	-2.85	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	402	CLA	CHC-C1C	2.85	1.42	1.35
15	bA	820	CLA	MG-ND	-2.85	2.00	2.05
15	c1	410	CLA	C4D-ND	-2.85	1.33	1.37
15	a3	415	CLA	CMB-C2B	-2.85	1.45	1.51
15	bB	812	CLA	C1D-ND	2.85	1.41	1.37
15	cX	102	CLA	CMB-C2B	-2.85	1.45	1.51
15	bB	820	CLA	CHC-C1C	2.85	1.42	1.35
15	cB	842	CLA	C3B-C2B	-2.85	1.36	1.40
15	cA	813	CLA	CMB-C2B	-2.85	1.45	1.51
15	c4	414	CLA	CHC-C1C	2.85	1.42	1.35
15	aA	812	CLA	C1D-ND	2.85	1.41	1.37
15	cA	827	CLA	CHC-C1C	2.85	1.42	1.35
15	cA	808	CLA	CHC-C1C	2.85	1.42	1.35
15	c6	408	CLA	CHC-C1C	2.85	1.42	1.35
15	aB	832	CLA	CMB-C2B	-2.85	1.45	1.51
15	cA	810	CLA	C1D-ND	2.85	1.41	1.37
15	cB	842	CLA	CHC-C1C	2.85	1.42	1.35
15	c3	410	CLA	CHC-C1C	2.85	1.42	1.35
18	cB	845	BCR	C1-C6	-2.85	1.49	1.53
18	c4	420	BCR	C30-C25	-2.85	1.49	1.53
15	aA	827	CLA	CHC-C1C	2.85	1.42	1.35
15	a1	404	CLA	CHC-C1C	2.85	1.42	1.35
15	aA	805	CLA	CHC-C1C	2.84	1.42	1.35
15	b2	405	CLA	CHC-C1C	2.84	1.42	1.35
18	bA	853	BCR	C1-C6	-2.84	1.49	1.53
15	c2	408	CLA	CHC-C1C	2.84	1.42	1.35
15	a5	405	CLA	CHC-C1C	2.84	1.42	1.35
15	a5	408	CLA	CHC-C1C	2.84	1.42	1.35
15	bA	833	CLA	CMB-C2B	-2.84	1.45	1.51
15	cB	838	CLA	CHC-C1C	2.84	1.42	1.35
15	c4	416	CLA	CMD-C2D	-2.84	1.44	1.50
15	a6	409	CLA	CHC-C1C	2.84	1.42	1.35
15	bA	811	CLA	CHC-C1C	2.84	1.42	1.35
18	bB	845	BCR	C1-C6	-2.84	1.49	1.53
18	aA	852	BCR	C1-C6	-2.84	1.49	1.53
18	a3	420	BCR	C30-C25	-2.84	1.49	1.53
15	aB	805	CLA	C1D-ND	2.84	1.41	1.37
15	bB	803	CLA	CMB-C2B	-2.84	1.45	1.51
15	bB	803	CLA	CHC-C1C	2.84	1.42	1.35
15	b1	405	CLA	CHC-C1C	2.84	1.42	1.35
15	aA	808	CLA	CHC-C1C	2.84	1.42	1.35
15	aB	838	CLA	CHC-C1C	2.84	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	820	CLA	CHC-C1C	2.84	1.42	1.35
15	bA	827	CLA	CHC-C1C	2.84	1.42	1.35
15	cA	812	CLA	C3B-C2B	-2.84	1.36	1.40
15	bA	805	CLA	CHC-C1C	2.84	1.42	1.35
15	b5	408	CLA	CHC-C1C	2.84	1.42	1.35
18	b6	401	BCR	C1-C6	-2.84	1.49	1.53
15	aA	804	CLA	CMB-C2B	-2.84	1.45	1.51
15	bB	834	CLA	CMB-C2B	-2.84	1.45	1.51
15	b1	410	CLA	C4D-ND	-2.84	1.33	1.37
15	aA	834	CLA	CMB-C2B	-2.84	1.45	1.51
15	a1	412	CLA	CHC-C1C	2.84	1.42	1.35
15	b6	409	CLA	CHC-C1C	2.84	1.42	1.35
15	aA	812	CLA	C3B-C2B	-2.84	1.36	1.40
15	aB	817	CLA	CHC-C1C	2.83	1.42	1.35
15	aA	806	CLA	CMC-C2C	-2.83	1.44	1.50
15	cB	803	CLA	CHC-C1C	2.83	1.42	1.35
15	c4	421	CLA	CHC-C1C	2.83	1.42	1.35
15	bA	808	CLA	CHC-C1C	2.83	1.42	1.35
15	b3	412	CLA	C3B-C2B	-2.83	1.36	1.40
15	cA	808	CLA	CMB-C2B	-2.83	1.45	1.51
15	b1	414	CLA	C4D-ND	-2.83	1.33	1.37
15	bA	809	CLA	CMB-C2B	-2.83	1.45	1.51
15	aB	828	CLA	CMD-C2D	-2.83	1.44	1.50
15	cB	804	CLA	CMD-C2D	-2.83	1.44	1.50
15	c5	405	CLA	CHC-C1C	2.83	1.42	1.35
15	bB	832	CLA	CMB-C2B	-2.83	1.45	1.51
15	bA	807	CLA	CMD-C2D	-2.83	1.44	1.50
18	c2	419	BCR	C40-C30	-2.83	1.48	1.53
18	b2	421	BCR	C30-C25	-2.83	1.49	1.53
15	cA	805	CLA	CHC-C1C	2.83	1.42	1.35
15	bA	803	CLA	CMC-C2C	-2.83	1.44	1.50
15	cB	834	CLA	CMB-C2B	-2.83	1.45	1.51
15	a2	408	CLA	CHC-C1C	2.83	1.42	1.35
18	c3	420	BCR	C30-C25	-2.83	1.49	1.53
15	b4	410	CLA	CMB-C2B	-2.83	1.45	1.51
15	bA	828	CLA	C3B-C2B	-2.83	1.36	1.40
15	cA	807	CLA	CMD-C2D	-2.83	1.44	1.50
15	aB	804	CLA	CMD-C2D	-2.83	1.44	1.50
15	a3	402	CLA	CHC-C1C	2.83	1.42	1.35
15	c1	410	CLA	CHC-C1C	2.83	1.42	1.35
15	aA	804	CLA	C3B-C2B	-2.83	1.36	1.40
15	bB	806	CLA	MG-ND	-2.83	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	407	CLA	CHC-C1C	2.83	1.42	1.35
18	aF	202	BCR	C30-C25	-2.83	1.49	1.53
15	cA	837	CLA	CHC-C1C	2.83	1.42	1.35
15	cA	833	CLA	CMB-C2B	-2.83	1.45	1.51
18	c6	401	BCR	C34-C9	-2.83	1.45	1.50
15	bA	806	CLA	CMC-C2C	-2.83	1.44	1.50
15	a3	403	CLA	C1D-ND	2.83	1.41	1.37
15	c6	412	CLA	CMB-C2B	-2.83	1.45	1.51
15	aB	842	CLA	CHC-C1C	2.83	1.42	1.35
15	a3	406	CLA	CHC-C1C	2.83	1.42	1.35
15	aB	804	CLA	CHC-C1C	2.83	1.42	1.35
15	aA	811	CLA	C1D-ND	2.82	1.41	1.37
15	a4	416	CLA	CMD-C2D	-2.82	1.44	1.50
15	c1	413	CLA	CHC-C1C	2.82	1.42	1.35
15	a2	422	CLA	MG-ND	-2.82	2.00	2.05
15	bA	830	CLA	CMB-C2B	-2.82	1.45	1.51
15	cA	830	CLA	CMB-C2B	-2.82	1.45	1.51
15	bA	804	CLA	CMB-C2B	-2.82	1.45	1.51
15	bA	825	CLA	CHC-C1C	2.82	1.42	1.35
15	aA	809	CLA	CMB-C2B	-2.82	1.45	1.51
15	bA	836	CLA	C1D-ND	2.82	1.41	1.37
15	bA	811	CLA	CMB-C2B	-2.82	1.45	1.51
15	aA	808	CLA	CMB-C2B	-2.82	1.45	1.51
15	cB	832	CLA	CMB-C2B	-2.82	1.45	1.51
15	aA	822	CLA	C3B-C2B	-2.82	1.36	1.40
18	aA	849	BCR	C1-C6	-2.82	1.49	1.53
18	bF	202	BCR	C30-C25	-2.82	1.49	1.53
15	bA	823	CLA	CHC-C1C	2.82	1.42	1.35
15	c4	413	CLA	CHC-C1C	2.82	1.42	1.35
15	c3	406	CLA	CHC-C1C	2.82	1.42	1.35
15	cB	827	CLA	CMC-C2C	-2.82	1.44	1.50
15	cB	812	CLA	C1D-ND	2.82	1.41	1.37
15	a6	408	CLA	CHC-C1C	2.82	1.42	1.35
15	cB	820	CLA	CHC-C1C	2.82	1.42	1.35
15	bB	804	CLA	CMD-C2D	-2.82	1.44	1.50
15	a1	407	CLA	CHC-C1C	2.82	1.42	1.35
15	b6	408	CLA	CHC-C1C	2.82	1.42	1.35
15	a3	412	CLA	C3B-C2B	-2.82	1.36	1.40
15	b3	406	CLA	CHC-C1C	2.82	1.42	1.35
15	a3	410	CLA	CHC-C1C	2.82	1.42	1.35
15	bB	842	CLA	CHC-C1C	2.82	1.42	1.35
15	aA	837	CLA	CHC-C1C	2.82	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	830	CLA	CMB-C2B	-2.82	1.45	1.51
18	a4	420	BCR	C30-C25	-2.82	1.49	1.53
15	a5	415	CLA	CMB-C2B	-2.82	1.45	1.51
15	cA	811	CLA	CMB-C2B	-2.82	1.45	1.51
18	b6	401	BCR	C34-C9	-2.82	1.45	1.50
15	b6	412	CLA	CMB-C2B	-2.81	1.45	1.51
15	cB	832	CLA	C1D-ND	2.81	1.41	1.37
15	aA	831	CLA	MG-ND	-2.81	2.00	2.05
15	aA	811	CLA	CMB-C2B	-2.81	1.45	1.51
15	c1	405	CLA	CHC-C1C	2.81	1.42	1.35
15	c1	408	CLA	CHC-C1C	2.81	1.42	1.35
18	cA	851	BCR	C1-C6	-2.81	1.49	1.53
15	b1	407	CLA	CHC-C1C	2.81	1.42	1.35
15	a2	411	CLA	CMB-C2B	-2.81	1.45	1.51
15	a4	415	CLA	CMB-C2B	-2.81	1.45	1.51
15	cA	825	CLA	CHC-C1C	2.81	1.42	1.35
15	c1	407	CLA	CHC-C1C	2.81	1.42	1.35
15	c4	406	CLA	CHC-C1C	2.81	1.42	1.35
15	a4	413	CLA	CHC-C1C	2.81	1.42	1.35
15	cA	803	CLA	CMC-C2C	-2.81	1.44	1.50
15	b4	410	CLA	CHC-C1C	2.81	1.42	1.35
15	bA	804	CLA	C3B-C2B	-2.81	1.36	1.40
15	b4	406	CLA	CHC-C1C	2.81	1.42	1.35
15	bB	838	CLA	CHC-C1C	2.81	1.42	1.35
18	bB	844	BCR	C30-C25	-2.81	1.49	1.53
15	aA	820	CLA	MG-ND	-2.81	2.00	2.05
15	b3	403	CLA	C1D-ND	2.81	1.41	1.37
15	cB	803	CLA	CMB-C2B	-2.81	1.45	1.51
15	bB	827	CLA	CMC-C2C	-2.81	1.44	1.50
15	c3	408	CLA	CMD-C2D	-2.81	1.44	1.50
15	cB	802	CLA	C1D-ND	2.81	1.41	1.37
15	b4	421	CLA	C4D-ND	-2.81	1.33	1.37
15	a6	413	CLA	C3B-C2B	-2.81	1.36	1.40
15	a1	409	CLA	CMB-C2B	-2.81	1.45	1.51
18	c1	401	BCR	C34-C9	-2.81	1.45	1.50
18	b5	419	BCR	C30-C25	-2.81	1.49	1.53
15	cA	843	CLA	CHC-C1C	2.81	1.42	1.35
15	bA	837	CLA	CHC-C1C	2.81	1.42	1.35
15	c2	409	CLA	CHC-C1C	2.81	1.42	1.35
15	c2	411	CLA	CHC-C1C	2.81	1.42	1.35
15	bB	842	CLA	CMB-C2B	-2.80	1.45	1.51
15	bJ	102	CLA	C4D-ND	-2.80	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	805	CLA	CMB-C2B	-2.80	1.45	1.51
15	aA	820	CLA	CHC-C1C	2.80	1.42	1.35
15	c5	407	CLA	CHC-C1C	2.80	1.42	1.35
15	c4	410	CLA	CMB-C2B	-2.80	1.45	1.51
15	c4	421	CLA	C4D-ND	-2.80	1.33	1.37
15	cB	817	CLA	MG-ND	-2.80	2.00	2.05
15	aA	830	CLA	CHC-C1C	2.80	1.42	1.35
15	a2	409	CLA	CHC-C1C	2.80	1.42	1.35
15	b6	407	CLA	CHC-C1C	2.80	1.42	1.35
15	c6	416	CLA	CMD-C2D	-2.80	1.44	1.50
15	c5	408	CLA	CHC-C1C	2.80	1.42	1.35
15	aA	823	CLA	CHC-C1C	2.80	1.42	1.35
18	a2	419	BCR	C40-C30	-2.80	1.48	1.53
15	c3	402	CLA	CHC-C1C	2.80	1.42	1.35
15	a1	401	CLA	CHC-C1C	2.80	1.42	1.35
15	a1	409	CLA	CHC-C1C	2.80	1.42	1.35
15	aB	803	CLA	CMB-C2B	-2.80	1.45	1.51
18	bA	850	BCR	C1-C6	-2.80	1.49	1.53
15	aA	819	CLA	CMB-C2B	-2.80	1.45	1.51
15	b1	408	CLA	CHC-C1C	2.80	1.42	1.35
15	a4	410	CLA	CMB-C2B	-2.80	1.45	1.51
15	cA	824	CLA	CHC-C1C	2.80	1.42	1.35
15	bA	810	CLA	C1D-ND	2.80	1.41	1.37
15	c5	415	CLA	CMB-C2B	-2.80	1.45	1.51
15	b2	408	CLA	CHC-C1C	2.80	1.42	1.35
15	aA	836	CLA	C1D-ND	2.80	1.41	1.37
15	c1	415	CLA	CMD-C2D	-2.80	1.44	1.50
18	b4	419	BCR	C1-C6	-2.80	1.49	1.53
15	bA	822	CLA	C3B-C2B	-2.80	1.36	1.40
15	aJ	202	CLA	CMB-C2B	-2.80	1.45	1.51
15	aB	827	CLA	CMC-C2C	-2.80	1.44	1.50
18	cF	204	BCR	C30-C25	-2.79	1.49	1.53
15	b3	408	CLA	CMD-C2D	-2.79	1.44	1.50
15	a4	406	CLA	CHC-C1C	2.79	1.42	1.35
15	bJ	101	CLA	CMB-C2B	-2.79	1.45	1.51
15	cA	816	CLA	CHC-C1C	2.79	1.42	1.35
15	bB	810	CLA	C3B-C2B	-2.79	1.36	1.40
15	c6	413	CLA	C3B-C2B	-2.79	1.36	1.40
18	cA	848	BCR	C1-C6	-2.79	1.49	1.53
15	a5	407	CLA	CHC-C1C	2.79	1.42	1.35
15	cB	822	CLA	CHC-C1C	2.79	1.42	1.35
15	c4	410	CLA	CHC-C1C	2.79	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	831	CLA	MG-ND	-2.79	2.00	2.05
15	bA	824	CLA	CHC-C1C	2.79	1.42	1.35
15	c5	406	CLA	CHC-C1C	2.79	1.42	1.35
15	b4	416	CLA	C4B-CHC	-2.79	1.33	1.41
15	c3	412	CLA	C3B-C2B	-2.79	1.36	1.40
15	aA	825	CLA	CHC-C1C	2.79	1.42	1.35
15	a6	416	CLA	CMD-C2D	-2.79	1.44	1.50
18	a4	419	BCR	C1-C6	-2.79	1.49	1.53
15	a1	412	CLA	C1D-ND	2.79	1.41	1.37
15	aA	803	CLA	CMC-C2C	-2.79	1.44	1.50
15	aB	842	CLA	C3B-C2B	-2.79	1.36	1.40
15	b3	421	CLA	CHC-C1C	2.79	1.42	1.35
15	c6	407	CLA	CHC-C1C	2.79	1.42	1.35
18	a6	401	BCR	C34-C9	-2.79	1.45	1.50
15	b1	410	CLA	CMB-C2B	-2.79	1.45	1.51
15	bA	816	CLA	CHC-C1C	2.79	1.42	1.35
15	aA	816	CLA	CHC-C1C	2.79	1.42	1.35
15	bA	844	CLA	CHC-C1C	2.79	1.42	1.35
15	cA	823	CLA	CHC-C1C	2.79	1.42	1.35
14	cA	801	CL0	C1C-NC	-2.79	1.33	1.37
15	aB	814	CLA	C1D-ND	2.79	1.41	1.37
15	b5	413	CLA	CHC-C1C	2.78	1.42	1.35
15	aA	824	CLA	CHC-C1C	2.78	1.42	1.35
15	b2	411	CLA	CHC-C1C	2.78	1.42	1.35
15	cA	811	CLA	C1D-ND	2.78	1.41	1.37
15	bA	840	CLA	MG-ND	-2.78	2.00	2.05
15	aB	817	CLA	MG-ND	-2.78	2.00	2.05
15	cB	806	CLA	MG-ND	-2.78	2.00	2.05
15	cB	810	CLA	C3B-C2B	-2.78	1.36	1.40
15	aA	814	CLA	CHC-C1C	2.78	1.42	1.35
15	cA	830	CLA	CHC-C1C	2.78	1.42	1.35
15	c1	402	CLA	CHC-C1C	2.78	1.42	1.35
15	aA	840	CLA	MG-ND	-2.78	2.00	2.05
15	cA	840	CLA	MG-ND	-2.78	2.00	2.05
15	a5	412	CLA	C3B-C2B	-2.78	1.36	1.40
15	c4	402	CLA	CHC-C1C	2.78	1.42	1.35
15	c3	416	CLA	C4B-CHC	-2.78	1.33	1.41
15	a1	414	CLA	CMD-C2D	-2.78	1.44	1.50
15	c3	405	CLA	CHC-C1C	2.78	1.42	1.35
14	bA	801	CL0	C1C-NC	-2.78	1.33	1.37
15	aB	802	CLA	CMD-C2D	-2.78	1.44	1.50
15	cA	820	CLA	MG-ND	-2.78	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	407	CLA	CHC-C1C	2.78	1.42	1.35
15	aA	844	CLA	CHC-C1C	2.78	1.42	1.35
15	c5	413	CLA	CHC-C1C	2.78	1.42	1.35
15	aB	832	CLA	C1D-ND	2.78	1.41	1.37
15	b5	415	CLA	CMB-C2B	-2.78	1.45	1.51
15	bB	842	CLA	C3B-C2B	-2.78	1.36	1.40
15	b5	412	CLA	C3B-C2B	-2.78	1.36	1.40
18	bI	102	BCR	C1-C6	-2.78	1.49	1.53
18	c2	401	BCR	C33-C5	-2.78	1.46	1.50
15	a1	406	CLA	CHC-C1C	2.78	1.42	1.35
18	aI	102	BCR	C1-C6	-2.78	1.50	1.53
15	cA	820	CLA	CHC-C1C	2.78	1.42	1.35
15	a2	422	CLA	CHC-C1C	2.78	1.42	1.35
15	cX	102	CLA	CHC-C1C	2.78	1.42	1.35
15	cA	828	CLA	C3B-C2B	-2.77	1.36	1.40
15	cB	831	CLA	CMB-C2B	-2.77	1.45	1.51
15	a6	412	CLA	CMB-C2B	-2.77	1.45	1.51
15	b4	415	CLA	CMB-C2B	-2.77	1.45	1.51
15	c2	422	CLA	MG-ND	-2.77	2.00	2.05
15	c4	416	CLA	C4B-CHC	-2.77	1.33	1.41
15	a3	421	CLA	CHC-C1C	2.77	1.42	1.35
15	c3	415	CLA	CMD-C2D	-2.77	1.44	1.50
15	aB	842	CLA	CMB-C2B	-2.77	1.45	1.51
15	cB	805	CLA	CMB-C2B	-2.77	1.45	1.51
15	a5	413	CLA	CHC-C1C	2.77	1.42	1.35
15	a4	410	CLA	CHC-C1C	2.77	1.42	1.35
15	a5	406	CLA	CHC-C1C	2.77	1.42	1.35
15	a4	402	CLA	CHC-C1C	2.77	1.42	1.35
15	a4	416	CLA	C4B-CHC	-2.77	1.33	1.41
15	cA	819	CLA	CMB-C2B	-2.77	1.45	1.51
15	cJ	102	CLA	CMB-C2B	-2.77	1.45	1.51
15	b1	402	CLA	CHC-C1C	2.77	1.42	1.35
15	b4	413	CLA	CHC-C1C	2.77	1.42	1.35
15	cA	820	CLA	C1D-ND	2.77	1.41	1.37
15	b1	411	CLA	CMB-C2B	-2.77	1.45	1.51
15	b1	415	CLA	CMD-C2D	-2.77	1.44	1.50
15	bA	820	CLA	CHC-C1C	2.77	1.42	1.35
15	cA	804	CLA	C3B-C2B	-2.77	1.36	1.40
15	b2	411	CLA	CMB-C2B	-2.77	1.45	1.51
15	bX	102	CLA	CHC-C1C	2.77	1.42	1.35
15	aJ	203	CLA	CMB-C2B	-2.77	1.45	1.51
15	c1	410	CLA	CMB-C2B	-2.77	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a4	408	CLA	CHC-C1C	2.77	1.42	1.35
15	b6	416	CLA	CMD-C2D	-2.77	1.44	1.50
15	aB	822	CLA	CHC-C1C	2.77	1.42	1.35
18	cI	102	BCR	C1-C6	-2.77	1.50	1.53
15	a5	408	CLA	CMD-C2D	-2.76	1.44	1.50
15	cA	819	CLA	CMC-C2C	-2.76	1.44	1.50
15	aA	820	CLA	C1D-ND	2.76	1.41	1.37
15	aA	832	CLA	CMD-C2D	-2.76	1.44	1.50
15	a2	411	CLA	CHC-C1C	2.76	1.42	1.35
15	bB	805	CLA	CMB-C2B	-2.76	1.45	1.51
15	b3	407	CLA	CHC-C1C	2.76	1.42	1.35
15	c3	421	CLA	CHC-C1C	2.76	1.42	1.35
15	b2	409	CLA	CHC-C1C	2.76	1.42	1.35
15	aA	810	CLA	CHC-C1C	2.76	1.42	1.35
15	cA	822	CLA	C3B-C2B	-2.76	1.36	1.40
15	aA	845	CLA	CMB-C2B	-2.76	1.45	1.51
15	c5	416	CLA	CMB-C2B	-2.76	1.45	1.51
15	bA	831	CLA	MG-ND	-2.76	2.00	2.05
15	c1	414	CLA	C4D-ND	-2.76	1.33	1.37
18	a4	401	BCR	C1-C6	-2.76	1.50	1.53
15	c5	412	CLA	C3B-C2B	-2.76	1.36	1.40
15	b4	408	CLA	CHC-C1C	2.76	1.42	1.35
15	bB	822	CLA	CHC-C1C	2.76	1.42	1.35
15	cB	802	CLA	CMD-C2D	-2.76	1.45	1.50
15	bA	845	CLA	CMB-C2B	-2.76	1.45	1.51
15	b5	406	CLA	CHC-C1C	2.76	1.42	1.35
15	bA	820	CLA	C1D-ND	2.76	1.41	1.37
15	bA	823	CLA	C1D-ND	2.76	1.41	1.37
15	bB	832	CLA	C1D-ND	2.76	1.41	1.37
15	b3	410	CLA	CHC-C1C	2.76	1.42	1.35
18	a6	420	BCR	C30-C25	-2.76	1.50	1.53
15	aA	810	CLA	C1D-ND	2.76	1.41	1.37
15	bA	830	CLA	CHC-C1C	2.76	1.42	1.35
15	bA	819	CLA	CMB-C2B	-2.76	1.45	1.51
15	b4	421	CLA	CMB-C2B	-2.76	1.45	1.51
15	bB	802	CLA	C1D-ND	2.76	1.41	1.37
15	bA	826	CLA	CMB-C2B	-2.76	1.45	1.51
15	a4	412	CLA	C3B-C2B	-2.76	1.36	1.40
15	bB	814	CLA	C1D-ND	2.75	1.41	1.37
15	bA	827	CLA	MG-ND	-2.75	2.00	2.05
18	b4	401	BCR	C1-C6	-2.75	1.50	1.53
15	cA	842	CLA	CMC-C2C	-2.75	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	810	CLA	CHC-C1C	2.75	1.42	1.35
15	b1	416	CLA	C4B-CHC	-2.75	1.33	1.41
15	aB	810	CLA	C3B-C2B	-2.75	1.36	1.40
15	aA	827	CLA	MG-ND	-2.75	2.00	2.05
15	bB	802	CLA	CMD-C2D	-2.75	1.45	1.50
15	a3	405	CLA	CHC-C1C	2.75	1.42	1.35
15	c4	415	CLA	CMB-C2B	-2.75	1.45	1.51
15	b5	408	CLA	CMD-C2D	-2.75	1.45	1.50
15	bB	817	CLA	MG-ND	-2.75	2.00	2.05
15	aL	202	CLA	CHC-C1C	2.75	1.42	1.35
15	c4	405	CLA	CHC-C1C	2.75	1.42	1.35
15	cA	814	CLA	CHC-C1C	2.75	1.42	1.35
15	c4	408	CLA	CHC-C1C	2.75	1.42	1.35
15	a3	416	CLA	C4B-CHC	-2.75	1.33	1.41
15	bB	831	CLA	CMB-C2B	-2.75	1.45	1.51
15	b4	402	CLA	CHC-C1C	2.75	1.42	1.35
18	a2	401	BCR	C33-C5	-2.75	1.46	1.50
18	aB	844	BCR	C30-C25	-2.75	1.50	1.53
15	b3	416	CLA	C4B-CHC	-2.75	1.33	1.41
15	b4	421	CLA	O1D-CGD	2.75	1.28	1.21
15	c3	407	CLA	CHC-C1C	2.75	1.42	1.35
15	a4	405	CLA	CHC-C1C	2.74	1.42	1.35
15	bA	832	CLA	CMD-C2D	-2.74	1.45	1.50
15	bA	812	CLA	C3B-C2B	-2.74	1.36	1.40
15	bB	834	CLA	CMC-C2C	-2.74	1.45	1.50
18	c4	401	BCR	C30-C25	-2.74	1.50	1.53
15	aB	830	CLA	MG-ND	-2.74	2.00	2.05
15	cJ	101	CLA	CMB-C2B	-2.74	1.45	1.51
15	c1	411	CLA	CMB-C2B	-2.74	1.45	1.51
15	bA	819	CLA	CMC-C2C	-2.74	1.45	1.50
15	aA	835	CLA	CHC-C1C	2.74	1.42	1.35
15	cB	842	CLA	CMB-C2B	-2.74	1.45	1.51
15	c2	411	CLA	CMB-C2B	-2.74	1.45	1.51
15	bA	818	CLA	CHC-C1C	2.74	1.42	1.35
15	a1	410	CLA	CMB-C2B	-2.74	1.45	1.51
15	c6	411	CLA	CMB-C2B	-2.74	1.45	1.51
15	cA	819	CLA	CHC-C1C	2.74	1.42	1.35
15	bL	203	CLA	CHC-C1C	2.74	1.42	1.35
14	aA	801	CL0	OBD-CAD	2.74	1.27	1.22
15	cB	821	CLA	CMB-C2B	-2.74	1.45	1.51
15	b5	416	CLA	C4B-CHC	-2.74	1.33	1.41
15	a5	408	CLA	CMB-C2B	-2.74	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	422	CLA	CHC-C1C	2.74	1.42	1.35
15	aB	809	CLA	CMD-C2D	-2.74	1.45	1.50
15	aA	826	CLA	CMB-C2B	-2.73	1.46	1.51
15	aB	807	CLA	CMB-C2B	-2.73	1.46	1.51
15	a5	416	CLA	C4B-CHC	-2.73	1.33	1.41
15	a4	407	CLA	CHC-C1C	2.73	1.42	1.35
15	cL	202	CLA	CHC-C1C	2.73	1.42	1.35
15	bA	843	CLA	CMC-C2C	-2.73	1.45	1.50
15	bA	810	CLA	CHC-C1C	2.73	1.42	1.35
15	cA	810	CLA	CMD-C2D	-2.73	1.45	1.50
15	bA	813	CLA	CHC-C1C	2.73	1.42	1.35
15	c5	416	CLA	C4B-CHC	-2.73	1.33	1.41
15	a1	415	CLA	C4B-CHC	-2.73	1.33	1.41
15	aA	843	CLA	CMC-C2C	-2.73	1.45	1.50
15	c4	421	CLA	O1D-CGD	2.73	1.28	1.21
15	aA	824	CLA	CMB-C2B	-2.73	1.46	1.51
15	cA	826	CLA	CMB-C2B	-2.73	1.46	1.51
15	aA	819	CLA	CMC-C2C	-2.73	1.45	1.50
15	aB	837	CLA	CMB-C2B	-2.73	1.46	1.51
15	a2	422	CLA	CMB-C2B	-2.73	1.46	1.51
15	aA	818	CLA	CHC-C1C	2.73	1.42	1.35
15	bB	818	CLA	CHC-C1C	2.73	1.42	1.35
15	aX	102	CLA	CHC-C1C	2.73	1.42	1.35
15	a6	407	CLA	CMB-C2B	-2.73	1.46	1.51
15	a6	411	CLA	CMB-C2B	-2.73	1.46	1.51
15	c5	410	CLA	CMB-C2B	-2.73	1.46	1.51
18	a1	417	BCR	C40-C30	-2.73	1.48	1.53
15	c5	408	CLA	CMD-C2D	-2.73	1.45	1.50
15	aA	838	CLA	MG-ND	-2.73	2.00	2.05
15	aB	831	CLA	CMB-C2B	-2.73	1.46	1.51
15	a1	413	CLA	C4D-ND	-2.73	1.33	1.37
15	aA	813	CLA	CHC-C1C	2.73	1.42	1.35
14	aA	801	CL0	C1C-NC	-2.73	1.33	1.37
15	a2	417	CLA	C1C-NC	-2.73	1.33	1.37
15	cB	837	CLA	CMB-C2B	-2.73	1.46	1.51
15	bA	814	CLA	CHC-C1C	2.73	1.42	1.35
15	bA	811	CLA	C1D-ND	2.73	1.41	1.37
15	aL	203	CLA	CHC-C1C	2.73	1.42	1.35
15	a3	408	CLA	CHC-C1C	2.73	1.42	1.35
15	aB	815	CLA	CMB-C2B	-2.73	1.46	1.51
15	aA	818	CLA	C1D-ND	2.73	1.41	1.37
15	aB	802	CLA	C1D-ND	2.73	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	844	CLA	CMB-C2B	-2.73	1.46	1.51
15	bA	810	CLA	CMD-C2D	-2.73	1.45	1.50
18	c4	401	BCR	C1-C6	-2.73	1.50	1.53
15	b5	416	CLA	CMB-C2B	-2.72	1.46	1.51
18	a6	401	BCR	C30-C25	-2.72	1.50	1.53
18	c4	419	BCR	C1-C6	-2.72	1.50	1.53
15	a4	421	CLA	O1D-CGD	2.72	1.28	1.21
15	aA	810	CLA	CMD-C2D	-2.72	1.45	1.50
18	b4	420	BCR	C30-C25	-2.72	1.50	1.53
15	bK	101	CLA	CHC-C1C	2.72	1.41	1.35
15	bL	204	CLA	CHC-C1C	2.72	1.41	1.35
15	b6	411	CLA	CMB-C2B	-2.72	1.46	1.51
15	b3	406	CLA	CMB-C2B	-2.72	1.46	1.51
18	cB	844	BCR	C30-C25	-2.72	1.50	1.53
15	aX	102	CLA	MG-ND	-2.72	2.00	2.05
15	cA	827	CLA	MG-ND	-2.72	2.00	2.05
15	aA	825	CLA	CMB-C2B	-2.72	1.46	1.51
15	c4	407	CLA	CHC-C1C	2.72	1.41	1.35
18	b2	401	BCR	C33-C5	-2.72	1.46	1.50
15	b6	413	CLA	C3B-C2B	-2.72	1.36	1.40
15	b6	409	CLA	CMD-C2D	-2.72	1.45	1.50
15	bB	815	CLA	CMB-C2B	-2.72	1.46	1.51
15	bJ	102	CLA	CMB-C2B	-2.72	1.46	1.51
15	aL	203	CLA	C3B-C2B	-2.72	1.36	1.40
15	bA	835	CLA	CHC-C1C	2.72	1.41	1.35
15	a3	407	CLA	CHC-C1C	2.72	1.41	1.35
15	bA	803	CLA	CMD-C2D	-2.72	1.45	1.50
15	b5	410	CLA	CMB-C2B	-2.72	1.46	1.51
15	cA	803	CLA	CMD-C2D	-2.72	1.45	1.50
15	a3	415	CLA	CMD-C2D	-2.72	1.45	1.50
15	b3	405	CLA	CHC-C1C	2.72	1.41	1.35
15	cB	834	CLA	CMC-C2C	-2.71	1.45	1.50
15	bA	802	CLA	CHC-C1C	2.71	1.41	1.35
15	cA	818	CLA	CHC-C1C	2.71	1.41	1.35
15	cB	835	CLA	C1D-ND	2.71	1.41	1.37
15	cA	827	CLA	CMB-C2B	-2.71	1.46	1.51
15	cB	809	CLA	CMD-C2D	-2.71	1.45	1.50
15	bB	835	CLA	CHC-C1C	2.71	1.41	1.35
15	a5	410	CLA	CMB-C2B	-2.71	1.46	1.51
15	a5	416	CLA	CMB-C2B	-2.71	1.46	1.51
15	cB	814	CLA	C1D-ND	2.71	1.41	1.37
15	bA	825	CLA	CMB-C2B	-2.71	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	408	CLA	CMB-C2B	-2.71	1.46	1.51
15	bL	202	CLA	CHC-C1C	2.71	1.41	1.35
15	c1	416	CLA	C4B-CHC	-2.71	1.33	1.41
15	bA	824	CLA	CMB-C2B	-2.71	1.46	1.51
15	bB	821	CLA	CMB-C2B	-2.71	1.46	1.51
18	b2	419	BCR	C40-C30	-2.71	1.48	1.53
15	cB	825	CLA	CMD-C2D	-2.71	1.45	1.50
15	b3	415	CLA	CMD-C2D	-2.71	1.45	1.50
15	aA	839	CLA	C3B-CAB	-2.71	1.42	1.47
15	aB	810	CLA	CMD-C2D	-2.71	1.45	1.50
15	a2	405	CLA	C1D-C2D	2.71	1.50	1.45
15	bA	812	CLA	CMC-C2C	-2.71	1.45	1.50
15	cA	832	CLA	CMD-C2D	-2.71	1.45	1.50
15	aB	835	CLA	CHC-C1C	2.71	1.41	1.35
15	aA	823	CLA	C1D-ND	2.71	1.41	1.37
15	bB	835	CLA	C1D-ND	2.71	1.41	1.37
15	bB	809	CLA	CMD-C2D	-2.71	1.45	1.50
15	cB	816	CLA	CHC-C1C	2.71	1.41	1.35
15	bA	839	CLA	C3B-CAB	-2.71	1.42	1.47
18	b1	418	BCR	C40-C30	-2.71	1.48	1.53
15	b6	407	CLA	CMB-C2B	-2.71	1.46	1.51
15	a4	421	CLA	CMB-C2B	-2.71	1.46	1.51
15	cB	807	CLA	CMB-C2B	-2.71	1.46	1.51
15	c2	417	CLA	C1C-NC	-2.71	1.33	1.37
15	cK	102	CLA	CHC-C1C	2.70	1.41	1.35
15	bA	827	CLA	CMB-C2B	-2.70	1.46	1.51
15	a2	417	CLA	C4B-CHC	-2.70	1.33	1.41
15	aK	102	CLA	CHC-C1C	2.70	1.41	1.35
15	aB	804	CLA	CMB-C2B	-2.70	1.46	1.51
15	bA	838	CLA	MG-ND	-2.70	2.00	2.05
15	c5	408	CLA	CMB-C2B	-2.70	1.46	1.51
18	c3	418	BCR	C33-C5	-2.70	1.46	1.50
15	cA	823	CLA	C1D-ND	2.70	1.41	1.37
15	b4	406	CLA	CMB-C2B	-2.70	1.46	1.51
15	bA	812	CLA	CHC-C1C	2.70	1.41	1.35
15	bB	807	CLA	CAA-C2A	-2.70	1.49	1.54
15	aB	826	CLA	CMB-C2B	-2.70	1.46	1.51
15	bA	812	CLA	CMB-C2B	-2.70	1.46	1.51
15	cB	815	CLA	CMB-C2B	-2.70	1.46	1.51
15	cA	838	CLA	MG-ND	-2.70	2.00	2.05
15	b2	417	CLA	C4B-CHC	-2.70	1.33	1.41
15	c4	421	CLA	CMB-C2B	-2.70	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	405	CLA	C1D-C2D	2.70	1.50	1.45
15	bX	102	CLA	MG-ND	-2.70	2.00	2.05
15	bB	825	CLA	CMD-C2D	-2.70	1.45	1.50
15	cB	810	CLA	CMD-C2D	-2.70	1.45	1.50
15	bB	837	CLA	CMB-C2B	-2.70	1.46	1.51
15	cA	835	CLA	CHC-C1C	2.70	1.41	1.35
15	aA	803	CLA	CMD-C2D	-2.70	1.45	1.50
15	bB	837	CLA	C1D-ND	2.70	1.41	1.37
15	cA	841	CLA	CMB-C2B	-2.70	1.46	1.51
15	a6	422	CLA	MG-ND	-2.70	2.00	2.05
15	aB	825	CLA	MG-ND	-2.70	2.00	2.05
14	cA	801	CL0	OBD-CAD	2.70	1.27	1.22
15	a6	409	CLA	CMD-C2D	-2.70	1.45	1.50
15	aB	821	CLA	C1D-ND	2.70	1.41	1.37
15	cB	807	CLA	CAA-C2A	-2.70	1.49	1.54
15	aL	201	CLA	CHC-C1C	2.70	1.41	1.35
15	c2	422	CLA	CHC-C1C	2.70	1.41	1.35
15	a6	406	CLA	CMB-C2B	-2.70	1.46	1.51
15	cA	842	CLA	CMD-C2D	-2.70	1.45	1.50
15	aB	821	CLA	CMB-C2B	-2.70	1.46	1.51
15	bA	843	CLA	CMD-C2D	-2.70	1.45	1.50
15	c4	406	CLA	CMB-C2B	-2.70	1.46	1.51
15	c6	406	CLA	CMB-C2B	-2.70	1.46	1.51
15	aB	835	CLA	C1D-ND	2.70	1.41	1.37
15	bA	840	CLA	C1D-ND	2.69	1.41	1.37
15	cA	840	CLA	C1D-ND	2.69	1.41	1.37
15	cA	812	CLA	CMB-C2B	-2.69	1.46	1.51
15	cA	821	CLA	CMB-C2B	-2.69	1.46	1.51
15	bB	807	CLA	CMB-C2B	-2.69	1.46	1.51
15	aB	834	CLA	CMC-C2C	-2.69	1.45	1.50
15	bA	829	CLA	CMD-C2D	-2.69	1.45	1.50
15	cL	203	CLA	CHC-C1C	2.69	1.41	1.35
15	b4	405	CLA	CHC-C1C	2.69	1.41	1.35
15	cB	818	CLA	CHC-C1C	2.69	1.41	1.35
15	c3	408	CLA	CHC-C1C	2.69	1.41	1.35
15	c2	417	CLA	C4B-CHC	-2.69	1.33	1.41
15	bB	830	CLA	MG-ND	-2.69	2.00	2.05
15	cB	820	CLA	C1D-ND	2.69	1.41	1.37
15	aB	840	CLA	CMD-C2D	-2.69	1.45	1.50
15	cA	839	CLA	CHC-C1C	2.69	1.41	1.35
15	cA	824	CLA	CMB-C2B	-2.69	1.46	1.51
15	cB	830	CLA	MG-ND	-2.69	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cX	102	CLA	MG-ND	-2.69	2.00	2.05
15	b3	408	CLA	CHC-C1C	2.69	1.41	1.35
15	cA	813	CLA	CHC-C1C	2.69	1.41	1.35
18	b4	401	BCR	C30-C25	-2.69	1.50	1.53
15	aB	828	CLA	C3B-C2B	-2.69	1.36	1.40
15	b4	421	CLA	MG-ND	-2.69	2.00	2.05
15	cA	830	CLA	MG-ND	-2.69	2.00	2.05
15	aA	841	CLA	CMB-C2B	-2.69	1.46	1.51
15	aA	829	CLA	CMD-C2D	-2.69	1.45	1.50
15	b2	413	CLA	C3B-C2B	-2.69	1.36	1.40
15	bA	839	CLA	CHC-C1C	2.69	1.41	1.35
15	cL	201	CLA	CHC-C1C	2.69	1.41	1.35
15	bA	830	CLA	MG-ND	-2.69	2.00	2.05
15	aA	812	CLA	CMB-C2B	-2.69	1.46	1.51
15	aB	829	CLA	CHC-C1C	2.69	1.41	1.35
18	c3	419	BCR	C1-C6	-2.69	1.50	1.53
15	cB	826	CLA	CMB-C2B	-2.69	1.46	1.51
15	aA	839	CLA	C1D-ND	2.69	1.41	1.37
15	bB	827	CLA	C1D-ND	2.69	1.41	1.37
15	bL	204	CLA	C3B-C2B	-2.69	1.36	1.40
15	bB	806	CLA	CMB-C2B	-2.69	1.46	1.51
15	cB	835	CLA	CHC-C1C	2.69	1.41	1.35
15	bA	819	CLA	CHC-C1C	2.69	1.41	1.35
18	b3	419	BCR	C1-C6	-2.69	1.50	1.53
18	c6	420	BCR	C30-C25	-2.69	1.50	1.53
15	aA	833	CLA	CHC-C1C	2.69	1.41	1.35
15	cA	833	CLA	CHC-C1C	2.69	1.41	1.35
15	cB	837	CLA	C1D-ND	2.69	1.41	1.37
15	aB	807	CLA	CAA-C2A	-2.69	1.49	1.54
15	aB	817	CLA	C3B-CAB	-2.69	1.42	1.47
15	cA	839	CLA	C3B-CAB	-2.69	1.42	1.47
15	a3	406	CLA	CMB-C2B	-2.69	1.46	1.51
15	bA	841	CLA	CMB-C2B	-2.69	1.46	1.51
15	bB	828	CLA	MG-ND	-2.69	2.00	2.05
15	cA	813	CLA	MG-ND	-2.69	2.00	2.05
15	a2	409	CLA	CMD-C2D	-2.69	1.45	1.50
15	c6	414	CLA	CHC-C1C	2.69	1.41	1.35
15	bB	816	CLA	CHC-C1C	2.68	1.41	1.35
15	aA	827	CLA	CMB-C2B	-2.68	1.46	1.51
15	bB	817	CLA	C3B-CAB	-2.68	1.42	1.47
15	a4	404	CLA	CMB-C2B	-2.68	1.46	1.51
15	aA	802	CLA	CHC-C1C	2.68	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	802	CLA	CHC-C1C	2.68	1.41	1.35
15	cA	812	CLA	CMC-C2C	-2.68	1.45	1.50
15	aA	814	CLA	CMD-C2D	-2.68	1.45	1.50
15	bF	201	CLA	C1D-ND	2.68	1.41	1.37
15	aB	825	CLA	CMD-C2D	-2.68	1.45	1.50
15	aA	819	CLA	CHC-C1C	2.68	1.41	1.35
18	b6	420	BCR	C30-C25	-2.68	1.50	1.53
18	c1	401	BCR	C1-C6	-2.68	1.50	1.53
14	bA	801	CL0	OBD-CAD	2.68	1.27	1.22
18	a5	418	BCR	C40-C30	-2.68	1.48	1.53
15	aA	812	CLA	CHC-C1C	2.68	1.41	1.35
15	cB	804	CLA	CMB-C2B	-2.68	1.46	1.51
15	cA	837	CLA	CMB-C2B	-2.68	1.46	1.51
15	bA	835	CLA	CMD-C2D	-2.68	1.45	1.50
15	bB	807	CLA	MG-ND	-2.68	2.00	2.05
15	b4	407	CLA	CHC-C1C	2.68	1.41	1.35
15	c2	422	CLA	CMB-C2B	-2.68	1.46	1.51
15	c6	407	CLA	CMB-C2B	-2.68	1.46	1.51
15	aA	839	CLA	CHC-C1C	2.68	1.41	1.35
15	aA	845	CLA	C1D-ND	2.68	1.41	1.37
15	b4	412	CLA	C3B-C2B	-2.68	1.36	1.40
15	c2	416	CLA	CMD-C2D	-2.68	1.45	1.50
15	bB	836	CLA	C1D-ND	2.68	1.41	1.37
18	b3	418	BCR	C33-C5	-2.68	1.46	1.50
15	cA	812	CLA	CHC-C1C	2.68	1.41	1.35
15	aA	830	CLA	MG-ND	-2.67	2.00	2.05
15	bA	813	CLA	MG-ND	-2.67	2.00	2.05
15	bB	826	CLA	CMB-C2B	-2.67	1.46	1.51
15	cA	829	CLA	CMD-C2D	-2.67	1.45	1.50
15	c6	409	CLA	CMD-C2D	-2.67	1.45	1.50
18	a1	420	BCR	C30-C25	-2.67	1.50	1.53
15	cB	829	CLA	CHC-C1C	2.67	1.41	1.35
15	aB	808	CLA	CMB-C2B	-2.67	1.46	1.51
15	aB	813	CLA	C1D-ND	2.67	1.41	1.37
15	cB	836	CLA	C1D-ND	2.67	1.41	1.37
15	bB	804	CLA	CMB-C2B	-2.67	1.46	1.51
15	aB	818	CLA	CHC-C1C	2.67	1.41	1.35
15	cB	821	CLA	C1D-ND	2.67	1.41	1.37
15	cB	808	CLA	CMB-C2B	-2.67	1.46	1.51
15	cA	817	CLA	C3B-C2B	-2.67	1.36	1.40
15	bB	836	CLA	MG-ND	-2.67	2.00	2.05
15	cA	813	CLA	C1D-ND	2.67	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	833	CLA	CHC-C1C	2.67	1.41	1.35
15	b3	404	CLA	CMB-C2B	-2.67	1.46	1.51
18	a1	420	BCR	C1-C6	-2.67	1.50	1.53
15	cB	840	CLA	CMD-C2D	-2.67	1.45	1.50
15	a4	421	CLA	MG-ND	-2.67	2.00	2.05
15	cB	806	CLA	CMB-C2B	-2.67	1.46	1.51
15	c2	405	CLA	CMB-C2B	-2.67	1.46	1.51
15	c3	406	CLA	CMB-C2B	-2.67	1.46	1.51
18	c5	418	BCR	C40-C30	-2.67	1.48	1.53
15	aA	837	CLA	CMB-C2B	-2.67	1.46	1.51
15	c4	412	CLA	C3B-C2B	-2.67	1.36	1.40
15	c2	405	CLA	C1D-C2D	2.67	1.50	1.45
18	b6	401	BCR	C30-C25	-2.67	1.50	1.53
15	a1	407	CLA	CMD-C2D	-2.67	1.45	1.50
18	a4	401	BCR	C30-C25	-2.67	1.50	1.53
15	bA	806	CLA	CHC-C1C	2.67	1.41	1.35
15	bF	201	CLA	MG-ND	-2.67	2.00	2.05
15	aB	836	CLA	MG-ND	-2.67	2.00	2.05
15	bB	820	CLA	C1D-ND	2.67	1.41	1.37
15	bA	837	CLA	CMB-C2B	-2.67	1.46	1.51
15	b4	404	CLA	CMB-C2B	-2.66	1.46	1.51
15	bA	813	CLA	C1D-ND	2.66	1.41	1.37
15	cA	825	CLA	CMB-C2B	-2.66	1.46	1.51
18	c1	418	BCR	C40-C30	-2.66	1.48	1.53
15	b6	417	CLA	C4B-CHC	-2.66	1.33	1.41
15	bL	202	CLA	C1D-ND	2.66	1.41	1.37
15	aA	835	CLA	CMD-C2D	-2.66	1.45	1.50
15	cA	826	CLA	C1D-ND	2.66	1.41	1.37
15	b6	406	CLA	CMB-C2B	-2.66	1.46	1.51
15	a3	404	CLA	CMB-C2B	-2.66	1.46	1.51
15	aA	812	CLA	CMC-C2C	-2.66	1.45	1.50
15	bB	840	CLA	CMD-C2D	-2.66	1.45	1.50
15	cB	817	CLA	C3B-CAB	-2.66	1.42	1.47
15	cL	203	CLA	C3B-C2B	-2.66	1.36	1.40
15	c4	421	CLA	MG-ND	-2.66	2.00	2.05
18	c1	401	BCR	C30-C25	-2.66	1.50	1.53
15	cB	807	CLA	MG-ND	-2.66	2.00	2.05
15	bB	810	CLA	CMD-C2D	-2.66	1.45	1.50
15	bB	818	CLA	CMB-C2B	-2.66	1.46	1.51
15	aA	840	CLA	C1D-ND	2.66	1.41	1.37
15	cA	839	CLA	C1D-ND	2.66	1.41	1.37
15	cB	827	CLA	CHC-C1C	2.66	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	814	CLA	CMD-C2D	-2.66	1.45	1.50
15	cA	836	CLA	CMD-C2D	-2.66	1.45	1.50
15	aJ	201	CLA	C1D-ND	2.66	1.41	1.37
15	c3	404	CLA	CMB-C2B	-2.66	1.46	1.51
15	bB	810	CLA	MG-ND	-2.65	2.00	2.05
15	cA	835	CLA	CMD-C2D	-2.65	1.45	1.50
15	aA	809	CLA	C3B-C2B	-2.65	1.36	1.40
15	cB	818	CLA	CMB-C2B	-2.65	1.46	1.51
15	aA	843	CLA	CMD-C2D	-2.65	1.45	1.50
15	bB	814	CLA	CMC-C2C	-2.65	1.45	1.50
15	c2	409	CLA	CMD-C2D	-2.65	1.45	1.50
15	aB	820	CLA	C1D-ND	2.65	1.41	1.37
15	a3	413	CLA	CHC-C1C	2.65	1.41	1.35
15	cB	813	CLA	C1D-ND	2.65	1.41	1.37
15	c3	413	CLA	CHC-C1C	2.65	1.41	1.35
15	cA	844	CLA	C1D-ND	2.65	1.41	1.37
15	aB	816	CLA	CHC-C1C	2.65	1.41	1.35
15	a2	413	CLA	C3B-C2B	-2.65	1.36	1.40
15	bB	825	CLA	MG-ND	-2.65	2.00	2.05
15	cB	836	CLA	MG-ND	-2.65	2.00	2.05
15	aB	834	CLA	C3B-C2B	-2.65	1.36	1.40
15	bJ	101	CLA	CHC-C1C	2.65	1.41	1.35
15	b2	416	CLA	CMD-C2D	-2.65	1.45	1.50
15	aA	822	CLA	CHC-C1C	2.65	1.41	1.35
15	cB	810	CLA	MG-ND	-2.65	2.00	2.05
15	cB	825	CLA	MG-ND	-2.65	2.00	2.05
18	c6	401	BCR	C30-C25	-2.65	1.50	1.53
18	b3	418	BCR	C40-C30	-2.64	1.48	1.53
15	bA	830	CLA	CMD-C2D	-2.64	1.45	1.50
15	aA	818	CLA	CMB-C2B	-2.64	1.46	1.51
15	c4	404	CLA	CMB-C2B	-2.64	1.46	1.51
15	bB	829	CLA	CHC-C1C	2.64	1.41	1.35
18	a3	419	BCR	C1-C6	-2.64	1.50	1.53
18	b1	401	BCR	C30-C25	-2.64	1.50	1.53
15	aA	839	CLA	CMD-C2D	-2.64	1.45	1.50
15	aA	806	CLA	C3B-C2B	-2.64	1.36	1.40
15	bB	813	CLA	C1D-ND	2.64	1.41	1.37
15	aA	842	CLA	CMB-C2B	-2.64	1.46	1.51
15	bA	818	CLA	C1D-ND	2.64	1.41	1.37
15	aB	828	CLA	MG-ND	-2.64	2.00	2.05
15	cA	814	CLA	CMD-C2D	-2.64	1.45	1.50
15	bF	201	CLA	C3B-C2B	-2.64	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	818	CLA	CMB-C2B	-2.64	1.46	1.51
15	bA	845	CLA	C1D-ND	2.64	1.41	1.37
15	bB	821	CLA	C1D-ND	2.64	1.41	1.37
15	b2	409	CLA	CMD-C2D	-2.64	1.45	1.50
15	cB	834	CLA	C3B-C2B	-2.64	1.36	1.40
15	aB	806	CLA	CMB-C2B	-2.64	1.46	1.51
15	aA	817	CLA	C3B-C2B	-2.64	1.36	1.40
15	b3	413	CLA	CHC-C1C	2.64	1.41	1.35
18	a4	418	BCR	C33-C5	-2.64	1.46	1.50
15	cB	814	CLA	CMC-C2C	-2.64	1.45	1.50
15	aA	813	CLA	MG-ND	-2.64	2.00	2.05
15	aA	837	CLA	C3B-C2B	-2.64	1.36	1.40
18	a3	418	BCR	C33-C5	-2.64	1.46	1.50
15	b6	422	CLA	CMB-C2B	-2.64	1.46	1.51
15	cB	828	CLA	C3B-C2B	-2.64	1.36	1.40
15	b1	412	CLA	C3B-C2B	-2.63	1.36	1.40
15	bB	808	CLA	CMB-C2B	-2.63	1.46	1.51
15	aJ	202	CLA	CHC-C1C	2.63	1.41	1.35
15	aB	810	CLA	CMC-C2C	-2.63	1.45	1.50
15	aB	836	CLA	C1D-ND	2.63	1.41	1.37
15	bA	843	CLA	CHC-C1C	2.63	1.41	1.35
15	a6	417	CLA	C4B-CHC	-2.63	1.33	1.41
15	cB	827	CLA	C1D-ND	2.63	1.41	1.37
18	c6	419	BCR	C40-C30	-2.63	1.48	1.53
15	aA	836	CLA	CMD-C2D	-2.63	1.45	1.50
15	aA	821	CLA	CMB-C2B	-2.63	1.46	1.51
15	bA	839	CLA	CMD-C2D	-2.63	1.45	1.50
15	bA	806	CLA	CMD-C2D	-2.63	1.45	1.50
15	a4	406	CLA	CMB-C2B	-2.63	1.46	1.51
15	aA	820	CLA	CMC-C2C	-2.63	1.45	1.50
15	bA	836	CLA	CMD-C2D	-2.63	1.45	1.50
15	aA	806	CLA	CHC-C1C	2.63	1.41	1.35
15	a6	422	CLA	C3B-C2B	-2.63	1.36	1.40
15	b4	407	CLA	CMB-C2B	-2.63	1.46	1.51
15	cB	832	CLA	CHC-C1C	2.63	1.41	1.35
15	aB	814	CLA	CMC-C2C	-2.63	1.45	1.50
15	cA	814	CLA	CMC-C2C	-2.63	1.45	1.50
15	b2	414	CLA	CHC-C1C	2.63	1.41	1.35
15	aB	810	CLA	MG-ND	-2.63	2.00	2.05
15	aB	827	CLA	C1D-ND	2.63	1.41	1.37
15	bB	803	CLA	C3B-CAB	-2.63	1.42	1.47
15	bA	818	CLA	CMB-C2B	-2.63	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	817	CLA	C3B-C2B	-2.63	1.36	1.40
15	bA	814	CLA	CMC-C2C	-2.63	1.45	1.50
15	a4	407	CLA	CMB-C2B	-2.63	1.46	1.51
15	cF	201	CLA	CMB-C2B	-2.63	1.46	1.51
15	aJ	201	CLA	C3B-C2B	-2.63	1.36	1.40
15	bB	827	CLA	CHC-C1C	2.63	1.41	1.35
15	aB	807	CLA	CMC-C2C	-2.63	1.45	1.50
15	bB	815	CLA	CMD-C2D	-2.63	1.45	1.50
15	a5	405	CLA	CMB-C2B	-2.63	1.46	1.51
15	cB	804	CLA	MG-ND	-2.63	2.00	2.05
15	aA	807	CLA	CHC-C1C	2.63	1.41	1.35
15	bB	834	CLA	C3B-C2B	-2.62	1.36	1.40
15	cA	807	CLA	CHC-C1C	2.62	1.41	1.35
15	aB	804	CLA	MG-ND	-2.62	2.00	2.05
15	cL	201	CLA	C1D-ND	2.62	1.41	1.37
15	a5	406	CLA	CMB-C2B	-2.62	1.46	1.51
15	bA	821	CLA	CMB-C2B	-2.62	1.46	1.51
15	b5	405	CLA	CMB-C2B	-2.62	1.46	1.51
15	bL	203	CLA	CMB-C2B	-2.62	1.46	1.51
15	cA	806	CLA	CMD-C2D	-2.62	1.45	1.50
15	c5	405	CLA	CMB-C2B	-2.62	1.46	1.51
15	aB	839	CLA	CMD-C2D	-2.62	1.45	1.50
15	aB	807	CLA	MG-ND	-2.62	2.00	2.05
15	bB	828	CLA	C3B-C2B	-2.62	1.36	1.40
15	aJ	201	CLA	MG-ND	-2.62	2.00	2.05
15	cA	820	CLA	CMC-C2C	-2.62	1.45	1.50
15	c1	408	CLA	CMD-C2D	-2.62	1.45	1.50
15	c4	408	CLA	CMD-C2D	-2.62	1.45	1.50
15	cA	806	CLA	C3B-C2B	-2.62	1.36	1.40
18	c5	401	BCR	C30-C25	-2.62	1.50	1.53
15	bA	822	CLA	CHC-C1C	2.62	1.41	1.35
15	aL	201	CLA	C1D-ND	2.62	1.41	1.37
15	c1	406	CLA	CMB-C2B	-2.62	1.46	1.51
15	bA	826	CLA	CHC-C1C	2.62	1.41	1.35
15	b1	404	CLA	CMB-C2B	-2.62	1.46	1.51
15	aA	843	CLA	CHC-C1C	2.62	1.41	1.35
15	aB	832	CLA	CHC-C1C	2.62	1.41	1.35
15	bA	842	CLA	CMB-C2B	-2.62	1.46	1.51
15	aA	806	CLA	CMD-C2D	-2.62	1.45	1.50
15	bA	806	CLA	C3B-C2B	-2.62	1.36	1.40
15	cF	203	CLA	C3B-C2B	-2.62	1.36	1.40
15	bB	807	CLA	CMC-C2C	-2.62	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	406	CLA	CMB-C2B	-2.62	1.46	1.51
15	cL	202	CLA	CMB-C2B	-2.62	1.46	1.51
15	bA	839	CLA	C1D-ND	2.62	1.41	1.37
15	cB	829	CLA	CMB-C2B	-2.61	1.46	1.51
15	bA	811	CLA	C3B-C2B	-2.61	1.36	1.40
15	cA	822	CLA	CHC-C1C	2.61	1.41	1.35
15	b2	405	CLA	CMB-C2B	-2.61	1.46	1.51
15	b4	408	CLA	CMB-C2B	-2.61	1.46	1.51
15	aB	829	CLA	CMB-C2B	-2.61	1.46	1.51
15	bB	830	CLA	C3B-C2B	-2.61	1.36	1.40
18	b4	418	BCR	C33-C5	-2.61	1.46	1.50
15	cF	203	CLA	MG-ND	-2.61	2.00	2.05
15	bA	820	CLA	CMC-C2C	-2.61	1.45	1.50
15	cB	815	CLA	CMD-C2D	-2.61	1.45	1.50
15	bB	825	CLA	CHC-C1C	2.61	1.41	1.35
18	b6	419	BCR	C40-C30	-2.61	1.48	1.53
18	b1	401	BCR	C34-C9	-2.61	1.45	1.50
15	cA	842	CLA	CHC-C1C	2.61	1.41	1.35
15	aB	834	CLA	CHC-C1C	2.61	1.41	1.35
15	cB	828	CLA	MG-ND	-2.61	2.00	2.05
15	aB	827	CLA	CHC-C1C	2.61	1.41	1.35
15	cF	203	CLA	C1D-ND	2.61	1.41	1.37
15	aB	803	CLA	C3B-CAB	-2.61	1.42	1.47
15	b2	422	CLA	CMB-C2B	-2.61	1.46	1.51
18	aF	203	BCR	C1-C6	-2.61	1.50	1.53
18	a5	401	BCR	C30-C25	-2.61	1.50	1.53
15	cA	806	CLA	CHC-C1C	2.61	1.41	1.35
15	b5	406	CLA	CMB-C2B	-2.61	1.46	1.51
15	cB	803	CLA	C3B-CAB	-2.61	1.42	1.47
15	cB	839	CLA	CMB-C2B	-2.61	1.46	1.51
15	cA	833	CLA	MG-ND	-2.61	2.00	2.05
18	c3	418	BCR	C40-C30	-2.61	1.48	1.53
15	cJ	101	CLA	CHC-C1C	2.61	1.41	1.35
15	aA	811	CLA	C3B-C2B	-2.61	1.36	1.40
15	bA	837	CLA	C3B-C2B	-2.61	1.36	1.40
15	aL	202	CLA	CMB-C2B	-2.60	1.46	1.51
15	aA	814	CLA	CMC-C2C	-2.60	1.45	1.50
15	bB	838	CLA	C1D-ND	2.60	1.41	1.37
15	c6	417	CLA	C4B-CHC	-2.60	1.33	1.41
15	cA	804	CLA	CMC-C2C	-2.60	1.45	1.50
15	a6	409	CLA	CMB-C2B	-2.60	1.46	1.51
15	bB	810	CLA	CMC-C2C	-2.60	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	809	CLA	C3B-C2B	-2.60	1.36	1.40
15	aA	826	CLA	CHC-C1C	2.60	1.41	1.35
15	cA	839	CLA	CMD-C2D	-2.60	1.45	1.50
15	b6	422	CLA	MG-ND	-2.60	2.00	2.05
15	cB	834	CLA	CHC-C1C	2.60	1.41	1.35
15	cA	818	CLA	C1D-ND	2.60	1.41	1.37
15	a1	401	CLA	CMB-C2B	-2.60	1.46	1.51
15	a4	408	CLA	CMD-C2D	-2.60	1.45	1.50
15	a1	422	CLA	MG-ND	-2.60	2.00	2.05
15	aB	825	CLA	CHC-C1C	2.60	1.41	1.35
15	cB	825	CLA	CHC-C1C	2.60	1.41	1.35
15	a2	416	CLA	CMD-C2D	-2.60	1.45	1.50
15	c6	409	CLA	CMB-C2B	-2.60	1.46	1.51
15	aA	821	CLA	CHC-C1C	2.60	1.41	1.35
18	cF	205	BCR	C1-C6	-2.60	1.50	1.53
15	b1	407	CLA	CMB-C2B	-2.60	1.46	1.51
15	bA	804	CLA	CMC-C2C	-2.60	1.45	1.50
15	a2	405	CLA	CMB-C2B	-2.60	1.46	1.51
15	cB	832	CLA	MG-ND	-2.60	2.00	2.05
15	cA	830	CLA	CMD-C2D	-2.60	1.45	1.50
18	c3	401	BCR	C30-C25	-2.60	1.50	1.53
15	b6	414	CLA	CHC-C1C	2.60	1.41	1.35
15	c5	403	CLA	CMD-C2D	-2.60	1.45	1.50
18	a3	418	BCR	C40-C30	-2.60	1.48	1.53
15	bA	807	CLA	CHC-C1C	2.60	1.41	1.35
15	aA	813	CLA	C1D-ND	2.60	1.41	1.37
15	bB	832	CLA	CHC-C1C	2.60	1.41	1.35
15	c2	414	CLA	CHC-C1C	2.60	1.41	1.35
15	cB	821	CLA	MG-ND	-2.60	2.00	2.05
15	c5	406	CLA	CMB-C2B	-2.60	1.46	1.51
18	a3	401	BCR	C30-C25	-2.60	1.50	1.53
18	a6	402	BCR	C1-C6	-2.60	1.50	1.53
18	b5	418	BCR	C40-C30	-2.60	1.48	1.53
15	cA	837	CLA	C3B-C2B	-2.60	1.36	1.40
15	bB	834	CLA	CHC-C1C	2.60	1.41	1.35
15	aA	834	CLA	CMD-C2D	-2.59	1.45	1.50
15	cA	826	CLA	CHC-C1C	2.59	1.41	1.35
15	aB	837	CLA	C3B-CAB	-2.59	1.42	1.47
15	cA	811	CLA	C3B-C2B	-2.59	1.36	1.40
15	c4	407	CLA	CMB-C2B	-2.59	1.46	1.51
18	b2	401	BCR	C30-C25	-2.59	1.50	1.53
15	aB	837	CLA	C1D-ND	2.59	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	413	CLA	C3B-C2B	-2.59	1.36	1.40
15	cB	839	CLA	CMD-C2D	-2.59	1.45	1.50
18	b5	401	BCR	C1-C6	-2.59	1.50	1.53
15	c1	402	CLA	CMB-C2B	-2.59	1.46	1.51
15	bA	826	CLA	C1D-ND	2.59	1.41	1.37
15	aA	802	CLA	CMD-C2D	-2.59	1.45	1.50
18	b6	419	BCR	C33-C5	-2.59	1.46	1.50
18	a4	419	BCR	C30-C25	-2.59	1.50	1.53
15	aA	826	CLA	C1D-ND	2.59	1.41	1.37
15	aB	838	CLA	C1D-ND	2.59	1.41	1.37
15	bA	838	CLA	C1D-ND	2.59	1.41	1.37
15	c5	420	CLA	CMB-C2B	-2.59	1.46	1.51
15	b4	408	CLA	CMD-C2D	-2.59	1.45	1.50
15	bB	829	CLA	CMB-C2B	-2.59	1.46	1.51
18	a2	401	BCR	C30-C25	-2.59	1.50	1.53
15	cA	818	CLA	CMB-C2B	-2.59	1.46	1.51
15	cB	837	CLA	C3B-CAB	-2.59	1.42	1.47
15	bB	837	CLA	C3B-CAB	-2.59	1.42	1.47
15	bA	802	CLA	CMC-C2C	-2.59	1.45	1.50
18	b1	401	BCR	C1-C6	-2.59	1.50	1.53
15	a3	414	CLA	CMB-C2B	-2.59	1.46	1.51
18	aA	848	BCR	C30-C25	-2.58	1.50	1.53
15	aA	804	CLA	CMC-C2C	-2.58	1.45	1.50
15	aA	830	CLA	CMD-C2D	-2.58	1.45	1.50
15	b5	403	CLA	CMD-C2D	-2.58	1.45	1.50
15	a2	414	CLA	CHC-C1C	2.58	1.41	1.35
15	bA	818	CLA	CMD-C2D	-2.58	1.45	1.50
15	b1	408	CLA	CMD-C2D	-2.58	1.45	1.50
15	cB	807	CLA	CMC-C2C	-2.58	1.45	1.50
15	cB	810	CLA	CMC-C2C	-2.58	1.45	1.50
15	bB	804	CLA	MG-ND	-2.58	2.00	2.05
15	aA	802	CLA	CMC-C2C	-2.58	1.45	1.50
15	a4	408	CLA	CMB-C2B	-2.58	1.46	1.51
15	b2	404	CLA	CMB-C2B	-2.58	1.46	1.51
15	bA	833	CLA	MG-ND	-2.58	2.00	2.05
15	aB	815	CLA	CMD-C2D	-2.58	1.45	1.50
15	cA	840	CLA	CMD-C2D	-2.58	1.45	1.50
15	a1	405	CLA	CMB-C2B	-2.58	1.46	1.51
15	aA	831	CLA	CMC-C2C	-2.58	1.45	1.50
15	cA	831	CLA	CMC-C2C	-2.58	1.45	1.50
15	aB	819	CLA	C1D-ND	2.58	1.41	1.37
15	c1	405	CLA	CMB-C2B	-2.58	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a5	420	CLA	CMB-C2B	-2.58	1.46	1.51
15	bA	831	CLA	CMC-C2C	-2.58	1.45	1.50
15	b6	409	CLA	CMB-C2B	-2.58	1.46	1.51
15	b1	402	CLA	CMB-C2B	-2.58	1.46	1.51
15	a4	414	CLA	CMB-C2B	-2.58	1.46	1.51
15	aA	815	CLA	C3B-C2B	-2.58	1.36	1.40
15	bB	839	CLA	CMB-C2B	-2.58	1.46	1.51
15	cA	815	CLA	CMB-C2B	-2.58	1.46	1.51
15	cL	203	CLA	MG-ND	-2.58	2.00	2.05
15	c1	404	CLA	CMB-C2B	-2.58	1.46	1.51
15	b5	404	CLA	CMB-C2B	-2.57	1.46	1.51
18	a6	419	BCR	C40-C30	-2.57	1.48	1.53
15	a6	403	CLA	CMB-C2B	-2.57	1.46	1.51
15	aB	821	CLA	MG-ND	-2.57	2.00	2.05
15	cB	816	CLA	CMB-C2B	-2.57	1.46	1.51
15	cA	834	CLA	CMD-C2D	-2.57	1.45	1.50
15	b3	414	CLA	CMB-C2B	-2.57	1.46	1.51
15	bB	821	CLA	MG-ND	-2.57	2.00	2.05
15	c4	408	CLA	CMB-C2B	-2.57	1.46	1.51
15	aB	825	CLA	CMB-C2B	-2.57	1.46	1.51
15	a1	407	CLA	CMB-C2B	-2.57	1.46	1.51
15	aB	829	CLA	C3B-CAB	-2.57	1.42	1.47
15	bA	834	CLA	CMD-C2D	-2.57	1.45	1.50
18	b4	419	BCR	C30-C25	-2.57	1.50	1.53
15	bB	814	CLA	CMB-C2B	-2.57	1.46	1.51
15	bB	819	CLA	C1D-ND	2.57	1.40	1.37
15	aB	839	CLA	CMB-C2B	-2.57	1.46	1.51
15	bA	815	CLA	CMB-C2B	-2.57	1.46	1.51
15	b1	405	CLA	CMB-C2B	-2.57	1.46	1.51
18	c6	402	BCR	C1-C6	-2.57	1.50	1.53
18	b6	402	BCR	C1-C6	-2.57	1.50	1.53
15	b2	417	CLA	C1C-NC	-2.57	1.34	1.37
15	cA	821	CLA	CHC-C1C	2.57	1.41	1.35
15	cB	802	CLA	MG-ND	-2.57	2.00	2.05
15	bA	802	CLA	CMD-C2D	-2.57	1.45	1.50
15	b4	402	CLA	CMB-C2B	-2.57	1.46	1.51
18	b3	401	BCR	C30-C25	-2.57	1.50	1.53
15	aA	807	CLA	C3B-C2B	-2.57	1.36	1.40
15	cA	840	CLA	C3B-C2B	-2.57	1.36	1.40
15	b6	403	CLA	CMB-C2B	-2.57	1.46	1.51
15	aB	832	CLA	MG-ND	-2.57	2.00	2.05
15	bA	822	CLA	MG-ND	-2.56	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	829	CLA	C3B-CAB	-2.56	1.42	1.47
15	bB	816	CLA	CMB-C2B	-2.56	1.46	1.51
15	c5	404	CLA	CMB-C2B	-2.56	1.46	1.51
15	c1	407	CLA	CMB-C2B	-2.56	1.46	1.51
15	b5	420	CLA	CMB-C2B	-2.56	1.46	1.51
15	b4	421	CLA	C2A-C1A	2.56	1.58	1.52
15	aA	833	CLA	MG-ND	-2.56	2.00	2.05
15	cA	806	CLA	MG-ND	-2.56	2.00	2.05
18	a5	401	BCR	C1-C6	-2.56	1.50	1.53
15	a5	403	CLA	CMD-C2D	-2.56	1.45	1.50
15	b5	414	CLA	CMB-C2B	-2.56	1.46	1.51
15	aB	802	CLA	MG-ND	-2.56	2.00	2.05
15	bB	832	CLA	MG-ND	-2.56	2.00	2.05
15	bL	204	CLA	MG-ND	-2.56	2.00	2.05
15	bB	839	CLA	CMD-C2D	-2.56	1.45	1.50
15	a1	404	CLA	CMB-C2B	-2.56	1.46	1.51
15	aL	203	CLA	MG-ND	-2.56	2.00	2.05
15	aA	833	CLA	C3B-C2B	-2.56	1.36	1.40
15	cA	809	CLA	C3B-C2B	-2.56	1.36	1.40
15	cB	823	CLA	CMB-C2B	-2.56	1.46	1.51
15	bA	818	CLA	CMC-C2C	-2.56	1.45	1.50
15	cA	802	CLA	CMD-C2D	-2.56	1.45	1.50
18	c4	418	BCR	C33-C5	-2.56	1.46	1.50
15	bB	829	CLA	C3B-CAB	-2.56	1.42	1.47
15	bA	829	CLA	CMB-C2B	-2.56	1.46	1.51
15	c5	414	CLA	CMB-C2B	-2.56	1.46	1.51
15	bA	803	CLA	CHC-C1C	2.56	1.41	1.35
15	b4	414	CLA	CMB-C2B	-2.55	1.46	1.51
15	a1	415	CLA	C3B-CAB	-2.55	1.42	1.47
15	aA	840	CLA	CMD-C2D	-2.55	1.45	1.50
15	bX	102	CLA	CMD-C2D	-2.55	1.45	1.50
15	cB	819	CLA	C1D-ND	2.55	1.40	1.37
15	c6	417	CLA	C3B-CAB	-2.55	1.42	1.47
15	b3	405	CLA	CMB-C2B	-2.55	1.46	1.51
15	aA	821	CLA	C3B-C2B	-2.55	1.36	1.40
15	cA	805	CLA	C1D-ND	2.55	1.40	1.37
15	c4	421	CLA	C2A-C1A	2.55	1.58	1.52
15	b1	408	CLA	CMB-C2B	-2.55	1.46	1.51
15	c6	403	CLA	CMB-C2B	-2.55	1.46	1.51
15	a3	421	CLA	CMD-C2D	-2.55	1.45	1.50
18	c4	419	BCR	C30-C25	-2.55	1.50	1.53
15	cA	815	CLA	C3B-C2B	-2.55	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	801	CLA	C3B-C2B	-2.55	1.36	1.40
15	b1	406	CLA	CMB-C2B	-2.55	1.46	1.51
15	bA	805	CLA	C1D-ND	2.55	1.40	1.37
18	a3	419	BCR	C30-C25	-2.55	1.50	1.53
18	c2	401	BCR	C30-C25	-2.55	1.50	1.53
15	c4	414	CLA	CMB-C2B	-2.55	1.46	1.51
15	cA	831	CLA	CMD-C2D	-2.55	1.45	1.50
18	c6	419	BCR	C33-C5	-2.55	1.46	1.50
18	bJ	105	BCR	C1-C6	-2.55	1.50	1.53
15	aB	801	CLA	C3B-C2B	-2.55	1.36	1.40
15	cA	807	CLA	CMC-C2C	-2.55	1.45	1.50
15	aA	815	CLA	CMB-C2B	-2.55	1.46	1.51
15	aB	814	CLA	CMB-C2B	-2.55	1.46	1.51
18	c5	401	BCR	C1-C6	-2.55	1.50	1.53
15	cA	818	CLA	CMD-C2D	-2.55	1.45	1.50
15	a1	403	CLA	CMB-C2B	-2.55	1.46	1.51
15	bA	815	CLA	C3B-C2B	-2.55	1.36	1.40
15	bB	802	CLA	MG-ND	-2.54	2.00	2.05
18	b5	418	BCR	C33-C5	-2.54	1.46	1.50
15	cA	803	CLA	CHC-C1C	2.54	1.41	1.35
15	a6	408	CLA	CMB-C2B	-2.54	1.46	1.51
15	c4	402	CLA	CMB-C2B	-2.54	1.46	1.51
15	bA	806	CLA	MG-ND	-2.54	2.00	2.05
15	b6	408	CLA	CMB-C2B	-2.54	1.46	1.51
15	cB	838	CLA	C1D-ND	2.54	1.40	1.37
15	cA	822	CLA	MG-ND	-2.54	2.00	2.05
15	aA	829	CLA	CMB-C2B	-2.54	1.46	1.51
15	aB	823	CLA	CMB-C2B	-2.54	1.46	1.51
15	cB	825	CLA	CMC-C2C	-2.54	1.45	1.50
15	a5	404	CLA	CMB-C2B	-2.54	1.46	1.51
15	bA	821	CLA	C3B-C2B	-2.54	1.36	1.40
15	aA	822	CLA	MG-ND	-2.54	2.00	2.05
15	a6	417	CLA	C3B-CAB	-2.54	1.42	1.47
15	aA	818	CLA	CMD-C2D	-2.54	1.45	1.50
15	aL	201	CLA	CMD-C2D	-2.54	1.45	1.50
15	c5	409	CLA	CMB-C2B	-2.54	1.46	1.51
18	a6	419	BCR	C33-C5	-2.54	1.46	1.50
15	a4	402	CLA	CMB-C2B	-2.54	1.46	1.51
18	cA	847	BCR	C30-C25	-2.54	1.50	1.53
15	cB	818	CLA	CMC-C2C	-2.54	1.45	1.50
15	cK	102	CLA	CMB-C2B	-2.54	1.46	1.51
15	cA	818	CLA	CMC-C2C	-2.54	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	830	CLA	C3B-C2B	-2.54	1.36	1.40
15	c3	409	CLA	CMB-C2B	-2.54	1.46	1.51
15	aA	803	CLA	CHC-C1C	2.54	1.41	1.35
15	cB	814	CLA	CMB-C2B	-2.54	1.46	1.51
15	bB	801	CLA	C3B-C2B	-2.54	1.36	1.40
15	cB	825	CLA	CMB-C2B	-2.54	1.46	1.51
15	aB	808	CLA	CHC-C1C	2.54	1.41	1.35
15	bB	809	CLA	CMC-C2C	-2.54	1.45	1.50
15	c3	414	CLA	CMB-C2B	-2.54	1.46	1.51
15	bB	826	CLA	C1D-ND	2.54	1.40	1.37
15	cA	821	CLA	C3B-C2B	-2.53	1.36	1.40
15	cA	833	CLA	C3B-C2B	-2.53	1.36	1.40
15	aA	831	CLA	CMD-C2D	-2.53	1.45	1.50
15	aB	820	CLA	CMD-C2D	-2.53	1.45	1.50
18	a1	420	BCR	C34-C9	-2.53	1.45	1.50
15	cA	838	CLA	C1D-ND	2.53	1.40	1.37
15	c3	407	CLA	CMB-C2B	-2.53	1.46	1.51
15	bB	825	CLA	CMB-C2B	-2.53	1.46	1.51
15	bA	840	CLA	CMD-C2D	-2.53	1.45	1.50
15	b3	409	CLA	CMB-C2B	-2.53	1.46	1.51
15	aA	841	CLA	C3B-C2B	-2.53	1.36	1.40
15	b3	416	CLA	C3B-CAB	-2.53	1.42	1.47
15	c2	413	CLA	MG-ND	-2.53	2.00	2.05
15	cA	829	CLA	CMB-C2B	-2.53	1.46	1.51
15	aA	806	CLA	MG-ND	-2.53	2.00	2.05
15	bA	831	CLA	CMD-C2D	-2.53	1.45	1.50
15	aB	818	CLA	CMC-C2C	-2.53	1.45	1.50
15	bJ	102	CLA	CHC-C1C	2.53	1.41	1.35
15	a6	414	CLA	CHC-C1C	2.53	1.41	1.35
15	bA	833	CLA	C3B-C2B	-2.53	1.36	1.40
18	b3	419	BCR	C30-C25	-2.53	1.50	1.53
15	b1	414	CLA	CMB-C2B	-2.53	1.46	1.51
15	aA	838	CLA	C1D-ND	2.53	1.40	1.37
15	a5	414	CLA	CMB-C2B	-2.53	1.46	1.51
15	a1	402	CLA	CMD-C2D	-2.53	1.45	1.50
18	b6	402	BCR	C30-C25	-2.53	1.50	1.53
15	cJ	102	CLA	CHC-C1C	2.53	1.41	1.35
15	aJ	203	CLA	CHC-C1C	2.53	1.41	1.35
15	b6	405	CLA	CMB-C2B	-2.53	1.46	1.51
15	bB	808	CLA	CHC-C1C	2.53	1.41	1.35
15	aK	102	CLA	CMB-C2B	-2.53	1.46	1.51
15	cA	807	CLA	C3B-C2B	-2.53	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	841	CLA	C3B-C2B	-2.53	1.36	1.40
15	bA	807	CLA	CMC-C2C	-2.53	1.45	1.50
15	aB	826	CLA	C1D-ND	2.53	1.40	1.37
18	a1	418	BCR	C30-C25	-2.53	1.50	1.53
15	cA	802	CLA	CMC-C2C	-2.53	1.45	1.50
15	aB	841	CLA	C3B-C2B	-2.53	1.36	1.40
15	aA	818	CLA	CMC-C2C	-2.52	1.45	1.50
15	aB	819	CLA	MG-ND	-2.52	2.00	2.05
15	b6	417	CLA	C3B-CAB	-2.52	1.42	1.47
15	c3	416	CLA	C3B-CAB	-2.52	1.42	1.47
18	aK	101	BCR	C30-C25	-2.52	1.50	1.53
15	a3	408	CLA	CMB-C2B	-2.52	1.46	1.51
18	b5	401	BCR	C30-C25	-2.52	1.50	1.53
15	a2	404	CLA	CMB-C2B	-2.52	1.46	1.51
15	a3	407	CLA	CMB-C2B	-2.52	1.46	1.51
15	bB	823	CLA	CMB-C2B	-2.52	1.46	1.51
15	a3	405	CLA	CMB-C2B	-2.52	1.46	1.51
15	bA	821	CLA	CHC-C1C	2.52	1.41	1.35
15	b5	409	CLA	CMB-C2B	-2.52	1.46	1.51
18	c3	419	BCR	C30-C25	-2.52	1.50	1.53
15	cB	801	CLA	CHC-C1C	2.52	1.41	1.35
15	a4	421	CLA	C2A-C1A	2.52	1.57	1.52
15	cA	814	CLA	CMB-C2B	-2.52	1.46	1.51
15	b1	403	CLA	CMD-C2D	-2.52	1.45	1.50
15	cL	203	CLA	CMD-C2D	-2.52	1.45	1.50
15	a3	416	CLA	C3B-CAB	-2.52	1.42	1.47
15	a2	406	CLA	MG-ND	-2.52	2.00	2.05
15	bA	840	CLA	C3B-C2B	-2.52	1.36	1.40
15	a4	416	CLA	C3B-CAB	-2.52	1.42	1.47
15	cA	826	CLA	MG-ND	-2.52	2.00	2.05
15	aL	203	CLA	CMD-C2D	-2.52	1.45	1.50
15	b3	407	CLA	CMB-C2B	-2.51	1.46	1.51
15	c3	421	CLA	C2A-C1A	2.51	1.57	1.52
15	c1	408	CLA	CMB-C2B	-2.51	1.46	1.51
15	aX	102	CLA	CMD-C2D	-2.51	1.45	1.50
15	cB	827	CLA	MG-ND	-2.51	2.00	2.05
15	c5	412	CLA	MG-ND	-2.51	2.00	2.05
15	c2	404	CLA	CMB-C2B	-2.51	1.46	1.51
15	aB	806	CLA	C1D-ND	2.51	1.40	1.37
15	c3	421	CLA	CMD-C2D	-2.51	1.45	1.50
15	c4	412	CLA	MG-ND	-2.51	2.00	2.05
15	b2	406	CLA	CAA-CBA	-2.51	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cF	203	CLA	CHC-C1C	2.51	1.41	1.35
15	aB	836	CLA	CMD-C2D	-2.51	1.45	1.50
15	cB	808	CLA	CHC-C1C	2.51	1.41	1.35
15	bB	825	CLA	CMC-C2C	-2.51	1.45	1.50
15	cB	819	CLA	MG-ND	-2.51	2.00	2.05
15	cL	201	CLA	CMD-C2D	-2.51	1.45	1.50
15	aB	816	CLA	CMB-C2B	-2.51	1.46	1.51
15	a5	402	CLA	CMB-C2B	-2.51	1.46	1.51
15	a3	421	CLA	C2A-C1A	2.51	1.57	1.52
15	a2	406	CLA	CAA-CBA	-2.51	1.45	1.52
15	cB	830	CLA	C3B-C2B	-2.51	1.36	1.40
15	c6	405	CLA	CMB-C2B	-2.51	1.46	1.51
18	a6	402	BCR	C30-C25	-2.51	1.50	1.53
15	aB	809	CLA	C1D-ND	2.51	1.40	1.37
15	c2	422	CLA	CMD-C2D	-2.51	1.45	1.50
15	cB	820	CLA	CMD-C2D	-2.51	1.45	1.50
15	c2	406	CLA	CMD-C2D	-2.51	1.45	1.50
15	a6	422	CLA	CAA-C2A	2.51	1.58	1.54
15	a5	416	CLA	C3B-CAB	-2.51	1.42	1.47
15	cB	826	CLA	C1D-ND	2.51	1.40	1.37
15	bB	811	CLA	C3B-CAB	-2.51	1.42	1.47
15	aA	807	CLA	CMC-C2C	-2.51	1.45	1.50
18	a5	418	BCR	C33-C5	-2.51	1.46	1.50
15	a6	406	CLA	C1D-C2D	2.51	1.50	1.45
15	aA	814	CLA	CMB-C2B	-2.51	1.46	1.51
15	aB	827	CLA	MG-ND	-2.51	2.00	2.05
15	cB	836	CLA	CMD-C2D	-2.51	1.45	1.50
15	c6	408	CLA	CMB-C2B	-2.51	1.46	1.51
15	b6	406	CLA	C1D-C2D	2.51	1.50	1.45
15	a6	405	CLA	CMB-C2B	-2.51	1.46	1.51
15	c3	402	CLA	CMB-C2B	-2.51	1.46	1.51
15	bB	820	CLA	CMD-C2D	-2.51	1.45	1.50
15	c4	403	CLA	CMD-C2D	-2.51	1.45	1.50
15	b5	416	CLA	C3B-CAB	-2.51	1.42	1.47
15	b3	402	CLA	CMB-C2B	-2.51	1.46	1.51
15	aB	825	CLA	CMC-C2C	-2.51	1.45	1.50
15	bB	827	CLA	MG-ND	-2.50	2.00	2.05
15	cB	819	CLA	CMB-C2B	-2.50	1.46	1.51
15	b3	421	CLA	CMD-C2D	-2.50	1.45	1.50
15	bL	202	CLA	CMD-C2D	-2.50	1.45	1.50
15	cB	835	CLA	CMC-C2C	-2.50	1.45	1.50
15	aB	803	CLA	CMC-C2C	-2.50	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	819	CLA	CMB-C2B	-2.50	1.46	1.51
15	bA	814	CLA	CMB-C2B	-2.50	1.46	1.51
15	b2	413	CLA	MG-ND	-2.50	2.00	2.05
15	a3	402	CLA	CMB-C2B	-2.50	1.46	1.51
15	c3	405	CLA	CMB-C2B	-2.50	1.46	1.51
15	bX	102	CLA	C3B-C2B	-2.50	1.36	1.40
15	c5	402	CLA	CMB-C2B	-2.50	1.46	1.51
15	a2	422	CLA	CMD-C2D	-2.50	1.45	1.50
15	c1	403	CLA	CMD-C2D	-2.50	1.45	1.50
15	cL	202	CLA	C3B-CAB	-2.50	1.42	1.47
15	aA	805	CLA	C1D-ND	2.50	1.40	1.37
15	bK	101	CLA	CMB-C2B	-2.50	1.46	1.51
15	bB	819	CLA	CMD-C2D	-2.50	1.45	1.50
15	b2	406	CLA	CMD-C2D	-2.50	1.45	1.50
15	cB	819	CLA	CMD-C2D	-2.50	1.45	1.50
15	b4	416	CLA	C3B-CAB	-2.50	1.42	1.47
15	aJ	201	CLA	CHC-C1C	2.50	1.41	1.35
15	a4	403	CLA	CMD-C2D	-2.50	1.45	1.50
15	bL	204	CLA	CMD-C2D	-2.50	1.45	1.50
15	aA	840	CLA	C3B-C2B	-2.50	1.36	1.40
15	cB	809	CLA	CMC-C2C	-2.50	1.45	1.50
15	cX	102	CLA	CMD-C2D	-2.50	1.45	1.50
15	a6	416	CLA	CHC-C1C	2.50	1.41	1.35
18	a2	420	BCR	C30-C25	-2.49	1.50	1.53
15	cL	202	CLA	CMC-C2C	-2.49	1.45	1.50
15	c1	414	CLA	CMB-C2B	-2.49	1.46	1.51
15	aB	809	CLA	CMC-C2C	-2.49	1.45	1.50
15	cB	811	CLA	C3B-CAB	-2.49	1.42	1.47
15	c4	416	CLA	C3B-CAB	-2.49	1.42	1.47
15	bA	835	CLA	CMC-C2C	-2.49	1.45	1.50
15	a3	409	CLA	CMB-C2B	-2.49	1.46	1.51
15	bF	201	CLA	CHC-C1C	2.49	1.41	1.35
15	b5	402	CLA	CMB-C2B	-2.49	1.46	1.51
15	bB	802	CLA	C3B-CAB	-2.49	1.42	1.47
15	b2	422	CLA	CMD-C2D	-2.49	1.45	1.50
15	a1	422	CLA	CMB-C2B	-2.49	1.46	1.51
15	aB	835	CLA	CMC-C2C	-2.49	1.45	1.50
18	b6	421	BCR	C1-C6	-2.49	1.50	1.53
15	aA	832	CLA	C3B-C2B	-2.49	1.36	1.40
15	b6	422	CLA	CMD-C2D	-2.49	1.45	1.50
15	bB	819	CLA	CMB-C2B	-2.49	1.46	1.51
15	c2	406	CLA	CAA-CBA	-2.49	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	818	CLA	CMC-C2C	-2.49	1.45	1.50
15	c4	405	CLA	CMB-C2B	-2.49	1.46	1.51
15	aL	202	CLA	CMC-C2C	-2.49	1.45	1.50
15	bB	801	CLA	CHC-C1C	2.49	1.41	1.35
15	bB	803	CLA	CMC-C2C	-2.49	1.45	1.50
15	cB	841	CLA	C3B-C2B	-2.49	1.36	1.40
15	c1	412	CLA	C3B-C2B	-2.49	1.36	1.40
15	cB	803	CLA	CMC-C2C	-2.48	1.45	1.50
15	cB	811	CLA	CMC-C2C	-2.48	1.45	1.50
15	a2	402	CLA	CMB-C2B	-2.48	1.46	1.51
15	a5	405	CLA	C1D-C2D	2.48	1.50	1.45
15	aB	811	CLA	CMC-C2C	-2.48	1.45	1.50
15	a4	412	CLA	MG-ND	-2.48	2.00	2.05
15	a2	413	CLA	MG-ND	-2.48	2.00	2.05
15	aA	814	CLA	MG-ND	-2.48	2.00	2.05
15	c5	416	CLA	C3B-CAB	-2.48	1.42	1.47
15	b3	408	CLA	CMB-C2B	-2.48	1.46	1.51
15	a2	406	CLA	CMD-C2D	-2.48	1.45	1.50
15	aA	803	CLA	MG-ND	-2.48	2.00	2.05
15	bB	811	CLA	CMC-C2C	-2.48	1.45	1.50
15	cF	201	CLA	C3B-C2B	-2.48	1.36	1.40
15	b4	412	CLA	MG-ND	-2.48	2.00	2.05
15	cL	201	CLA	C3B-CAB	-2.48	1.42	1.47
15	b4	405	CLA	CMB-C2B	-2.48	1.46	1.51
15	aB	809	CLA	CHC-C1C	2.48	1.41	1.35
15	bB	810	CLA	C4B-CHC	-2.48	1.34	1.41
15	a2	415	CLA	CMB-C2B	-2.48	1.46	1.51
15	bB	809	CLA	CHC-C1C	2.48	1.41	1.35
15	bA	807	CLA	C3B-C2B	-2.48	1.36	1.40
15	a4	405	CLA	CMB-C2B	-2.48	1.46	1.51
15	cB	809	CLA	CHC-C1C	2.48	1.41	1.35
15	bA	814	CLA	MG-ND	-2.48	2.00	2.05
15	a1	413	CLA	CMB-C2B	-2.48	1.46	1.51
15	bA	824	CLA	C3B-C2B	-2.48	1.36	1.40
15	aA	835	CLA	CMC-C2C	-2.48	1.45	1.50
15	a5	412	CLA	MG-ND	-2.48	2.00	2.05
15	bB	820	CLA	C3B-C2B	-2.48	1.36	1.40
15	aB	801	CLA	CHC-C1C	2.48	1.41	1.35
15	bB	809	CLA	C1D-ND	2.48	1.40	1.37
15	aB	826	CLA	CMD-C2D	-2.48	1.45	1.50
15	b3	416	CLA	C4C-C3C	2.48	1.49	1.45
18	c6	402	BCR	C30-C25	-2.48	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	833	CLA	CMD-C2D	-2.47	1.45	1.50
15	aB	803	CLA	C3B-C2B	-2.47	1.36	1.40
15	a5	407	CLA	CMB-C2B	-2.47	1.46	1.51
15	a4	405	CLA	C1D-C2D	2.47	1.50	1.45
15	a5	409	CLA	CMB-C2B	-2.47	1.46	1.51
15	cX	102	CLA	C3B-C2B	-2.47	1.36	1.40
15	b2	406	CLA	MG-ND	-2.47	2.00	2.05
18	c2	420	BCR	C30-C25	-2.47	1.50	1.53
15	cL	202	CLA	CMD-C2D	-2.47	1.45	1.50
15	cB	802	CLA	C3B-CAB	-2.47	1.42	1.47
15	c3	405	CLA	C1D-C2D	2.47	1.50	1.45
15	cB	810	CLA	C4B-CHC	-2.47	1.34	1.41
15	cA	836	CLA	CHC-C1C	2.47	1.41	1.35
15	b2	402	CLA	CMB-C2B	-2.47	1.46	1.51
15	c3	408	CLA	CMB-C2B	-2.47	1.46	1.51
18	bA	849	BCR	C30-C25	-2.47	1.50	1.53
15	aB	811	CLA	C3B-CAB	-2.47	1.42	1.47
15	bA	836	CLA	CHC-C1C	2.47	1.41	1.35
15	aB	802	CLA	C3B-CAB	-2.47	1.42	1.47
15	cA	821	CLA	MG-ND	-2.47	2.00	2.05
15	aA	842	CLA	C3B-C2B	-2.47	1.36	1.40
15	bB	836	CLA	CMD-C2D	-2.47	1.45	1.50
15	cA	835	CLA	CMC-C2C	-2.47	1.45	1.50
15	aA	826	CLA	MG-ND	-2.47	2.00	2.05
15	bA	826	CLA	MG-ND	-2.47	2.00	2.05
15	aB	810	CLA	C4B-CHC	-2.47	1.34	1.41
18	bB	845	BCR	C30-C25	-2.47	1.50	1.53
15	b2	415	CLA	CMB-C2B	-2.47	1.46	1.51
15	bA	832	CLA	C3B-C2B	-2.47	1.36	1.40
15	bA	841	CLA	C3B-C2B	-2.47	1.36	1.40
15	b5	416	CLA	C3C-C2C	2.47	1.42	1.36
15	bB	806	CLA	C1D-ND	2.47	1.40	1.37
15	aA	805	CLA	CMC-C2C	-2.47	1.45	1.50
15	bL	203	CLA	CMD-C2D	-2.47	1.45	1.50
15	aA	836	CLA	CHC-C1C	2.47	1.41	1.35
15	a4	412	CLA	CMC-C2C	-2.46	1.45	1.50
15	c4	405	CLA	C1D-C2D	2.46	1.50	1.45
15	bB	835	CLA	CMC-C2C	-2.46	1.45	1.50
15	bB	803	CLA	C3B-C2B	-2.46	1.36	1.40
15	cB	809	CLA	C1D-ND	2.46	1.40	1.37
15	bA	842	CLA	C3B-C2B	-2.46	1.37	1.40
15	aL	201	CLA	C3B-CAB	-2.46	1.42	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	403	CLA	CMD-C2D	-2.46	1.45	1.50
15	bB	841	CLA	C3B-C2B	-2.46	1.37	1.40
15	bB	802	CLA	CHC-C1C	2.46	1.41	1.35
15	a3	416	CLA	C4C-C3C	2.46	1.49	1.45
18	c1	419	BCR	C30-C25	-2.46	1.50	1.53
15	a1	422	CLA	CMD-C2D	-2.46	1.45	1.50
15	cB	803	CLA	C3B-C2B	-2.46	1.37	1.40
15	cB	820	CLA	C3B-C2B	-2.46	1.37	1.40
15	c4	412	CLA	CMC-C2C	-2.46	1.45	1.50
15	aX	102	CLA	C3B-C2B	-2.46	1.37	1.40
15	bA	815	CLA	C3B-CAB	-2.46	1.42	1.47
15	aB	820	CLA	C3B-C2B	-2.46	1.37	1.40
15	cA	833	CLA	CMD-C2D	-2.46	1.45	1.50
15	b5	412	CLA	MG-ND	-2.46	2.00	2.05
15	bB	822	CLA	CMB-C2B	-2.46	1.46	1.51
15	bB	819	CLA	MG-ND	-2.46	2.00	2.05
15	bB	837	CLA	CMC-C2C	-2.46	1.45	1.50
15	aA	821	CLA	MG-ND	-2.46	2.00	2.05
15	bL	203	CLA	CMC-C2C	-2.46	1.45	1.50
15	aA	835	CLA	C3B-CAB	-2.46	1.42	1.47
18	aB	845	BCR	C30-C25	-2.46	1.50	1.53
15	b4	412	CLA	CMC-C2C	-2.46	1.45	1.50
18	c5	418	BCR	C33-C5	-2.46	1.46	1.50
18	b1	419	BCR	C30-C25	-2.46	1.50	1.53
15	b2	406	CLA	CMB-C2B	-2.46	1.46	1.51
15	cB	826	CLA	CMD-C2D	-2.46	1.45	1.50
15	cB	837	CLA	CMC-C2C	-2.46	1.45	1.50
15	c6	416	CLA	CHC-C1C	2.46	1.41	1.35
15	a5	416	CLA	C3C-C2C	2.46	1.41	1.36
18	aB	849	BCR	C38-C26	-2.46	1.46	1.50
18	cB	845	BCR	C30-C25	-2.45	1.50	1.53
15	b3	421	CLA	C2A-C1A	2.45	1.57	1.52
15	bL	203	CLA	C3B-CAB	-2.45	1.42	1.47
15	aB	819	CLA	CMD-C2D	-2.45	1.45	1.50
15	cB	838	CLA	CMD-C2D	-2.45	1.45	1.50
15	aL	202	CLA	CMD-C2D	-2.45	1.45	1.50
15	aB	808	CLA	C1D-ND	2.45	1.40	1.37
15	b6	416	CLA	CHC-C1C	2.45	1.41	1.35
15	b3	412	CLA	MG-ND	-2.45	2.00	2.05
15	bA	807	CLA	CMB-C2B	-2.45	1.46	1.51
15	bB	840	CLA	C4B-CHC	-2.45	1.34	1.41
15	bB	838	CLA	CMD-C2D	-2.45	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aL	202	CLA	C3B-CAB	-2.45	1.42	1.47
15	aB	838	CLA	CMD-C2D	-2.45	1.45	1.50
15	aB	840	CLA	C4B-CHC	-2.45	1.34	1.41
15	cB	828	CLA	CMC-C2C	-2.45	1.45	1.50
15	b1	416	CLA	C3C-C2C	2.45	1.41	1.36
15	bA	844	CLA	CMB-C2B	-2.45	1.46	1.51
15	cA	824	CLA	C3B-C2B	-2.45	1.37	1.40
15	aA	816	CLA	CMB-C2B	-2.45	1.46	1.51
15	bL	202	CLA	C3B-CAB	-2.45	1.42	1.47
15	bA	828	CLA	C1D-ND	2.45	1.40	1.37
15	bB	828	CLA	CMC-C2C	-2.45	1.45	1.50
15	cB	811	CLA	CMD-C2D	-2.45	1.45	1.50
15	aB	809	CLA	MG-ND	-2.45	2.00	2.05
15	a6	415	CLA	CMB-C2B	-2.45	1.46	1.51
15	c3	412	CLA	MG-ND	-2.45	2.00	2.05
15	c2	402	CLA	CMB-C2B	-2.45	1.46	1.51
15	a1	411	CLA	C3B-C2B	-2.45	1.37	1.40
15	cB	840	CLA	C4B-CHC	-2.45	1.34	1.41
15	bA	821	CLA	MG-ND	-2.45	2.00	2.05
15	aB	830	CLA	C4B-CHC	-2.45	1.34	1.41
15	cB	802	CLA	CHC-C1C	2.44	1.41	1.35
15	c2	406	CLA	MG-ND	-2.44	2.00	2.05
15	aB	815	CLA	CMC-C2C	-2.44	1.45	1.50
15	aB	837	CLA	CMC-C2C	-2.44	1.45	1.50
15	c6	406	CLA	C1D-C2D	2.44	1.50	1.45
15	bA	833	CLA	CMD-C2D	-2.44	1.45	1.50
15	cA	815	CLA	C3B-CAB	-2.44	1.43	1.47
15	cA	828	CLA	C1D-ND	2.44	1.40	1.37
15	aA	844	CLA	CMB-C2B	-2.44	1.46	1.51
15	bB	824	CLA	CMB-C2B	-2.44	1.46	1.51
15	cA	807	CLA	CMB-C2B	-2.44	1.46	1.51
15	cA	830	CLA	CMC-C2C	-2.44	1.45	1.50
15	a6	413	CLA	MG-ND	-2.44	2.00	2.05
15	aA	807	CLA	CMB-C2B	-2.44	1.46	1.51
15	c2	415	CLA	CMB-C2B	-2.44	1.46	1.51
15	aB	802	CLA	CHC-C1C	2.44	1.41	1.35
15	aB	811	CLA	CMD-C2D	-2.44	1.45	1.50
15	aB	828	CLA	CMC-C2C	-2.44	1.45	1.50
15	bB	815	CLA	CMC-C2C	-2.44	1.45	1.50
15	bA	807	CLA	C3B-CAB	-2.44	1.43	1.47
15	aA	812	CLA	CMD-C2D	-2.44	1.45	1.50
15	cA	832	CLA	C3B-C2B	-2.44	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	806	CLA	C1D-ND	2.44	1.40	1.37
15	a2	406	CLA	CMB-C2B	-2.44	1.46	1.51
15	c3	416	CLA	C4C-C3C	2.44	1.49	1.45
15	bA	803	CLA	MG-ND	-2.44	2.01	2.05
15	b3	415	CLA	C3B-CAB	-2.44	1.43	1.47
15	a4	421	CLA	CMD-C2D	-2.44	1.45	1.50
15	bB	811	CLA	CMD-C2D	-2.44	1.45	1.50
15	aA	824	CLA	C3B-C2B	-2.44	1.37	1.40
15	cB	809	CLA	MG-ND	-2.44	2.01	2.05
15	aA	819	CLA	CMD-C2D	-2.44	1.45	1.50
15	aB	814	CLA	MG-ND	-2.44	2.01	2.05
15	cB	822	CLA	CMB-C2B	-2.44	1.46	1.51
15	aA	813	CLA	CMD-C2D	-2.44	1.45	1.50
15	aB	831	CLA	C3B-C2B	-2.44	1.37	1.40
15	a1	415	CLA	C3C-C2C	2.44	1.41	1.36
15	cA	838	CLA	C4B-CHC	-2.44	1.34	1.41
15	cA	805	CLA	CMC-C2C	-2.44	1.45	1.50
15	c2	416	CLA	CHC-C1C	2.44	1.41	1.35
15	bB	831	CLA	C3B-C2B	-2.44	1.37	1.40
15	a6	413	CLA	CMC-C2C	-2.43	1.45	1.50
15	bA	804	CLA	MG-ND	-2.43	2.01	2.05
15	a3	412	CLA	MG-ND	-2.43	2.01	2.05
15	cA	825	CLA	CMD-C2D	-2.43	1.45	1.50
15	aA	838	CLA	C4B-CHC	-2.43	1.34	1.41
18	bB	850	BCR	C38-C26	-2.43	1.46	1.50
15	b5	407	CLA	CMB-C2B	-2.43	1.46	1.51
15	c5	416	CLA	C3C-C2C	2.43	1.41	1.36
15	bA	812	CLA	CMD-C2D	-2.43	1.45	1.50
15	bB	830	CLA	C4B-CHC	-2.43	1.34	1.41
15	bA	805	CLA	CMC-C2C	-2.43	1.45	1.50
15	bB	826	CLA	CMD-C2D	-2.43	1.45	1.50
15	c6	413	CLA	MG-ND	-2.43	2.01	2.05
15	cA	835	CLA	C3B-CAB	-2.43	1.43	1.47
18	a1	421	BCR	C1-C6	-2.43	1.50	1.53
15	b1	405	CLA	C1D-C2D	2.43	1.50	1.45
15	c2	406	CLA	CMB-C2B	-2.43	1.46	1.51
15	b6	415	CLA	CMB-C2B	-2.43	1.46	1.51
15	bB	809	CLA	MG-ND	-2.43	2.01	2.05
15	a1	404	CLA	C1D-C2D	2.43	1.50	1.45
15	aA	828	CLA	C1D-ND	2.43	1.40	1.37
15	a6	422	CLA	CMD-C2D	-2.43	1.45	1.50
15	c5	405	CLA	C1D-C2D	2.43	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	cB	849	BCR	C38-C26	-2.43	1.46	1.50
15	c5	407	CLA	CMB-C2B	-2.43	1.46	1.51
18	b2	420	BCR	C30-C25	-2.43	1.50	1.53
15	c4	421	CLA	CMD-C2D	-2.43	1.45	1.50
15	bB	831	CLA	CMD-C2D	-2.43	1.45	1.50
15	cB	827	CLA	CMD-C2D	-2.43	1.45	1.50
15	a3	416	CLA	C3C-C2C	2.43	1.41	1.36
15	b2	408	CLA	CMB-C2B	-2.43	1.46	1.51
15	cB	830	CLA	C4B-CHC	-2.42	1.34	1.41
18	b6	421	BCR	C33-C5	-2.42	1.47	1.50
15	cA	842	CLA	MG-ND	-2.42	2.01	2.05
15	bA	838	CLA	C4B-CHC	-2.42	1.34	1.41
15	bA	813	CLA	C3B-C2B	-2.42	1.37	1.40
15	aB	831	CLA	CMD-C2D	-2.42	1.45	1.50
15	bA	809	CLA	CMD-C2D	-2.42	1.45	1.50
15	cA	812	CLA	CMD-C2D	-2.42	1.45	1.50
15	c1	412	CLA	MG-ND	-2.42	2.01	2.05
15	c1	416	CLA	C3C-C2C	2.42	1.41	1.36
15	aA	820	CLA	CMD-C2D	-2.42	1.45	1.50
15	cB	832	CLA	CMD-C2D	-2.42	1.45	1.50
18	a5	401	BCR	C33-C5	-2.42	1.47	1.50
15	cA	803	CLA	MG-ND	-2.42	2.01	2.05
15	cA	819	CLA	CMD-C2D	-2.42	1.45	1.50
15	bA	816	CLA	CMC-C2C	-2.42	1.45	1.50
15	cA	820	CLA	CMD-C2D	-2.42	1.45	1.50
15	bA	843	CLA	MG-ND	-2.42	2.01	2.05
15	cA	813	CLA	CMD-C2D	-2.42	1.45	1.50
15	cB	823	CLA	CMD-C2D	-2.42	1.45	1.50
15	bB	833	CLA	MG-ND	-2.42	2.01	2.05
15	bA	830	CLA	CMC-C2C	-2.42	1.45	1.50
15	aA	815	CLA	C3B-CAB	-2.42	1.43	1.47
15	aA	804	CLA	MG-ND	-2.42	2.01	2.05
15	aB	822	CLA	CMB-C2B	-2.42	1.46	1.51
15	c6	415	CLA	CMB-C2B	-2.42	1.46	1.51
15	aA	843	CLA	MG-ND	-2.42	2.01	2.05
15	bA	819	CLA	CMD-C2D	-2.42	1.45	1.50
15	cB	839	CLA	CMC-C2C	-2.42	1.45	1.50
15	cA	814	CLA	MG-ND	-2.42	2.01	2.05
15	b4	405	CLA	C1D-C2D	2.42	1.50	1.45
15	aB	817	CLA	C1D-ND	2.42	1.40	1.37
15	cA	830	CLA	C1D-ND	2.42	1.40	1.37
15	c1	409	CLA	CMB-C2B	-2.42	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	829	CLA	C3B-C2B	-2.42	1.37	1.40
18	cK	101	BCR	C30-C25	-2.42	1.50	1.53
15	c1	405	CLA	C1D-C2D	2.42	1.50	1.45
15	c2	417	CLA	C4C-C3C	2.42	1.49	1.45
15	bA	840	CLA	C4B-CHC	-2.42	1.34	1.41
18	c5	401	BCR	C33-C5	-2.42	1.47	1.50
15	aB	814	CLA	CMD-C2D	-2.42	1.45	1.50
15	aB	827	CLA	CMD-C2D	-2.42	1.45	1.50
15	bJ	102	CLA	C3B-C2B	-2.41	1.37	1.40
15	aA	825	CLA	CMD-C2D	-2.41	1.45	1.50
15	b6	413	CLA	CMC-C2C	-2.41	1.45	1.50
15	cB	831	CLA	CMD-C2D	-2.41	1.45	1.50
15	cA	843	CLA	CMB-C2B	-2.41	1.46	1.51
15	b5	405	CLA	C1D-C2D	2.41	1.50	1.45
15	b3	412	CLA	CMC-C2C	-2.41	1.45	1.50
15	a1	412	CLA	C3B-C2B	-2.41	1.37	1.40
15	aB	824	CLA	CMB-C2B	-2.41	1.46	1.51
15	c4	417	CLA	C4D-ND	-2.41	1.34	1.37
18	bB	848	BCR	C33-C5	-2.41	1.47	1.50
18	b1	418	BCR	C33-C5	-2.41	1.47	1.50
15	bA	830	CLA	C1D-ND	2.41	1.40	1.37
15	b3	415	CLA	MG-ND	-2.41	2.01	2.05
15	cA	840	CLA	C4B-CHC	-2.41	1.34	1.41
15	c1	416	CLA	C3B-CAB	-2.41	1.43	1.47
15	aA	810	CLA	MG-ND	-2.41	2.01	2.05
15	bB	814	CLA	MG-ND	-2.41	2.01	2.05
15	cB	805	CLA	CMC-C2C	-2.41	1.45	1.50
15	aA	807	CLA	C3B-CAB	-2.41	1.43	1.47
15	b1	409	CLA	CMB-C2B	-2.41	1.46	1.51
15	cB	812	CLA	CMB-C2B	-2.41	1.46	1.51
15	c2	410	CLA	CMB-C2B	-2.41	1.46	1.51
15	aA	845	CLA	CMD-C2D	-2.41	1.45	1.50
15	bB	827	CLA	CMD-C2D	-2.41	1.45	1.50
15	aA	830	CLA	CMC-C2C	-2.41	1.45	1.50
15	c6	413	CLA	CMC-C2C	-2.41	1.45	1.50
15	cL	202	CLA	MG-ND	-2.41	2.01	2.05
15	cB	821	CLA	CMD-C2D	-2.41	1.45	1.50
15	b4	416	CLA	C3C-C2C	2.41	1.41	1.36
15	cA	844	CLA	CMD-C2D	-2.41	1.45	1.50
15	bA	832	CLA	CHC-C1C	2.41	1.41	1.35
15	a3	405	CLA	C1D-C2D	2.41	1.50	1.45
15	aA	830	CLA	C1D-ND	2.41	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	416	CLA	C3B-CAB	-2.41	1.43	1.47
15	cA	807	CLA	C3B-CAB	-2.41	1.43	1.47
15	aB	832	CLA	CMD-C2D	-2.41	1.45	1.50
15	cA	804	CLA	MG-ND	-2.41	2.01	2.05
15	bB	805	CLA	CMC-C2C	-2.41	1.45	1.50
15	bA	816	CLA	CMB-C2B	-2.40	1.46	1.51
15	aB	805	CLA	CMC-C2C	-2.40	1.45	1.50
15	b5	403	CLA	CMB-C2B	-2.40	1.46	1.51
15	cA	809	CLA	CMD-C2D	-2.40	1.45	1.50
15	aA	832	CLA	CHC-C1C	2.40	1.41	1.35
15	aA	839	CLA	CMC-C2C	-2.40	1.45	1.50
15	aB	834	CLA	CMD-C2D	-2.40	1.45	1.50
15	a1	411	CLA	MG-ND	-2.40	2.01	2.05
15	a5	420	CLA	MG-ND	-2.40	2.01	2.05
15	aB	823	CLA	CMD-C2D	-2.40	1.45	1.50
15	bA	813	CLA	CMD-C2D	-2.40	1.45	1.50
15	b1	413	CLA	C3B-C2B	-2.40	1.37	1.40
15	cA	832	CLA	CHC-C1C	2.40	1.41	1.35
15	c2	408	CLA	CMB-C2B	-2.40	1.46	1.51
15	bA	820	CLA	CMD-C2D	-2.40	1.45	1.50
15	b1	412	CLA	CMC-C2C	-2.40	1.45	1.50
15	cA	816	CLA	CMC-C2C	-2.40	1.45	1.50
15	b2	417	CLA	C4C-C3C	2.40	1.49	1.45
18	b5	401	BCR	C33-C5	-2.40	1.47	1.50
15	c4	416	CLA	C3C-C2C	2.40	1.41	1.36
15	bB	812	CLA	CMB-C2B	-2.40	1.46	1.51
15	cA	823	CLA	CMB-C2B	-2.40	1.46	1.51
15	aA	808	CLA	C3B-C2B	-2.40	1.37	1.40
15	aB	828	CLA	CHC-C1C	2.40	1.41	1.35
15	cB	833	CLA	CMD-C2D	-2.40	1.45	1.50
15	c5	412	CLA	CMC-C2C	-2.40	1.45	1.50
15	bB	821	CLA	CMD-C2D	-2.40	1.45	1.50
15	bB	834	CLA	CMD-C2D	-2.40	1.45	1.50
15	b6	413	CLA	MG-ND	-2.40	2.01	2.05
15	bA	835	CLA	C3B-CAB	-2.40	1.43	1.47
15	aB	833	CLA	MG-ND	-2.40	2.01	2.05
15	a4	416	CLA	C3C-C2C	2.40	1.41	1.36
15	cA	810	CLA	MG-ND	-2.40	2.01	2.05
15	aA	816	CLA	CMC-C2C	-2.40	1.45	1.50
18	c1	418	BCR	C33-C5	-2.40	1.47	1.50
15	cA	816	CLA	CMB-C2B	-2.40	1.46	1.51
15	cB	831	CLA	C3B-C2B	-2.40	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	814	CLA	MG-ND	-2.40	2.01	2.05
15	bA	834	CLA	CHC-C1C	2.40	1.41	1.35
15	bA	845	CLA	C3B-C2B	-2.40	1.37	1.40
15	bB	833	CLA	CMD-C2D	-2.40	1.45	1.50
18	a1	418	BCR	C33-C5	-2.40	1.47	1.50
15	cB	840	CLA	C3B-CAB	-2.40	1.43	1.47
15	cB	824	CLA	CMB-C2B	-2.40	1.46	1.51
15	cB	832	CLA	C3B-C2B	-2.39	1.37	1.40
15	aB	839	CLA	CMC-C2C	-2.39	1.45	1.50
15	bB	832	CLA	CMD-C2D	-2.39	1.45	1.50
15	a3	415	CLA	MG-ND	-2.39	2.01	2.05
15	c6	404	CLA	CMD-C2D	-2.39	1.45	1.50
15	aA	840	CLA	C4B-CHC	-2.39	1.34	1.41
15	a4	417	CLA	C4D-ND	-2.39	1.34	1.37
15	c1	413	CLA	C3B-C2B	-2.39	1.37	1.40
18	bA	848	BCR	C30-C25	-2.39	1.50	1.53
15	aJ	203	CLA	C3B-C2B	-2.39	1.37	1.40
15	c3	416	CLA	C3C-C2C	2.39	1.41	1.36
15	b2	416	CLA	C3B-CAB	-2.39	1.43	1.47
15	a5	403	CLA	CMB-C2B	-2.39	1.46	1.51
15	bB	829	CLA	C3B-C2B	-2.39	1.37	1.40
15	a5	412	CLA	CMC-C2C	-2.39	1.45	1.50
15	cB	814	CLA	CMD-C2D	-2.39	1.45	1.50
18	a1	417	BCR	C33-C5	-2.39	1.47	1.50
15	bA	823	CLA	CMB-C2B	-2.39	1.46	1.51
15	bA	825	CLA	CMD-C2D	-2.39	1.45	1.50
15	bA	845	CLA	CMD-C2D	-2.39	1.45	1.50
15	b1	403	CLA	CMB-C2B	-2.39	1.46	1.51
15	aB	803	CLA	CMD-C2D	-2.39	1.45	1.50
15	b5	412	CLA	CMC-C2C	-2.39	1.45	1.50
15	cB	825	CLA	CAC-C3C	-2.39	1.45	1.51
15	bB	817	CLA	C1D-ND	2.39	1.40	1.37
15	cA	834	CLA	CHC-C1C	2.39	1.41	1.35
15	bL	203	CLA	MG-ND	-2.39	2.01	2.05
15	cL	201	CLA	MG-ND	-2.39	2.01	2.05
15	aB	833	CLA	CMD-C2D	-2.39	1.45	1.50
15	cB	815	CLA	CMC-C2C	-2.39	1.45	1.50
15	a2	416	CLA	CHC-C1C	2.39	1.41	1.35
15	b2	409	CLA	CMB-C2B	-2.39	1.46	1.51
15	a6	417	CLA	C3C-C2C	2.39	1.41	1.36
15	bB	825	CLA	CAC-C3C	-2.39	1.45	1.51
15	aA	809	CLA	CMD-C2D	-2.39	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	829	CLA	MG-ND	-2.39	2.01	2.05
15	bB	803	CLA	CMD-C2D	-2.39	1.45	1.50
15	aB	825	CLA	CAC-C3C	-2.39	1.45	1.51
18	b1	419	BCR	C33-C5	-2.39	1.47	1.50
15	cB	821	CLA	C3B-C2B	-2.39	1.37	1.40
15	cB	819	CLA	CAC-C3C	-2.39	1.45	1.51
15	aL	202	CLA	MG-ND	-2.39	2.01	2.05
15	aB	821	CLA	CMD-C2D	-2.38	1.45	1.50
15	aB	819	CLA	CAC-C3C	-2.38	1.45	1.51
15	c6	413	CLA	CHC-C1C	2.38	1.41	1.35
15	bA	804	CLA	C1D-ND	2.38	1.40	1.37
15	aB	829	CLA	MG-ND	-2.38	2.01	2.05
15	cB	813	CLA	C3B-C2B	-2.38	1.37	1.40
15	b5	420	CLA	MG-ND	-2.38	2.01	2.05
15	bA	826	CLA	CMD-C2D	-2.38	1.45	1.50
15	cB	806	CLA	CMD-C2D	-2.38	1.45	1.50
15	b3	405	CLA	C1D-C2D	2.38	1.50	1.45
15	c1	403	CLA	CMB-C2B	-2.38	1.46	1.51
15	aB	807	CLA	CHC-C1C	2.38	1.41	1.35
15	cA	833	CLA	C3B-CAB	-2.38	1.43	1.47
15	aA	826	CLA	CMD-C2D	-2.38	1.45	1.50
15	b4	421	CLA	CMD-C2D	-2.38	1.45	1.50
15	bA	810	CLA	MG-ND	-2.38	2.01	2.05
15	aB	840	CLA	MG-ND	-2.38	2.01	2.05
15	c3	415	CLA	MG-ND	-2.38	2.01	2.05
15	c5	403	CLA	CMB-C2B	-2.38	1.46	1.51
15	a6	413	CLA	CHC-C1C	2.38	1.41	1.35
15	cA	805	CLA	CMD-C2D	-2.38	1.45	1.50
15	c5	420	CLA	MG-ND	-2.38	2.01	2.05
15	aA	834	CLA	CHC-C1C	2.38	1.41	1.35
15	bB	807	CLA	CHC-C1C	2.38	1.41	1.35
15	b6	413	CLA	CHC-C1C	2.38	1.41	1.35
15	bA	811	CLA	CMD-C2D	-2.38	1.45	1.50
15	cA	826	CLA	CMD-C2D	-2.38	1.45	1.50
15	a1	402	CLA	CMB-C2B	-2.38	1.46	1.51
15	b4	403	CLA	CMB-C2B	-2.38	1.46	1.51
15	b1	416	CLA	C3B-CAB	-2.38	1.43	1.47
15	cA	839	CLA	CMC-C2C	-2.38	1.45	1.50
15	a3	421	CLA	CMB-C2B	-2.38	1.46	1.51
15	bB	823	CLA	CMD-C2D	-2.38	1.45	1.50
15	cA	811	CLA	CMD-C2D	-2.38	1.45	1.50
15	bB	840	CLA	C3B-CAB	-2.38	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	803	CLA	CMD-C2D	-2.38	1.45	1.50
15	bB	828	CLA	CHC-C1C	2.38	1.41	1.35
15	c3	403	CLA	CMD-C2D	-2.38	1.45	1.50
15	cA	813	CLA	C3B-C2B	-2.38	1.37	1.40
15	bB	832	CLA	C3B-C2B	-2.37	1.37	1.40
15	a3	412	CLA	CMC-C2C	-2.37	1.45	1.50
15	bB	832	CLA	CMC-C2C	-2.37	1.45	1.50
15	c2	408	CLA	CMD-C2D	-2.37	1.45	1.50
15	cA	805	CLA	MG-ND	-2.37	2.01	2.05
15	bB	808	CLA	C1D-ND	2.37	1.40	1.37
15	cB	808	CLA	C1D-ND	2.37	1.40	1.37
15	cB	828	CLA	CHC-C1C	2.37	1.41	1.35
15	b2	410	CLA	CMB-C2B	-2.37	1.46	1.51
15	a1	415	CLA	C1C-NC	-2.37	1.34	1.37
15	cA	830	CLA	C3B-CAB	-2.37	1.43	1.47
15	a2	403	CLA	CMB-C2B	-2.37	1.46	1.51
15	aA	823	CLA	CMB-C2B	-2.37	1.46	1.51
15	a2	410	CLA	CMB-C2B	-2.37	1.46	1.51
15	c4	409	CLA	CMB-C2B	-2.37	1.46	1.51
15	cF	203	CLA	CMD-C2D	-2.37	1.45	1.50
15	aA	842	CLA	MG-ND	-2.37	2.01	2.05
15	aB	801	CLA	CMD-C2D	-2.37	1.45	1.50
15	a1	408	CLA	CMB-C2B	-2.37	1.46	1.51
15	a1	411	CLA	CMC-C2C	-2.37	1.45	1.50
15	bA	806	CLA	C3B-CAB	-2.37	1.43	1.47
15	bB	829	CLA	MG-ND	-2.37	2.01	2.05
15	cA	844	CLA	C3B-C2B	-2.37	1.37	1.40
15	a4	403	CLA	CMB-C2B	-2.37	1.46	1.51
15	bA	831	CLA	C4B-CHC	-2.37	1.34	1.41
15	bA	842	CLA	MG-ND	-2.37	2.01	2.05
15	a2	408	CLA	CMB-C2B	-2.36	1.46	1.51
15	c1	416	CLA	C4C-C3C	2.36	1.49	1.45
18	aF	201	BCR	C32-C1	-2.36	1.49	1.53
15	bK	101	CLA	MG-ND	-2.36	2.01	2.05
15	b3	416	CLA	C3C-C2C	2.36	1.41	1.36
15	b2	416	CLA	CHC-C1C	2.36	1.41	1.35
15	cB	832	CLA	CMC-C2C	-2.36	1.45	1.50
18	c1	419	BCR	C33-C5	-2.36	1.47	1.50
15	bB	814	CLA	CMD-C2D	-2.36	1.45	1.50
15	a2	422	CLA	C3B-C2B	-2.36	1.37	1.40
15	cF	201	CLA	MG-ND	-2.36	2.01	2.05
15	bB	810	CLA	CAA-C2A	-2.36	1.49	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	403	CLA	CMD-C2D	-2.36	1.45	1.50
15	cB	834	CLA	CMD-C2D	-2.36	1.45	1.50
15	c3	412	CLA	CMC-C2C	-2.36	1.45	1.50
15	b4	409	CLA	CMB-C2B	-2.36	1.46	1.51
15	c6	410	CLA	CMB-C2B	-2.36	1.46	1.51
15	bB	840	CLA	MG-ND	-2.36	2.01	2.05
15	bL	202	CLA	MG-ND	-2.36	2.01	2.05
15	c4	403	CLA	CMB-C2B	-2.36	1.46	1.51
18	a3	401	BCR	C4-C5	-2.36	1.46	1.51
15	bA	833	CLA	C3B-CAB	-2.36	1.43	1.47
15	aB	837	CLA	C3B-C2B	-2.36	1.37	1.40
15	a2	403	CLA	CMD-C2D	-2.36	1.45	1.50
15	bA	830	CLA	C3B-CAB	-2.36	1.43	1.47
15	a1	409	CLA	C3C-C2C	2.36	1.41	1.36
15	cB	833	CLA	MG-ND	-2.36	2.01	2.05
15	cB	801	CLA	CMD-C2D	-2.36	1.45	1.50
15	a6	410	CLA	CMB-C2B	-2.36	1.46	1.51
15	bB	819	CLA	CAC-C3C	-2.36	1.45	1.51
15	cJ	102	CLA	C3B-C2B	-2.36	1.37	1.40
15	aB	806	CLA	CHC-C1C	2.36	1.41	1.35
15	bB	806	CLA	CHC-C1C	2.36	1.41	1.35
15	c2	407	CLA	CMB-C2B	-2.36	1.46	1.51
15	aB	829	CLA	C1D-ND	2.36	1.40	1.37
15	bB	829	CLA	C1D-ND	2.36	1.40	1.37
15	a2	409	CLA	CMB-C2B	-2.36	1.46	1.51
15	aJ	201	CLA	C3B-CAB	-2.36	1.43	1.47
18	a2	419	BCR	C33-C5	-2.36	1.47	1.50
15	aB	812	CLA	CMB-C2B	-2.36	1.46	1.51
15	aB	829	CLA	C3B-C2B	-2.36	1.37	1.40
15	aB	832	CLA	C3B-C2B	-2.36	1.37	1.40
15	aA	822	CLA	CMD-C2D	-2.36	1.45	1.50
15	aB	806	CLA	CMD-C2D	-2.36	1.45	1.50
15	b1	412	CLA	MG-ND	-2.35	2.01	2.05
15	b6	404	CLA	CMD-C2D	-2.35	1.45	1.50
15	aA	831	CLA	C4B-CHC	-2.35	1.34	1.41
15	bB	801	CLA	CMD-C2D	-2.35	1.45	1.50
15	aA	845	CLA	C3B-C2B	-2.35	1.37	1.40
15	b4	421	CLA	C3B-C2B	-2.35	1.37	1.40
15	bA	805	CLA	MG-ND	-2.35	2.01	2.05
15	bA	839	CLA	CMC-C2C	-2.35	1.45	1.50
15	a6	411	CLA	C3C-C2C	2.35	1.41	1.36
15	aA	811	CLA	CMD-C2D	-2.35	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	417	CLA	C4C-C3C	2.35	1.49	1.45
15	a2	408	CLA	CMD-C2D	-2.35	1.45	1.50
18	aB	848	BCR	C33-C5	-2.35	1.47	1.50
15	bB	806	CLA	CMD-C2D	-2.35	1.45	1.50
15	bB	840	CLA	CMC-C2C	-2.35	1.45	1.50
15	c2	409	CLA	CMB-C2B	-2.35	1.46	1.51
15	b2	403	CLA	CMB-C2B	-2.35	1.46	1.51
15	bB	837	CLA	C3B-C2B	-2.35	1.37	1.40
15	aA	837	CLA	CMD-C2D	-2.35	1.45	1.50
15	aA	805	CLA	CMD-C2D	-2.35	1.45	1.50
15	a3	407	CLA	MG-ND	-2.35	2.01	2.05
15	aA	824	CLA	CMD-C2D	-2.35	1.45	1.50
15	a2	407	CLA	CMB-C2B	-2.35	1.46	1.51
15	aA	813	CLA	C3B-C2B	-2.35	1.37	1.40
15	aB	840	CLA	C3B-CAB	-2.35	1.43	1.47
15	aA	833	CLA	C3B-CAB	-2.35	1.43	1.47
15	b6	410	CLA	CMB-C2B	-2.35	1.46	1.51
15	c3	407	CLA	MG-ND	-2.35	2.01	2.05
15	bA	824	CLA	CMD-C2D	-2.35	1.45	1.50
18	a6	421	BCR	C33-C5	-2.35	1.47	1.50
15	bA	805	CLA	CMD-C2D	-2.35	1.45	1.50
15	aB	832	CLA	CMC-C2C	-2.35	1.45	1.50
15	cF	203	CLA	C3B-CAB	-2.34	1.43	1.47
15	c3	415	CLA	C3B-CAB	-2.34	1.43	1.47
15	c2	403	CLA	CMB-C2B	-2.34	1.46	1.51
15	cB	840	CLA	MG-ND	-2.34	2.01	2.05
15	bA	808	CLA	C3B-C2B	-2.34	1.37	1.40
15	cB	817	CLA	C1D-ND	2.34	1.40	1.37
15	bB	839	CLA	CMC-C2C	-2.34	1.45	1.50
18	bB	849	BCR	C32-C1	-2.34	1.49	1.53
15	bB	831	CLA	CHC-C1C	2.34	1.41	1.35
15	aB	810	CLA	CAA-C2A	-2.34	1.49	1.54
15	a1	415	CLA	C4C-C3C	2.34	1.49	1.45
15	b4	415	CLA	C3B-CAB	-2.34	1.43	1.47
15	aB	813	CLA	C3B-C2B	-2.34	1.37	1.40
15	cB	806	CLA	CHC-C1C	2.34	1.41	1.35
15	cA	804	CLA	C1D-ND	2.34	1.40	1.37
15	cB	807	CLA	CHC-C1C	2.34	1.41	1.35
15	b2	403	CLA	CMD-C2D	-2.34	1.45	1.50
15	aA	822	CLA	CMC-C2C	-2.34	1.45	1.50
15	b4	417	CLA	C4D-ND	-2.34	1.34	1.37
15	aA	806	CLA	C3B-CAB	-2.34	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	830	CLA	C3B-CAB	-2.34	1.43	1.47
15	cA	809	CLA	C3B-CAB	-2.34	1.43	1.47
15	cB	810	CLA	CAA-C2A	-2.34	1.49	1.54
15	cA	831	CLA	C4B-CHC	-2.34	1.34	1.41
15	bB	836	CLA	CHC-C1C	2.34	1.41	1.35
15	cA	838	CLA	CHC-C1C	2.34	1.41	1.35
15	bB	805	CLA	CMD-C2D	-2.34	1.45	1.50
15	bA	813	CLA	CMC-C2C	-2.33	1.45	1.50
15	bB	836	CLA	C3B-CAB	-2.33	1.43	1.47
15	cB	831	CLA	CHC-C1C	2.33	1.40	1.35
15	bA	822	CLA	CMD-C2D	-2.33	1.45	1.50
15	aA	813	CLA	CMC-C2C	-2.33	1.45	1.50
15	aB	801	CLA	MG-ND	-2.33	2.01	2.05
15	bB	813	CLA	C3B-C2B	-2.33	1.37	1.40
15	aA	805	CLA	MG-ND	-2.33	2.01	2.05
15	b3	407	CLA	MG-ND	-2.33	2.01	2.05
15	bB	810	CLA	CHC-C1C	2.33	1.40	1.35
15	b2	402	CLA	CMD-C2D	-2.33	1.45	1.50
15	a4	409	CLA	CMB-C2B	-2.33	1.46	1.51
15	bF	201	CLA	C3B-CAB	-2.33	1.43	1.47
15	bB	808	CLA	CMD-C2D	-2.33	1.45	1.50
15	b5	416	CLA	C4C-C3C	2.33	1.49	1.45
15	cA	824	CLA	CMD-C2D	-2.33	1.45	1.50
15	cA	839	CLA	MG-ND	-2.33	2.01	2.05
18	c2	419	BCR	C33-C5	-2.33	1.47	1.50
15	bF	201	CLA	CMD-C2D	-2.33	1.45	1.50
15	c2	414	CLA	MG-ND	-2.33	2.01	2.05
18	b3	401	BCR	C4-C5	-2.33	1.46	1.51
15	aL	201	CLA	MG-ND	-2.33	2.01	2.05
15	aB	839	CLA	C3B-C2B	-2.33	1.37	1.40
15	b3	402	CLA	CMD-C2D	-2.33	1.45	1.50
15	cB	808	CLA	CMD-C2D	-2.33	1.45	1.50
15	cA	837	CLA	CMD-C2D	-2.33	1.45	1.50
15	b6	414	CLA	C3B-C2B	-2.33	1.37	1.40
15	cK	102	CLA	MG-ND	-2.33	2.01	2.05
15	a5	416	CLA	C4C-C3C	2.33	1.49	1.45
15	aA	833	CLA	CMC-C2C	-2.33	1.45	1.50
15	aB	805	CLA	CMD-C2D	-2.33	1.45	1.50
15	aJ	201	CLA	CMD-C2D	-2.33	1.45	1.50
15	a2	414	CLA	MG-ND	-2.32	2.01	2.05
15	a6	404	CLA	CMD-C2D	-2.32	1.45	1.50
15	aB	831	CLA	CHC-C1C	2.32	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	407	CLA	MG-ND	-2.32	2.01	2.05
15	c6	417	CLA	C3C-C2C	2.32	1.41	1.36
15	aA	822	CLA	C1D-ND	2.32	1.40	1.37
15	cB	805	CLA	CMD-C2D	-2.32	1.45	1.50
15	cA	806	CLA	C3B-CAB	-2.32	1.43	1.47
15	a6	422	CLA	O2D-CGD	2.32	1.38	1.33
18	b2	420	BCR	C34-C9	-2.32	1.46	1.50
15	aB	804	CLA	C3B-CAB	-2.32	1.43	1.47
15	aA	819	CLA	C3B-C2B	-2.32	1.37	1.40
15	bA	809	CLA	C3B-CAB	-2.32	1.43	1.47
15	c2	403	CLA	CMD-C2D	-2.32	1.45	1.50
15	bB	839	CLA	C3B-C2B	-2.32	1.37	1.40
18	a6	421	BCR	C1-C6	-2.32	1.50	1.53
15	bA	819	CLA	C3B-C2B	-2.32	1.37	1.40
15	aK	102	CLA	MG-ND	-2.32	2.01	2.05
15	cB	804	CLA	C3B-CAB	-2.32	1.43	1.47
15	bA	838	CLA	CHC-C1C	2.32	1.40	1.35
15	cB	801	CLA	MG-ND	-2.32	2.01	2.05
15	bA	802	CLA	C3B-CAB	-2.32	1.43	1.47
15	c1	410	CLA	C3C-C2C	2.32	1.41	1.36
15	b6	417	CLA	C3C-C2C	2.32	1.41	1.36
15	b2	414	CLA	MG-ND	-2.32	2.01	2.05
15	cB	839	CLA	C3B-C2B	-2.32	1.37	1.40
15	b2	408	CLA	CMD-C2D	-2.32	1.45	1.50
15	cA	822	CLA	CMD-C2D	-2.32	1.45	1.50
15	cB	826	CLA	C3B-CAB	-2.32	1.43	1.47
15	c5	416	CLA	C4C-C3C	2.32	1.49	1.45
15	b6	411	CLA	C3C-C2C	2.32	1.41	1.36
18	c3	401	BCR	C4-C5	-2.32	1.46	1.51
15	cK	102	CLA	CMD-C2D	-2.32	1.45	1.50
15	a3	415	CLA	C3B-CAB	-2.32	1.43	1.47
15	aA	839	CLA	MG-ND	-2.32	2.01	2.05
15	b3	403	CLA	CMD-C2D	-2.32	1.45	1.50
15	bA	837	CLA	CMD-C2D	-2.32	1.45	1.50
15	c3	402	CLA	CMD-C2D	-2.32	1.45	1.50
15	aA	832	CLA	C1D-ND	2.32	1.40	1.37
15	cB	829	CLA	C1D-ND	2.32	1.40	1.37
15	c2	422	CLA	C3B-C2B	-2.32	1.37	1.40
15	b1	410	CLA	C3C-C2C	2.32	1.41	1.36
15	a5	415	CLA	CHC-C1C	2.32	1.40	1.35
15	aB	807	CLA	C1D-ND	2.31	1.40	1.37
15	bB	826	CLA	C3B-CAB	-2.31	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	806	CLA	CMC-C2C	-2.31	1.45	1.50
15	cA	840	CLA	CHC-C1C	2.31	1.40	1.35
15	c5	415	CLA	CHC-C1C	2.31	1.40	1.35
15	bK	101	CLA	CMD-C2D	-2.31	1.45	1.50
15	aA	804	CLA	C1D-ND	2.31	1.40	1.37
15	a3	403	CLA	CMB-C2B	-2.31	1.46	1.51
15	c1	412	CLA	CMC-C2C	-2.31	1.45	1.50
15	aA	838	CLA	CHC-C1C	2.31	1.40	1.35
15	bA	834	CLA	CMC-C2C	-2.31	1.45	1.50
15	cA	813	CLA	CMC-C2C	-2.31	1.45	1.50
15	a6	414	CLA	C3B-C2B	-2.31	1.37	1.40
15	cB	837	CLA	C3B-C2B	-2.31	1.37	1.40
15	b2	416	CLA	MG-ND	-2.31	2.01	2.05
15	c3	403	CLA	CMB-C2B	-2.31	1.46	1.51
15	aA	834	CLA	CMC-C2C	-2.31	1.45	1.50
15	cA	833	CLA	CMC-C2C	-2.31	1.45	1.50
15	cA	808	CLA	C3B-C2B	-2.31	1.37	1.40
18	cF	202	BCR	C32-C1	-2.31	1.49	1.53
15	bB	801	CLA	CMC-C2C	-2.31	1.45	1.50
15	cB	808	CLA	CMC-C2C	-2.31	1.45	1.50
15	c6	411	CLA	C3C-C2C	2.31	1.41	1.36
15	bB	804	CLA	C3B-CAB	-2.31	1.43	1.47
15	b3	408	CLA	CMC-C2C	-2.31	1.45	1.50
15	c2	411	CLA	C3C-C2C	2.31	1.41	1.36
15	b3	403	CLA	CMB-C2B	-2.31	1.46	1.51
15	bB	821	CLA	C3B-C2B	-2.31	1.37	1.40
15	cB	807	CLA	C1D-ND	2.31	1.40	1.37
15	aA	809	CLA	C3B-CAB	-2.31	1.43	1.47
15	bA	808	CLA	CMD-C2D	-2.31	1.45	1.50
15	bA	833	CLA	CMC-C2C	-2.31	1.45	1.50
15	bA	839	CLA	MG-ND	-2.31	2.01	2.05
15	aB	810	CLA	CHC-C1C	2.31	1.40	1.35
15	aA	802	CLA	C3B-CAB	-2.31	1.43	1.47
15	aB	821	CLA	C3B-C2B	-2.31	1.37	1.40
15	bB	841	CLA	CMD-C2D	-2.31	1.45	1.50
15	a4	407	CLA	MG-ND	-2.31	2.01	2.05
18	cB	848	BCR	C33-C5	-2.31	1.47	1.50
15	aB	840	CLA	CMC-C2C	-2.30	1.45	1.50
15	a2	416	CLA	C3B-CAB	-2.30	1.43	1.47
15	cA	808	CLA	CMD-C2D	-2.30	1.45	1.50
15	c4	416	CLA	C4C-C3C	2.30	1.49	1.45
15	cA	802	CLA	C3B-CAB	-2.30	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	837	CLA	CMD-C2D	-2.30	1.45	1.50
15	bA	832	CLA	C1D-ND	2.30	1.40	1.37
15	aB	826	CLA	C3B-CAB	-2.30	1.43	1.47
15	aB	837	CLA	CMD-C2D	-2.30	1.45	1.50
15	aB	836	CLA	CHC-C1C	2.30	1.40	1.35
15	bA	822	CLA	CMC-C2C	-2.30	1.45	1.50
15	b3	407	CLA	CMD-C2D	-2.30	1.45	1.50
15	a1	414	CLA	MG-ND	-2.30	2.01	2.05
15	a2	416	CLA	MG-ND	-2.30	2.01	2.05
15	cA	822	CLA	CMC-C2C	-2.30	1.45	1.50
15	c2	402	CLA	CMD-C2D	-2.30	1.45	1.50
15	c6	403	CLA	CMD-C2D	-2.30	1.45	1.50
15	a4	410	CLA	C3C-C2C	2.30	1.41	1.36
15	c4	410	CLA	C3C-C2C	2.30	1.41	1.36
15	b2	416	CLA	C3B-C2B	-2.30	1.37	1.40
15	cB	806	CLA	CMC-C2C	-2.30	1.45	1.50
15	aB	808	CLA	CMD-C2D	-2.30	1.45	1.50
15	aA	828	CLA	CMD-C2D	-2.30	1.45	1.50
15	cB	836	CLA	C3B-CAB	-2.30	1.43	1.47
15	bB	808	CLA	CMC-C2C	-2.30	1.45	1.50
15	b2	407	CLA	CMB-C2B	-2.30	1.46	1.51
15	b2	411	CLA	C3C-C2C	2.30	1.41	1.36
15	a3	403	CLA	MG-ND	-2.30	2.01	2.05
15	bB	837	CLA	MG-ND	-2.30	2.01	2.05
15	cB	836	CLA	CHC-C1C	2.30	1.40	1.35
15	bB	807	CLA	C1D-ND	2.30	1.40	1.37
15	c1	415	CLA	MG-ND	-2.30	2.01	2.05
15	aB	808	CLA	CMC-C2C	-2.30	1.45	1.50
15	aB	836	CLA	C3B-CAB	-2.30	1.43	1.47
15	b3	421	CLA	CMB-C2B	-2.30	1.46	1.51
15	cA	822	CLA	C1D-ND	2.30	1.40	1.37
15	cB	810	CLA	CHC-C1C	2.30	1.40	1.35
15	cB	810	CLA	C1D-ND	2.29	1.40	1.37
15	aA	820	CLA	C3B-C2B	-2.29	1.37	1.40
15	a4	421	CLA	C3B-C2B	-2.29	1.37	1.40
15	b1	416	CLA	C4C-C3C	2.29	1.49	1.45
15	aK	102	CLA	CMD-C2D	-2.29	1.45	1.50
15	bB	801	CLA	MG-ND	-2.29	2.01	2.05
15	aX	102	CLA	C1D-ND	2.29	1.40	1.37
15	cA	807	CLA	CAA-C2A	-2.29	1.49	1.54
15	c3	407	CLA	CMD-C2D	-2.29	1.45	1.50
15	c2	416	CLA	MG-ND	-2.29	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	810	CLA	C1D-ND	2.29	1.40	1.37
15	bB	810	CLA	C1D-ND	2.29	1.40	1.37
15	c3	403	CLA	MG-ND	-2.29	2.01	2.05
18	a2	420	BCR	C34-C9	-2.29	1.46	1.50
15	bB	806	CLA	CMC-C2C	-2.29	1.45	1.50
15	aB	840	CLA	C1D-ND	2.29	1.40	1.37
15	c4	415	CLA	C3B-CAB	-2.29	1.43	1.47
18	b2	419	BCR	C33-C5	-2.29	1.47	1.50
15	a6	417	CLA	C4C-C3C	2.29	1.49	1.45
15	cB	836	CLA	CMC-C2C	-2.29	1.46	1.50
15	b5	415	CLA	CHC-C1C	2.29	1.40	1.35
15	cB	840	CLA	CMC-C2C	-2.29	1.46	1.50
15	bA	822	CLA	C1D-ND	2.29	1.40	1.37
15	bA	828	CLA	CMD-C2D	-2.29	1.46	1.50
15	cB	801	CLA	CMC-C2C	-2.29	1.46	1.50
15	cA	828	CLA	CMD-C2D	-2.28	1.46	1.50
15	c4	407	CLA	MG-ND	-2.28	2.01	2.05
15	c6	417	CLA	C4C-C3C	2.28	1.49	1.45
15	b1	415	CLA	C3B-CAB	-2.28	1.43	1.47
15	bA	840	CLA	CHC-C1C	2.28	1.40	1.35
15	b1	415	CLA	CHC-C1C	2.28	1.40	1.35
15	bB	838	CLA	C3B-CAB	-2.28	1.43	1.47
15	b1	415	CLA	MG-ND	-2.28	2.01	2.05
15	cA	836	CLA	MG-ND	-2.28	2.01	2.05
15	c4	415	CLA	MG-ND	-2.28	2.01	2.05
15	aA	840	CLA	CHC-C1C	2.28	1.40	1.35
15	bB	836	CLA	CMC-C2C	-2.28	1.46	1.50
15	b2	411	CLA	MG-ND	-2.28	2.01	2.05
15	aB	841	CLA	CMD-C2D	-2.28	1.46	1.50
15	cA	832	CLA	C1D-ND	2.28	1.40	1.37
15	cA	836	CLA	C3B-CAB	-2.28	1.43	1.47
15	cA	809	CLA	CMC-C2C	-2.28	1.46	1.50
15	bX	102	CLA	C1D-ND	2.28	1.40	1.37
15	a3	402	CLA	CMD-C2D	-2.28	1.46	1.50
15	a2	411	CLA	C3C-C2C	2.28	1.41	1.36
15	a5	410	CLA	C3C-C2C	2.28	1.41	1.36
15	aA	825	CLA	MG-ND	-2.28	2.01	2.05
15	a5	415	CLA	MG-ND	-2.28	2.01	2.05
15	a4	415	CLA	C3B-CAB	-2.28	1.43	1.47
18	bB	849	BCR	C33-C5	-2.27	1.47	1.50
15	b4	410	CLA	C3C-C2C	2.27	1.41	1.36
15	cB	840	CLA	C1D-ND	2.27	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c6	402	BCR	C4-C5	-2.27	1.46	1.51
15	cB	841	CLA	CMD-C2D	-2.27	1.46	1.50
15	cA	825	CLA	MG-ND	-2.27	2.01	2.05
15	cB	813	CLA	MG-ND	-2.27	2.01	2.05
15	b5	415	CLA	MG-ND	-2.27	2.01	2.05
15	bA	812	CLA	C3B-CAB	-2.27	1.43	1.47
15	a4	416	CLA	C4C-C3C	2.27	1.48	1.45
15	b4	409	CLA	CMD-C2D	-2.27	1.46	1.50
15	a6	403	CLA	CMD-C2D	-2.27	1.46	1.50
15	aB	801	CLA	CMC-C2C	-2.27	1.46	1.50
15	bA	836	CLA	MG-ND	-2.27	2.01	2.05
15	b4	416	CLA	C4C-C3C	2.27	1.48	1.45
15	bA	836	CLA	C3B-CAB	-2.27	1.43	1.47
15	cA	823	CLA	CMD-C2D	-2.27	1.46	1.50
15	b4	415	CLA	MG-ND	-2.27	2.01	2.05
18	cF	202	BCR	C33-C5	-2.27	1.47	1.50
15	bA	807	CLA	CAA-C2A	-2.27	1.49	1.54
15	b5	410	CLA	MG-ND	-2.27	2.01	2.05
15	c5	415	CLA	MG-ND	-2.27	2.01	2.05
15	c1	412	CLA	C4B-CHC	-2.27	1.34	1.41
15	a4	415	CLA	MG-ND	-2.27	2.01	2.05
15	a3	407	CLA	CMD-C2D	-2.27	1.46	1.50
15	bA	823	CLA	CMD-C2D	-2.27	1.46	1.50
15	c5	412	CLA	CHC-C1C	2.27	1.40	1.35
15	a2	422	CLA	CMC-C2C	-2.26	1.46	1.50
18	aM	101	BCR	C30-C25	-2.26	1.50	1.53
15	b6	417	CLA	C4C-C3C	2.26	1.48	1.45
15	bA	841	CLA	CMC-C2C	-2.26	1.46	1.50
15	c1	413	CLA	MG-ND	-2.26	2.01	2.05
15	a4	409	CLA	CMD-C2D	-2.26	1.46	1.50
15	a5	417	CLA	C4D-ND	-2.26	1.34	1.37
18	c2	420	BCR	C34-C9	-2.26	1.46	1.50
15	bB	840	CLA	C1D-ND	2.26	1.40	1.37
15	aB	806	CLA	C4B-CHC	-2.26	1.34	1.41
15	b5	412	CLA	CHC-C1C	2.26	1.40	1.35
15	a2	411	CLA	MG-ND	-2.26	2.01	2.05
18	aI	103	BCR	C33-C5	-2.26	1.47	1.50
18	b6	402	BCR	C4-C5	-2.26	1.46	1.51
15	a3	408	CLA	CMC-C2C	-2.26	1.46	1.50
15	b6	403	CLA	CMD-C2D	-2.26	1.46	1.50
15	bB	806	CLA	C4B-CHC	-2.26	1.34	1.41
15	aB	837	CLA	MG-ND	-2.26	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	833	CLA	CMC-C2C	-2.26	1.46	1.50
15	b5	402	CLA	CMD-C2D	-2.26	1.46	1.50
15	c3	408	CLA	CMC-C2C	-2.26	1.46	1.50
15	b2	417	CLA	C3C-C2C	2.26	1.41	1.36
15	cB	837	CLA	MG-ND	-2.26	2.01	2.05
15	aA	808	CLA	CMD-C2D	-2.26	1.46	1.50
15	c4	407	CLA	CMD-C2D	-2.26	1.46	1.50
15	c1	415	CLA	CHC-C1C	2.26	1.40	1.35
15	cA	809	CLA	MG-ND	-2.26	2.01	2.05
15	bB	837	CLA	CMD-C2D	-2.26	1.46	1.50
15	cA	834	CLA	CMC-C2C	-2.26	1.46	1.50
18	aA	851	BCR	C38-C26	-2.26	1.47	1.50
15	bA	806	CLA	CMA-C3A	-2.26	1.48	1.53
15	cA	819	CLA	C3B-C2B	-2.26	1.37	1.40
15	b2	413	CLA	CHC-C1C	2.26	1.40	1.35
15	cJ	101	CLA	C3B-C2B	-2.25	1.37	1.40
18	a6	402	BCR	C4-C5	-2.25	1.46	1.51
15	bA	821	CLA	C3B-CAB	-2.25	1.43	1.47
18	bA	852	BCR	C38-C26	-2.25	1.47	1.50
15	cB	830	CLA	CMC-C2C	-2.25	1.46	1.50
15	c5	402	CLA	CMD-C2D	-2.25	1.46	1.50
15	c5	420	CLA	CMD-C2D	-2.25	1.46	1.50
15	a1	414	CLA	CHC-C1C	2.25	1.40	1.35
15	a3	410	CLA	MG-ND	-2.25	2.01	2.05
15	a2	402	CLA	CMD-C2D	-2.25	1.46	1.50
15	b3	403	CLA	MG-ND	-2.25	2.01	2.05
15	bB	829	CLA	CMC-C2C	-2.25	1.46	1.50
18	cM	101	BCR	C30-C25	-2.25	1.50	1.53
15	bB	842	CLA	CMD-C2D	-2.25	1.46	1.50
15	a5	412	CLA	CHC-C1C	2.25	1.40	1.35
15	aA	838	CLA	CMC-C2C	-2.25	1.46	1.50
15	cA	834	CLA	C1D-ND	2.25	1.40	1.37
15	bB	833	CLA	CMC-C2C	-2.25	1.46	1.50
15	aA	809	CLA	MG-ND	-2.25	2.01	2.05
15	c6	411	CLA	MG-ND	-2.25	2.01	2.05
15	c6	414	CLA	C3B-C2B	-2.25	1.37	1.40
15	aA	809	CLA	CMC-C2C	-2.25	1.46	1.50
15	bA	831	CLA	CHC-C1C	2.25	1.40	1.35
15	c4	415	CLA	CHC-C1C	2.25	1.40	1.35
15	aA	823	CLA	CMD-C2D	-2.25	1.46	1.50
15	b6	404	CLA	CMB-C2B	-2.25	1.47	1.51
15	c5	417	CLA	C4D-ND	-2.25	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	838	CLA	C3B-CAB	-2.25	1.43	1.47
15	c1	415	CLA	C3B-CAB	-2.25	1.43	1.47
15	c4	410	CLA	MG-ND	-2.25	2.01	2.05
15	cA	821	CLA	C3B-CAB	-2.25	1.43	1.47
15	b6	404	CLA	MG-ND	-2.25	2.01	2.05
15	b2	409	CLA	CMC-C2C	-2.25	1.46	1.50
15	c2	413	CLA	CMC-C2C	-2.25	1.46	1.50
15	a6	411	CLA	MG-ND	-2.25	2.01	2.05
15	c3	417	CLA	C4D-ND	-2.25	1.34	1.37
15	cA	841	CLA	CMC-C2C	-2.25	1.46	1.50
15	aA	836	CLA	C3B-CAB	-2.25	1.43	1.47
15	a5	420	CLA	CMC-C2C	-2.24	1.46	1.50
15	b3	412	CLA	CHC-C1C	2.24	1.40	1.35
15	cB	838	CLA	C3B-C2B	-2.24	1.37	1.40
15	aA	831	CLA	CHC-C1C	2.24	1.40	1.35
15	c4	409	CLA	CMD-C2D	-2.24	1.46	1.50
15	a1	412	CLA	MG-ND	-2.24	2.01	2.05
18	a6	421	BCR	C30-C25	-2.24	1.50	1.53
15	a2	409	CLA	CMC-C2C	-2.24	1.46	1.50
15	bA	809	CLA	MG-ND	-2.24	2.01	2.05
15	aB	842	CLA	CMD-C2D	-2.24	1.46	1.50
15	a5	402	CLA	CMD-C2D	-2.24	1.46	1.50
15	cA	806	CLA	CMA-C3A	-2.24	1.48	1.53
15	b1	413	CLA	MG-ND	-2.24	2.01	2.05
15	cX	102	CLA	C1D-ND	2.24	1.40	1.37
15	aB	836	CLA	CMC-C2C	-2.24	1.46	1.50
15	c5	408	CLA	CMC-C2C	-2.24	1.46	1.50
18	a1	421	BCR	C33-C5	-2.24	1.47	1.50
15	a3	409	CLA	CMD-C2D	-2.24	1.46	1.50
15	c5	410	CLA	C3C-C2C	2.24	1.41	1.36
15	aA	807	CLA	CAA-C2A	-2.24	1.49	1.54
15	bA	829	CLA	MG-ND	-2.24	2.01	2.05
15	a1	411	CLA	C4B-CHC	-2.24	1.34	1.41
15	aB	829	CLA	CMC-C2C	-2.24	1.46	1.50
15	c3	421	CLA	CMB-C2B	-2.24	1.47	1.51
15	a5	415	CLA	C3B-CAB	-2.24	1.43	1.47
15	a6	409	CLA	CMC-C2C	-2.24	1.46	1.50
15	cA	817	CLA	CMD-C2D	-2.24	1.46	1.50
15	bA	825	CLA	MG-ND	-2.24	2.01	2.05
15	c6	404	CLA	MG-ND	-2.24	2.01	2.05
15	cB	817	CLA	CMD-C2D	-2.24	1.46	1.50
15	cB	842	CLA	CMD-C2D	-2.24	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b6	421	BCR	C30-C25	-2.24	1.50	1.53
15	b4	415	CLA	CHC-C1C	2.24	1.40	1.35
18	cA	850	BCR	C38-C26	-2.24	1.47	1.50
15	aA	812	CLA	C3B-CAB	-2.24	1.43	1.47
15	bA	820	CLA	C3B-C2B	-2.24	1.37	1.40
15	bB	835	CLA	CMD-C2D	-2.24	1.46	1.50
15	c4	410	CLA	CMD-C2D	-2.24	1.46	1.50
15	a4	415	CLA	CHC-C1C	2.24	1.40	1.35
15	cB	806	CLA	C4B-CHC	-2.24	1.34	1.41
15	a5	410	CLA	MG-ND	-2.24	2.01	2.05
15	a3	415	CLA	CHC-C1C	2.24	1.40	1.35
15	bB	834	CLA	MG-ND	-2.24	2.01	2.05
15	b2	422	CLA	CMC-C2C	-2.24	1.46	1.50
15	a5	409	CLA	CMD-C2D	-2.24	1.46	1.50
15	c2	422	CLA	CMC-C2C	-2.24	1.46	1.50
15	bA	809	CLA	CMC-C2C	-2.23	1.46	1.50
15	b6	411	CLA	MG-ND	-2.23	2.01	2.05
15	cB	809	CLA	C3B-CAB	-2.23	1.43	1.47
15	bB	817	CLA	CMD-C2D	-2.23	1.46	1.50
15	aB	832	CLA	C3B-CAB	-2.23	1.43	1.47
15	cA	838	CLA	CMC-C2C	-2.23	1.46	1.50
15	aA	836	CLA	MG-ND	-2.23	2.01	2.05
15	aA	810	CLA	C3B-C2B	-2.23	1.37	1.40
15	bA	839	CLA	C4B-CHC	-2.23	1.34	1.41
15	bB	831	CLA	MG-ND	-2.23	2.01	2.05
15	bB	830	CLA	CMC-C2C	-2.23	1.46	1.50
15	c3	409	CLA	CMD-C2D	-2.23	1.46	1.50
18	bM	101	BCR	C30-C25	-2.23	1.50	1.53
15	aA	827	CLA	C3B-CAB	-2.23	1.43	1.47
15	b5	417	CLA	C4D-ND	-2.23	1.34	1.37
15	bJ	101	CLA	C3B-C2B	-2.23	1.37	1.40
15	bA	838	CLA	CMC-C2C	-2.23	1.46	1.50
15	b1	402	CLA	CMD-C2D	-2.23	1.46	1.50
15	aB	838	CLA	C3B-C2B	-2.23	1.37	1.40
15	aB	809	CLA	C3B-CAB	-2.23	1.43	1.47
15	a3	412	CLA	CHC-C1C	2.23	1.40	1.35
15	b4	402	CLA	CMD-C2D	-2.23	1.46	1.50
15	aA	821	CLA	C4B-CHC	-2.23	1.34	1.41
15	bB	828	CLA	C1D-ND	2.23	1.40	1.37
15	aB	813	CLA	MG-ND	-2.23	2.01	2.05
15	b1	417	CLA	CMD-C2D	-2.23	1.46	1.50
15	b5	408	CLA	CMC-C2C	-2.23	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	810	CLA	C3B-C2B	-2.23	1.37	1.40
15	a2	417	CLA	C3C-C2C	2.23	1.41	1.36
15	cB	824	CLA	CMD-C2D	-2.23	1.46	1.50
15	bA	834	CLA	C1D-ND	2.23	1.40	1.37
15	bB	819	CLA	CMC-C2C	-2.23	1.46	1.50
15	b2	413	CLA	CMC-C2C	-2.23	1.46	1.50
15	a2	418	CLA	C4D-ND	-2.23	1.34	1.37
15	cB	820	CLA	MG-ND	-2.23	2.01	2.05
15	b5	410	CLA	C3C-C2C	2.23	1.41	1.36
15	a5	420	CLA	CMD-C2D	-2.23	1.46	1.50
15	aB	821	CLA	CMC-C2C	-2.23	1.46	1.50
15	cB	833	CLA	CMC-C2C	-2.23	1.46	1.50
15	bB	811	CLA	CHC-C1C	2.23	1.40	1.35
15	cB	834	CLA	MG-ND	-2.23	2.01	2.05
15	a3	411	CLA	CMC-C2C	-2.22	1.46	1.50
15	a4	413	CLA	CMD-C2D	-2.22	1.46	1.50
15	b4	407	CLA	CMD-C2D	-2.22	1.46	1.50
15	aB	828	CLA	C4B-CHC	-2.22	1.34	1.41
15	bB	828	CLA	C4B-CHC	-2.22	1.34	1.41
15	cA	839	CLA	C4B-CHC	-2.22	1.34	1.41
15	b2	418	CLA	CMC-C2C	-2.22	1.46	1.50
15	b5	409	CLA	CMD-C2D	-2.22	1.46	1.50
15	aB	834	CLA	MG-ND	-2.22	2.01	2.05
15	a6	404	CLA	MG-ND	-2.22	2.01	2.05
15	c6	409	CLA	CMC-C2C	-2.22	1.46	1.50
15	c2	417	CLA	C3C-C2C	2.22	1.41	1.36
18	aF	201	BCR	C33-C5	-2.22	1.47	1.50
15	a2	416	CLA	C3B-C2B	-2.22	1.37	1.40
15	cB	828	CLA	C4B-CHC	-2.22	1.34	1.41
15	a5	408	CLA	CMC-C2C	-2.22	1.46	1.50
15	b4	410	CLA	CMD-C2D	-2.22	1.46	1.50
15	cB	835	CLA	CMD-C2D	-2.22	1.46	1.50
15	a6	414	CLA	C4B-CHC	-2.22	1.34	1.41
15	cA	812	CLA	C3B-CAB	-2.22	1.43	1.47
15	b2	422	CLA	C3B-C2B	-2.22	1.37	1.40
15	c2	409	CLA	CMC-C2C	-2.22	1.46	1.50
15	bB	815	CLA	C3B-C2B	-2.22	1.37	1.40
15	bA	817	CLA	CMD-C2D	-2.22	1.46	1.50
15	aB	835	CLA	CMD-C2D	-2.22	1.46	1.50
15	cJ	101	CLA	CMD-C2D	-2.22	1.46	1.50
15	c5	410	CLA	MG-ND	-2.22	2.01	2.05
15	bB	813	CLA	MG-ND	-2.22	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	805	CLA	C3B-C2B	-2.22	1.37	1.40
15	aA	817	CLA	CMD-C2D	-2.22	1.46	1.50
15	aB	830	CLA	CMC-C2C	-2.22	1.46	1.50
15	b4	408	CLA	CMC-C2C	-2.22	1.46	1.50
15	a3	410	CLA	C3B-C2B	-2.22	1.37	1.40
15	bF	201	CLA	CMC-C2C	-2.22	1.46	1.50
15	aA	806	CLA	CMA-C3A	-2.22	1.48	1.53
15	bB	808	CLA	C3B-C2B	-2.22	1.37	1.40
15	cA	810	CLA	C3B-C2B	-2.22	1.37	1.40
15	cF	203	CLA	CMC-C2C	-2.22	1.46	1.50
18	cL	204	BCR	C33-C5	-2.22	1.47	1.50
15	aB	817	CLA	CMD-C2D	-2.21	1.46	1.50
15	bA	834	CLA	C4B-CHC	-2.21	1.34	1.41
15	a6	405	CLA	CMD-C2D	-2.21	1.46	1.50
15	bJ	102	CLA	CMC-C2C	-2.21	1.46	1.50
15	b4	410	CLA	C3B-C2B	-2.21	1.37	1.40
15	a4	402	CLA	CMD-C2D	-2.21	1.46	1.50
15	a6	422	CLA	C3B-CAB	-2.21	1.43	1.47
15	aB	838	CLA	C3B-CAB	-2.21	1.43	1.47
15	a1	409	CLA	MG-ND	-2.21	2.01	2.05
15	a4	405	CLA	CMD-C2D	-2.21	1.46	1.50
15	b4	405	CLA	CMD-C2D	-2.21	1.46	1.50
15	cA	827	CLA	C3B-CAB	-2.21	1.43	1.47
15	b6	422	CLA	C3B-C2B	-2.21	1.37	1.40
15	cA	834	CLA	C4B-CHC	-2.21	1.34	1.41
15	c3	412	CLA	CHC-C1C	2.21	1.40	1.35
15	bB	838	CLA	C3B-C2B	-2.21	1.37	1.40
15	b5	415	CLA	C3B-CAB	-2.21	1.43	1.47
15	bA	841	CLA	CMD-C2D	-2.21	1.46	1.50
15	aL	202	CLA	C3B-C2B	-2.21	1.37	1.40
15	cA	820	CLA	C3B-C2B	-2.21	1.37	1.40
15	a4	408	CLA	CMC-C2C	-2.21	1.46	1.50
15	cB	838	CLA	MG-ND	-2.21	2.01	2.05
15	a2	413	CLA	CHC-C1C	2.21	1.40	1.35
15	cB	811	CLA	CHC-C1C	2.21	1.40	1.35
15	a6	404	CLA	CMB-C2B	-2.21	1.47	1.51
15	aJ	201	CLA	CMC-C2C	-2.21	1.46	1.50
15	b3	411	CLA	CMD-C2D	-2.21	1.46	1.50
15	c1	409	CLA	CMD-C2D	-2.21	1.46	1.50
15	c4	402	CLA	CMD-C2D	-2.21	1.46	1.50
15	aA	821	CLA	C3B-CAB	-2.21	1.43	1.47
15	cB	832	CLA	C3B-CAB	-2.21	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a4	410	CLA	MG-ND	-2.21	2.01	2.05
15	aJ	202	CLA	C3B-C2B	-2.21	1.37	1.40
15	b3	410	CLA	C3B-C2B	-2.21	1.37	1.40
15	b3	411	CLA	CMC-C2C	-2.21	1.46	1.50
15	b5	420	CLA	CMD-C2D	-2.21	1.46	1.50
15	cA	841	CLA	CMD-C2D	-2.21	1.46	1.50
18	cL	204	BCR	C38-C26	-2.21	1.47	1.50
15	b3	415	CLA	CHC-C1C	2.21	1.40	1.35
15	bB	820	CLA	MG-ND	-2.21	2.01	2.05
15	bB	838	CLA	MG-ND	-2.21	2.01	2.05
15	cB	829	CLA	CMC-C2C	-2.21	1.46	1.50
18	bL	205	BCR	C33-C5	-2.21	1.47	1.50
15	cA	832	CLA	C3B-CAB	-2.21	1.43	1.47
15	c2	418	CLA	C4D-ND	-2.21	1.34	1.37
15	bB	807	CLA	C4B-CHC	-2.21	1.34	1.41
15	cA	821	CLA	C4B-CHC	-2.21	1.34	1.41
15	aA	829	CLA	MG-ND	-2.21	2.01	2.05
15	c2	403	CLA	MG-ND	-2.21	2.01	2.05
15	aL	203	CLA	CMC-C2C	-2.21	1.46	1.50
15	c5	415	CLA	C3B-CAB	-2.21	1.43	1.47
15	aA	821	CLA	CAC-C3C	-2.21	1.45	1.51
18	aF	202	BCR	C33-C5	-2.21	1.47	1.50
15	aA	841	CLA	CMC-C2C	-2.20	1.46	1.50
15	b4	413	CLA	CMD-C2D	-2.20	1.46	1.50
15	aB	811	CLA	C3B-C2B	-2.20	1.37	1.40
15	b1	409	CLA	CMD-C2D	-2.20	1.46	1.50
15	bA	821	CLA	C4B-CHC	-2.20	1.34	1.41
15	a4	407	CLA	CMD-C2D	-2.20	1.46	1.50
15	c3	411	CLA	CMC-C2C	-2.20	1.46	1.50
15	cA	829	CLA	MG-ND	-2.20	2.01	2.05
15	a1	408	CLA	CMD-C2D	-2.20	1.46	1.50
15	c2	418	CLA	CMC-C2C	-2.20	1.46	1.50
15	c3	411	CLA	CMD-C2D	-2.20	1.46	1.50
15	aA	839	CLA	C4B-CHC	-2.20	1.34	1.41
15	b6	405	CLA	CMD-C2D	-2.20	1.46	1.50
15	aB	819	CLA	CMC-C2C	-2.20	1.46	1.50
15	aJ	202	CLA	CMD-C2D	-2.20	1.46	1.50
15	cB	831	CLA	CMC-C2C	-2.20	1.46	1.50
15	aA	834	CLA	C4B-CHC	-2.20	1.34	1.41
15	bA	803	CLA	C4B-CHC	-2.20	1.34	1.41
15	a4	412	CLA	CHC-C1C	2.20	1.40	1.35
15	b2	406	CLA	C3B-CAB	-2.20	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	412	CLA	CHC-C1C	2.20	1.40	1.35
15	cB	819	CLA	CMC-C2C	-2.20	1.46	1.50
18	cF	204	BCR	C33-C5	-2.20	1.47	1.50
15	c1	403	CLA	MG-ND	-2.20	2.01	2.05
15	c1	410	CLA	MG-ND	-2.20	2.01	2.05
15	a2	413	CLA	CMC-C2C	-2.20	1.46	1.50
15	c2	406	CLA	CMC-C2C	-2.20	1.46	1.50
15	c4	405	CLA	CMD-C2D	-2.20	1.46	1.50
15	bA	834	CLA	CMA-C3A	-2.20	1.48	1.53
15	aB	815	CLA	C3B-C2B	-2.20	1.37	1.40
15	aB	828	CLA	C1D-ND	2.20	1.40	1.37
18	a1	421	BCR	C30-C25	-2.20	1.50	1.53
15	aB	813	CLA	CMC-C2C	-2.20	1.46	1.50
15	cA	831	CLA	CHC-C1C	2.20	1.40	1.35
15	cB	819	CLA	CHC-C1C	2.20	1.40	1.35
15	cA	836	CLA	CMC-C2C	-2.20	1.46	1.50
15	cB	813	CLA	CMD-C2D	-2.20	1.46	1.50
15	a2	413	CLA	C4B-CHC	-2.20	1.34	1.41
15	c2	411	CLA	MG-ND	-2.20	2.01	2.05
15	c2	413	CLA	CHC-C1C	2.20	1.40	1.35
15	a3	413	CLA	C3B-C2B	-2.20	1.37	1.40
15	aB	838	CLA	MG-ND	-2.20	2.01	2.05
15	aA	834	CLA	C3B-CAB	-2.20	1.43	1.47
15	c4	421	CLA	C3B-C2B	-2.20	1.37	1.40
15	cA	808	CLA	C3B-CAB	-2.20	1.43	1.47
15	cB	807	CLA	C4B-CHC	-2.20	1.34	1.41
15	c3	413	CLA	MG-ND	-2.20	2.01	2.05
15	cB	808	CLA	C3B-C2B	-2.20	1.37	1.40
15	c2	416	CLA	C3B-C2B	-2.20	1.37	1.40
15	aB	819	CLA	CHC-C1C	2.20	1.40	1.35
15	cA	824	CLA	CMC-C2C	-2.19	1.46	1.50
15	cA	826	CLA	CMC-C2C	-2.19	1.46	1.50
15	c1	410	CLA	CMD-C2D	-2.19	1.46	1.50
15	b2	418	CLA	C4D-ND	-2.19	1.34	1.37
15	bB	811	CLA	C3B-C2B	-2.19	1.37	1.40
15	aB	831	CLA	MG-ND	-2.19	2.01	2.05
15	a1	414	CLA	C3B-CAB	-2.19	1.43	1.47
15	bA	827	CLA	C3B-CAB	-2.19	1.43	1.47
15	a3	411	CLA	CMD-C2D	-2.19	1.46	1.50
15	c4	412	CLA	CHC-C1C	2.19	1.40	1.35
15	bB	809	CLA	C3B-CAB	-2.19	1.43	1.47
15	bB	813	CLA	CMC-C2C	-2.19	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c4	413	CLA	CMD-C2D	-2.19	1.46	1.50
15	cA	842	CLA	C1D-ND	2.19	1.40	1.37
15	b4	410	CLA	MG-ND	-2.19	2.01	2.05
15	a2	410	CLA	CMD-C2D	-2.19	1.46	1.50
15	bA	836	CLA	CMC-C2C	-2.19	1.46	1.50
15	c6	404	CLA	CMB-C2B	-2.19	1.47	1.51
15	bA	808	CLA	C3B-CAB	-2.19	1.43	1.47
15	bJ	101	CLA	CMD-C2D	-2.19	1.46	1.50
15	b6	409	CLA	CMC-C2C	-2.19	1.46	1.50
15	b1	415	CLA	C3B-C2B	-2.19	1.37	1.40
15	aA	834	CLA	C1D-ND	2.19	1.40	1.37
15	c4	408	CLA	CMC-C2C	-2.19	1.46	1.50
15	c3	415	CLA	CHC-C1C	2.19	1.40	1.35
15	aA	832	CLA	C3B-CAB	-2.19	1.43	1.47
15	c3	411	CLA	MG-ND	-2.19	2.01	2.05
15	a3	404	CLA	CMD-C2D	-2.19	1.46	1.50
15	bA	827	CLA	CMC-C2C	-2.19	1.46	1.50
15	b1	410	CLA	MG-ND	-2.19	2.01	2.05
15	c3	410	CLA	C3B-C2B	-2.19	1.37	1.40
14	cA	801	CL0	C4D-CHA	2.19	1.46	1.38
15	cB	828	CLA	C3B-CAB	-2.19	1.43	1.47
15	aA	836	CLA	CMC-C2C	-2.19	1.46	1.50
15	cA	822	CLA	C3B-CAB	-2.19	1.43	1.47
15	c1	406	CLA	CMC-C2C	-2.19	1.46	1.50
15	bA	821	CLA	CAC-C3C	-2.19	1.45	1.51
15	bA	829	CLA	CMC-C2C	-2.19	1.46	1.50
15	c3	410	CLA	C3C-C2C	2.19	1.41	1.36
15	cA	834	CLA	CMA-C3A	-2.19	1.48	1.53
15	bB	813	CLA	CMD-C2D	-2.19	1.46	1.50
15	b6	414	CLA	C4B-CHC	-2.19	1.34	1.41
15	bB	831	CLA	CMC-C2C	-2.19	1.46	1.50
18	bF	202	BCR	C33-C5	-2.19	1.47	1.50
15	aA	829	CLA	CMC-C2C	-2.19	1.46	1.50
15	b1	406	CLA	CMD-C2D	-2.19	1.46	1.50
15	b5	406	CLA	CMD-C2D	-2.19	1.46	1.50
15	b3	408	CLA	MG-ND	-2.19	2.01	2.05
15	aB	828	CLA	C1C-NC	-2.19	1.34	1.37
15	b5	420	CLA	CMC-C2C	-2.19	1.46	1.50
15	aA	828	CLA	MG-ND	-2.19	2.01	2.05
15	c6	405	CLA	CMD-C2D	-2.19	1.46	1.50
15	b2	413	CLA	C4B-CHC	-2.19	1.34	1.41
15	aB	811	CLA	CHC-C1C	2.18	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	cB	813	CLA	CMC-C2C	-2.18	1.46	1.50
15	b1	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	aA	803	CLA	C4B-CHC	-2.18	1.34	1.41
15	aA	827	CLA	CMC-C2C	-2.18	1.46	1.50
15	bB	824	CLA	CMD-C2D	-2.18	1.46	1.50
15	cB	828	CLA	C1C-NC	-2.18	1.34	1.37
15	cA	803	CLA	C4B-CHC	-2.18	1.34	1.41
15	b1	404	CLA	MG-ND	-2.18	2.01	2.05
15	bA	840	CLA	C3B-CAB	-2.18	1.43	1.47
15	aB	807	CLA	C4B-CHC	-2.18	1.34	1.41
15	a4	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	b2	404	CLA	MG-ND	-2.18	2.01	2.05
15	aA	834	CLA	CMA-C3A	-2.18	1.48	1.53
15	bB	828	CLA	C3B-CAB	-2.18	1.43	1.47
15	aA	811	CLA	CMC-C2C	-2.18	1.46	1.50
15	a3	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	bB	821	CLA	CMC-C2C	-2.18	1.46	1.50
15	c1	417	CLA	CMD-C2D	-2.18	1.46	1.50
15	aA	840	CLA	C3B-CAB	-2.18	1.43	1.47
15	bA	811	CLA	CMC-C2C	-2.18	1.46	1.50
15	b3	409	CLA	CMD-C2D	-2.18	1.46	1.50
15	aA	833	CLA	C1B-NB	-2.18	1.33	1.35
15	cB	805	CLA	C3B-C2B	-2.18	1.37	1.40
15	bA	822	CLA	C3B-CAB	-2.18	1.43	1.47
15	c3	421	CLA	MG-NA	2.18	2.11	2.06
15	aB	824	CLA	CMD-C2D	-2.18	1.46	1.50
15	c5	411	CLA	MG-ND	-2.18	2.01	2.05
15	a4	411	CLA	CMC-C2C	-2.18	1.46	1.50
15	cL	203	CLA	CMC-C2C	-2.18	1.46	1.50
15	b3	413	CLA	MG-ND	-2.18	2.01	2.05
15	bB	832	CLA	C3B-CAB	-2.18	1.43	1.47
15	b6	415	CLA	CMD-C2D	-2.18	1.46	1.50
15	bA	828	CLA	MG-ND	-2.18	2.01	2.05
15	bA	816	CLA	CMD-C2D	-2.18	1.46	1.50
15	cJ	102	CLA	CMC-C2C	-2.18	1.46	1.50
15	a4	413	CLA	C3B-C2B	-2.18	1.37	1.40
15	c4	413	CLA	C3B-C2B	-2.18	1.37	1.40
15	c1	417	CLA	C4D-ND	-2.18	1.34	1.37
15	aA	808	CLA	C3B-CAB	-2.18	1.43	1.47
15	aB	820	CLA	C3B-CAB	-2.18	1.43	1.47
15	b3	417	CLA	CMC-C2C	-2.18	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c5	417	CLA	CMC-C2C	-2.18	1.46	1.50
15	bA	826	CLA	CMC-C2C	-2.18	1.46	1.50
15	c5	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	a5	417	CLA	CMC-C2C	-2.17	1.46	1.50
15	aB	808	CLA	C3B-C2B	-2.17	1.37	1.40
15	aB	812	CLA	CMD-C2D	-2.17	1.46	1.50
15	b6	408	CLA	CMD-C2D	-2.17	1.46	1.50
15	c5	420	CLA	CMC-C2C	-2.17	1.46	1.50
15	bL	202	CLA	CMC-C2C	-2.17	1.46	1.50
15	c5	409	CLA	CMD-C2D	-2.17	1.46	1.50
15	bB	826	CLA	MG-ND	-2.17	2.01	2.05
15	aB	835	CLA	C3B-C2B	-2.17	1.37	1.40
15	bB	804	CLA	C4B-CHC	-2.17	1.34	1.41
15	bB	819	CLA	CHC-C1C	2.17	1.40	1.35
15	a2	403	CLA	MG-ND	-2.17	2.01	2.05
15	cA	821	CLA	CAC-C3C	-2.17	1.45	1.51
15	c4	411	CLA	CMC-C2C	-2.17	1.46	1.50
15	aA	832	CLA	C4B-CHC	-2.17	1.35	1.41
18	a4	401	BCR	C33-C5	-2.17	1.47	1.50
15	c5	406	CLA	CMD-C2D	-2.17	1.46	1.50
15	b3	417	CLA	C4D-ND	-2.17	1.34	1.37
15	c2	406	CLA	C3B-CAB	-2.17	1.43	1.47
15	a6	408	CLA	CMD-C2D	-2.17	1.46	1.50
15	bA	824	CLA	CMC-C2C	-2.17	1.46	1.50
15	cB	828	CLA	C1D-ND	2.17	1.40	1.37
15	aB	802	CLA	C4B-CHC	-2.17	1.35	1.41
14	bA	801	CL0	C4D-CHA	2.17	1.46	1.38
15	b3	404	CLA	CMD-C2D	-2.17	1.46	1.50
15	bA	832	CLA	C3B-CAB	-2.17	1.43	1.47
15	aA	824	CLA	CMC-C2C	-2.17	1.46	1.50
15	cL	202	CLA	C3B-C2B	-2.17	1.37	1.40
15	cB	802	CLA	CAA-C2A	-2.17	1.50	1.54
15	b3	411	CLA	MG-ND	-2.17	2.01	2.05
18	bB	850	BCR	C33-C5	-2.17	1.47	1.50
15	aA	822	CLA	C3B-CAB	-2.17	1.43	1.47
15	b5	411	CLA	MG-ND	-2.17	2.01	2.05
15	aA	841	CLA	CMD-C2D	-2.17	1.46	1.50
15	aB	828	CLA	C3B-CAB	-2.17	1.43	1.47
15	bA	834	CLA	C3B-CAB	-2.17	1.43	1.47
15	b2	403	CLA	MG-ND	-2.17	2.01	2.05
18	bL	205	BCR	C38-C26	-2.17	1.47	1.50
15	aB	820	CLA	MG-ND	-2.17	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	404	CLA	MG-ND	-2.17	2.01	2.05
15	a3	411	CLA	MG-ND	-2.17	2.01	2.05
15	cB	839	CLA	C3B-CAB	-2.17	1.43	1.47
15	bA	831	CLA	C1D-ND	2.17	1.40	1.37
15	aB	802	CLA	CAA-C2A	-2.17	1.50	1.54
15	bB	802	CLA	C4B-CHC	-2.17	1.35	1.41
15	cB	820	CLA	C3B-CAB	-2.17	1.43	1.47
15	a1	403	CLA	MG-ND	-2.17	2.01	2.05
15	b2	414	CLA	C3B-C2B	-2.17	1.37	1.40
18	b4	401	BCR	C33-C5	-2.17	1.47	1.50
15	bA	832	CLA	C4B-CHC	-2.17	1.35	1.41
15	a1	409	CLA	CMD-C2D	-2.17	1.46	1.50
15	bB	841	CLA	CMC-C2C	-2.17	1.46	1.50
15	bB	820	CLA	C3B-CAB	-2.17	1.43	1.47
15	c6	408	CLA	CMD-C2D	-2.17	1.46	1.50
15	a5	413	CLA	C3B-C2B	-2.17	1.37	1.40
15	cB	815	CLA	C3B-C2B	-2.17	1.37	1.40
15	c1	417	CLA	CMC-C2C	-2.17	1.46	1.50
18	cB	849	BCR	C33-C5	-2.17	1.47	1.50
15	c4	417	CLA	CMC-C2C	-2.16	1.46	1.50
15	bA	843	CLA	C1D-ND	2.16	1.40	1.37
15	b1	406	CLA	CMC-C2C	-2.16	1.46	1.50
15	a3	408	CLA	MG-ND	-2.16	2.01	2.05
15	a5	411	CLA	MG-ND	-2.16	2.01	2.05
15	cA	832	CLA	C4B-CHC	-2.16	1.35	1.41
15	a2	406	CLA	CMC-C2C	-2.16	1.46	1.50
15	b3	410	CLA	CMD-C2D	-2.16	1.46	1.50
15	aB	813	CLA	CMD-C2D	-2.16	1.46	1.50
15	aB	826	CLA	MG-ND	-2.16	2.01	2.05
15	a3	413	CLA	MG-ND	-2.16	2.01	2.05
15	cA	828	CLA	MG-ND	-2.16	2.01	2.05
15	bL	203	CLA	C3B-C2B	-2.16	1.37	1.40
15	cB	821	CLA	CMC-C2C	-2.16	1.46	1.50
15	c2	404	CLA	CMD-C2D	-2.16	1.46	1.50
15	aA	843	CLA	C1D-ND	2.16	1.40	1.37
15	b1	412	CLA	C4B-CHC	-2.16	1.35	1.41
15	b2	404	CLA	CMD-C2D	-2.16	1.46	1.50
15	cB	811	CLA	C3B-C2B	-2.16	1.37	1.40
15	c2	404	CLA	MG-ND	-2.16	2.01	2.05
15	bB	828	CLA	C1C-NC	-2.16	1.34	1.37
15	aA	815	CLA	CMD-C2D	-2.16	1.46	1.50
15	b3	405	CLA	CMD-C2D	-2.16	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	bL	206	BCR	C30-C25	-2.16	1.50	1.53
15	aJ	203	CLA	CMC-C2C	-2.16	1.46	1.50
15	cB	804	CLA	C4B-CHC	-2.16	1.35	1.41
15	b3	410	CLA	MG-ND	-2.16	2.01	2.05
15	aB	830	CLA	CHC-C1C	2.16	1.40	1.35
15	bA	833	CLA	C1B-NB	-2.16	1.33	1.35
15	b6	422	CLA	C3B-CAB	-2.16	1.43	1.47
15	aA	808	CLA	CMC-C2C	-2.16	1.46	1.50
15	a4	417	CLA	CMC-C2C	-2.16	1.46	1.50
15	cA	834	CLA	C3B-CAB	-2.16	1.43	1.47
15	aA	831	CLA	C1D-ND	2.16	1.40	1.37
15	aB	819	CLA	C3B-CAB	-2.16	1.43	1.47
15	bA	831	CLA	C3B-CAB	-2.16	1.43	1.47
15	cA	840	CLA	C3B-CAB	-2.16	1.43	1.47
15	b4	414	CLA	CMD-C2D	-2.16	1.46	1.50
15	cB	841	CLA	CMC-C2C	-2.16	1.46	1.50
15	bL	204	CLA	CMC-C2C	-2.16	1.46	1.50
15	c3	404	CLA	CMD-C2D	-2.16	1.46	1.50
18	aI	103	BCR	C38-C26	-2.16	1.47	1.50
15	a1	405	CLA	CMD-C2D	-2.16	1.46	1.50
15	b5	417	CLA	CMC-C2C	-2.16	1.46	1.50
15	b5	413	CLA	C3B-C2B	-2.16	1.37	1.40
15	cA	811	CLA	CMC-C2C	-2.16	1.46	1.50
15	c4	406	CLA	CMD-C2D	-2.16	1.46	1.50
15	bB	812	CLA	CMD-C2D	-2.15	1.46	1.50
15	a5	406	CLA	CMD-C2D	-2.15	1.46	1.50
15	cB	812	CLA	CMD-C2D	-2.15	1.46	1.50
15	c4	404	CLA	CMD-C2D	-2.15	1.46	1.50
15	a6	414	CLA	MG-ND	-2.15	2.01	2.05
18	cB	847	BCR	C12-C13	-2.15	1.44	1.50
15	c3	410	CLA	CMD-C2D	-2.15	1.46	1.50
15	aA	826	CLA	CMC-C2C	-2.15	1.46	1.50
15	a2	418	CLA	CMC-C2C	-2.15	1.46	1.50
15	cA	829	CLA	CMC-C2C	-2.15	1.46	1.50
14	aA	801	CL0	C4D-CHA	2.15	1.46	1.38
15	b2	406	CLA	CMC-C2C	-2.15	1.46	1.50
15	b4	413	CLA	C3B-C2B	-2.15	1.37	1.40
15	cB	811	CLA	C4B-CHC	-2.15	1.35	1.41
15	c3	405	CLA	CMD-C2D	-2.15	1.46	1.50
15	a3	417	CLA	C4D-ND	-2.15	1.34	1.37
15	aB	810	CLA	C3B-CAB	-2.15	1.43	1.47
15	bB	810	CLA	C3B-CAB	-2.15	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	410	CLA	CMD-C2D	-2.15	1.46	1.50
15	cA	808	CLA	CMC-C2C	-2.15	1.46	1.50
15	a4	412	CLA	C4B-CHC	-2.15	1.35	1.41
15	bL	203	CLA	C4B-CHC	-2.15	1.35	1.41
15	cA	844	CLA	C3B-CAB	-2.15	1.43	1.47
15	cB	831	CLA	MG-ND	-2.15	2.01	2.05
15	cB	830	CLA	CHC-C1C	2.15	1.40	1.35
15	cA	831	CLA	C1D-ND	2.15	1.40	1.37
15	b4	417	CLA	CMC-C2C	-2.15	1.46	1.50
15	c1	404	CLA	MG-ND	-2.15	2.01	2.05
15	aA	816	CLA	CMD-C2D	-2.15	1.46	1.50
15	a3	421	CLA	MG-NA	2.15	2.11	2.06
15	cA	816	CLA	MG-ND	-2.15	2.01	2.05
18	cM	101	BCR	C33-C5	-2.15	1.47	1.50
15	a3	417	CLA	CMC-C2C	-2.15	1.46	1.50
15	aA	845	CLA	C3B-CAB	-2.15	1.43	1.47
15	aL	203	CLA	C3B-CAB	-2.15	1.43	1.47
15	cA	833	CLA	C1B-NB	-2.15	1.33	1.35
15	aB	804	CLA	C4B-CHC	-2.15	1.35	1.41
15	aB	841	CLA	CMC-C2C	-2.15	1.46	1.50
15	c5	413	CLA	C3B-C2B	-2.15	1.37	1.40
15	aB	811	CLA	C4B-CHC	-2.15	1.35	1.41
15	c3	408	CLA	MG-ND	-2.15	2.01	2.05
15	a1	405	CLA	CMC-C2C	-2.15	1.46	1.50
15	bB	818	CLA	CMD-C2D	-2.15	1.46	1.50
15	bL	204	CLA	C3B-CAB	-2.15	1.43	1.47
15	a2	404	CLA	CMD-C2D	-2.15	1.46	1.50
15	b1	417	CLA	CMC-C2C	-2.15	1.46	1.50
15	b4	405	CLA	CMC-C2C	-2.15	1.46	1.50
15	cA	816	CLA	CMD-C2D	-2.15	1.46	1.50
15	c1	406	CLA	CMD-C2D	-2.15	1.46	1.50
15	a5	410	CLA	CMD-C2D	-2.15	1.46	1.50
15	b1	403	CLA	MG-ND	-2.15	2.01	2.05
15	c3	413	CLA	C3B-C2B	-2.15	1.37	1.40
15	cA	807	CLA	C1D-ND	2.14	1.40	1.37
15	a1	402	CLA	MG-ND	-2.14	2.01	2.05
15	c1	402	CLA	CMD-C2D	-2.14	1.46	1.50
15	b3	413	CLA	C3B-C2B	-2.14	1.37	1.40
15	bB	839	CLA	C3B-CAB	-2.14	1.43	1.47
15	c5	404	CLA	MG-ND	-2.14	2.01	2.05
18	c2	401	BCR	C4-C5	-2.14	1.46	1.51
15	bB	802	CLA	CAA-C2A	-2.14	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aJ	203	CLA	CMD-C2D	-2.14	1.46	1.50
15	cB	818	CLA	CMD-C2D	-2.14	1.46	1.50
15	c2	413	CLA	C4B-CHC	-2.14	1.35	1.41
18	aB	849	BCR	C33-C5	-2.14	1.47	1.50
15	bB	835	CLA	C3B-C2B	-2.14	1.37	1.40
15	aB	831	CLA	CMC-C2C	-2.14	1.46	1.50
15	b6	415	CLA	CMC-C2C	-2.14	1.46	1.50
18	aB	847	BCR	C12-C13	-2.14	1.44	1.50
15	aA	825	CLA	C3B-C2B	-2.14	1.37	1.40
15	a4	414	CLA	CMD-C2D	-2.14	1.46	1.50
15	cA	815	CLA	CMD-C2D	-2.14	1.46	1.50
15	a2	412	CLA	MG-ND	-2.14	2.01	2.05
15	b4	404	CLA	CMD-C2D	-2.14	1.46	1.50
15	cA	827	CLA	CMC-C2C	-2.14	1.46	1.50
15	c6	410	CLA	CMD-C2D	-2.14	1.46	1.50
15	c2	408	CLA	MG-ND	-2.14	2.01	2.05
15	cB	802	CLA	C4B-CHC	-2.14	1.35	1.41
15	c4	412	CLA	C4B-CHC	-2.14	1.35	1.41
15	bB	816	CLA	CMC-C2C	-2.14	1.46	1.50
15	cA	818	CLA	C3B-C2B	-2.14	1.37	1.40
15	bB	830	CLA	CHC-C1C	2.14	1.40	1.35
15	a4	404	CLA	CMD-C2D	-2.14	1.46	1.50
15	b4	403	CLA	MG-ND	-2.14	2.01	2.05
15	cB	826	CLA	MG-ND	-2.14	2.01	2.05
15	b3	421	CLA	MG-NA	2.14	2.11	2.06
15	cA	837	CLA	CMC-C2C	-2.14	1.46	1.50
15	b5	404	CLA	MG-ND	-2.14	2.01	2.05
15	b1	412	CLA	CHC-C1C	2.14	1.40	1.35
15	c6	416	CLA	C3B-CAB	-2.14	1.43	1.47
15	a1	416	CLA	CMD-C2D	-2.14	1.46	1.50
15	cA	838	CLA	C3B-C2B	-2.14	1.37	1.40
15	cB	819	CLA	C4B-CHC	-2.14	1.35	1.41
15	c6	408	CLA	MG-ND	-2.14	2.01	2.05
15	a4	406	CLA	CMD-C2D	-2.14	1.46	1.50
15	b4	411	CLA	CMC-C2C	-2.14	1.46	1.50
15	bB	811	CLA	C4B-CHC	-2.14	1.35	1.41
15	c2	412	CLA	MG-ND	-2.14	2.01	2.05
15	a6	415	CLA	CMC-C2C	-2.14	1.46	1.50
15	b3	404	CLA	MG-ND	-2.14	2.01	2.05
15	a3	412	CLA	CMD-C2D	-2.14	1.46	1.50
15	bB	819	CLA	C4B-CHC	-2.14	1.35	1.41
15	cB	824	CLA	C3B-C2B	-2.14	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	410	CLA	CMC-C2C	-2.14	1.46	1.50
15	c3	410	CLA	MG-ND	-2.14	2.01	2.05
15	aL	202	CLA	C4B-CHC	-2.14	1.35	1.41
15	cA	822	CLA	C4B-CHC	-2.13	1.35	1.41
15	a4	403	CLA	MG-ND	-2.13	2.01	2.05
15	c3	405	CLA	CMC-C2C	-2.13	1.46	1.50
15	bB	833	CLA	C1D-ND	2.13	1.40	1.37
15	a5	405	CLA	CMD-C2D	-2.13	1.46	1.50
15	cB	831	CLA	C4B-CHC	-2.13	1.35	1.41
15	c4	411	CLA	CMD-C2D	-2.13	1.46	1.50
15	aB	833	CLA	C1D-ND	2.13	1.40	1.37
15	aB	805	CLA	C3B-C2B	-2.13	1.37	1.40
15	a5	411	CLA	CMC-C2C	-2.13	1.46	1.50
15	cJ	102	CLA	CMD-C2D	-2.13	1.46	1.50
15	c6	407	CLA	CMD-C2D	-2.13	1.46	1.50
15	b4	412	CLA	C4B-CHC	-2.13	1.35	1.41
15	cL	202	CLA	C4B-CHC	-2.13	1.35	1.41
18	bB	847	BCR	C12-C13	-2.13	1.44	1.50
15	bA	844	CLA	CMD-C2D	-2.13	1.46	1.50
15	c5	404	CLA	CMD-C2D	-2.13	1.46	1.50
15	a1	409	CLA	C3B-C2B	-2.13	1.37	1.40
15	a1	422	CLA	C3B-CAB	-2.13	1.43	1.47
15	a6	416	CLA	C3B-CAB	-2.13	1.43	1.47
15	b2	412	CLA	MG-ND	-2.13	2.01	2.05
18	aA	850	BCR	C33-C5	-2.13	1.47	1.50
18	bL	201	BCR	C30-C25	-2.13	1.50	1.53
15	aA	832	CLA	CMC-C2C	-2.13	1.46	1.50
15	b3	412	CLA	CMD-C2D	-2.13	1.46	1.50
15	b4	406	CLA	CMD-C2D	-2.13	1.46	1.50
15	b4	411	CLA	CMD-C2D	-2.13	1.46	1.50
15	aB	839	CLA	C3B-CAB	-2.13	1.43	1.47
15	cA	831	CLA	C3B-CAB	-2.13	1.43	1.47
15	bJ	102	CLA	CMD-C2D	-2.13	1.46	1.50
15	b1	402	CLA	CMC-C2C	-2.13	1.46	1.50
15	c5	414	CLA	CMD-C2D	-2.13	1.46	1.50
15	aA	807	CLA	C1D-ND	2.13	1.40	1.37
15	cA	807	CLA	CAC-C3C	-2.13	1.45	1.51
15	c6	412	CLA	MG-ND	-2.13	2.01	2.05
15	c5	411	CLA	CMC-C2C	-2.13	1.46	1.50
19	cA	853	LHG	O8-C6	-2.13	1.40	1.45
15	a2	406	CLA	C3B-CAB	-2.13	1.43	1.47
15	a1	411	CLA	CMD-C2D	-2.13	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a4	405	CLA	CMC-C2C	-2.13	1.46	1.50
15	b5	414	CLA	CMD-C2D	-2.13	1.46	1.50
18	cB	844	BCR	C33-C5	-2.13	1.47	1.50
15	a3	405	CLA	MG-ND	-2.13	2.01	2.05
15	b1	408	CLA	CMC-C2C	-2.13	1.46	1.50
15	aB	816	CLA	CMC-C2C	-2.13	1.46	1.50
15	cL	201	CLA	CMC-C2C	-2.13	1.46	1.50
18	bM	101	BCR	C33-C5	-2.13	1.47	1.50
15	cB	816	CLA	C4B-CHC	-2.13	1.35	1.41
15	aB	822	CLA	CMD-C2D	-2.13	1.46	1.50
15	aB	838	CLA	CMC-C2C	-2.13	1.46	1.50
15	a1	416	CLA	CMC-C2C	-2.13	1.46	1.50
15	cA	821	CLA	CMD-C2D	-2.13	1.46	1.50
15	cJ	101	CLA	MG-ND	-2.13	2.01	2.05
15	c4	414	CLA	CMD-C2D	-2.13	1.46	1.50
15	c1	412	CLA	CHC-C1C	2.13	1.40	1.35
15	bB	822	CLA	CMD-C2D	-2.13	1.46	1.50
18	a6	421	BCR	C4-C5	-2.12	1.46	1.51
15	bA	808	CLA	CMC-C2C	-2.12	1.46	1.50
15	a6	415	CLA	CMD-C2D	-2.12	1.46	1.50
15	bA	815	CLA	CMD-C2D	-2.12	1.46	1.50
15	b5	410	CLA	CMD-C2D	-2.12	1.46	1.50
15	b5	411	CLA	CMC-C2C	-2.12	1.46	1.50
15	aB	831	CLA	C4B-CHC	-2.12	1.35	1.41
15	cB	829	CLA	C4B-CHC	-2.12	1.35	1.41
15	a6	407	CLA	CMD-C2D	-2.12	1.46	1.50
15	c1	414	CLA	CMD-C2D	-2.12	1.46	1.50
15	c3	409	CLA	CMC-C2C	-2.12	1.46	1.50
15	b3	405	CLA	MG-ND	-2.12	2.01	2.05
15	aB	818	CLA	CMD-C2D	-2.12	1.46	1.50
15	a6	414	CLA	CAC-C3C	-2.12	1.45	1.51
15	aB	832	CLA	C4B-CHC	-2.12	1.35	1.41
15	cB	826	CLA	CMC-C2C	-2.12	1.46	1.50
15	c1	404	CLA	CMD-C2D	-2.12	1.46	1.50
15	bJ	101	CLA	MG-ND	-2.12	2.01	2.05
15	bA	820	CLA	C3B-CAB	-2.12	1.43	1.47
15	b6	416	CLA	C3B-CAB	-2.12	1.43	1.47
18	c4	401	BCR	C33-C5	-2.12	1.47	1.50
15	c4	405	CLA	CMC-C2C	-2.12	1.46	1.50
15	bA	816	CLA	MG-ND	-2.12	2.01	2.05
19	cX	101	LHG	P-O6	2.12	1.67	1.59
15	cB	819	CLA	C3B-CAB	-2.12	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	405	CLA	CMC-C2C	-2.12	1.46	1.50
15	aA	807	CLA	CAC-C3C	-2.12	1.45	1.51
19	bX	101	LHG	P-O6	2.12	1.67	1.59
15	bA	825	CLA	C3B-CAB	-2.12	1.43	1.47
15	bB	805	CLA	MG-ND	-2.12	2.01	2.05
15	cB	816	CLA	CMD-C2D	-2.12	1.46	1.50
15	c1	414	CLA	CMC-C2C	-2.12	1.46	1.50
18	a2	401	BCR	C4-C5	-2.12	1.46	1.51
15	a4	411	CLA	CMD-C2D	-2.12	1.46	1.50
15	c2	410	CLA	CMD-C2D	-2.12	1.46	1.50
15	cB	832	CLA	C4B-CHC	-2.12	1.35	1.41
15	c5	408	CLA	MG-ND	-2.12	2.01	2.05
15	bA	818	CLA	C3B-C2B	-2.12	1.37	1.40
18	aM	101	BCR	C33-C5	-2.12	1.47	1.50
15	aB	830	CLA	C1B-NB	-2.12	1.33	1.35
15	b3	415	CLA	C3B-C2B	-2.12	1.37	1.40
15	aK	102	CLA	CMC-C2C	-2.12	1.46	1.50
15	a3	406	CLA	CMC-C2C	-2.12	1.46	1.50
15	b6	412	CLA	MG-ND	-2.12	2.01	2.05
15	bA	845	CLA	C3B-CAB	-2.12	1.43	1.47
19	aX	101	LHG	P-O6	2.12	1.67	1.59
15	bA	822	CLA	C4B-CHC	-2.12	1.35	1.41
15	c2	422	CLA	C3B-CAB	-2.12	1.43	1.47
15	bB	838	CLA	CMC-C2C	-2.12	1.46	1.50
15	c1	408	CLA	CMC-C2C	-2.12	1.46	1.50
18	aI	102	BCR	C34-C9	-2.12	1.46	1.50
15	c6	414	CLA	C4B-CHC	-2.12	1.35	1.41
15	a6	412	CLA	MG-ND	-2.12	2.01	2.05
15	c4	413	CLA	MG-ND	-2.12	2.01	2.05
15	a3	404	CLA	C3B-C2B	-2.12	1.37	1.40
15	b1	407	CLA	CMD-C2D	-2.12	1.46	1.50
15	a6	408	CLA	MG-ND	-2.12	2.01	2.05
15	cB	805	CLA	MG-ND	-2.12	2.01	2.05
15	a5	414	CLA	CMC-C2C	-2.12	1.46	1.50
15	cB	835	CLA	C3B-C2B	-2.12	1.37	1.40
15	aB	819	CLA	C4B-CHC	-2.12	1.35	1.41
15	bA	803	CLA	CAC-C3C	-2.12	1.45	1.51
15	b4	412	CLA	CMD-C2D	-2.12	1.46	1.50
15	b5	407	CLA	CMD-C2D	-2.12	1.46	1.50
15	bB	816	CLA	C4B-CHC	-2.12	1.35	1.41
15	aA	821	CLA	CMD-C2D	-2.11	1.46	1.50
15	b2	408	CLA	MG-ND	-2.11	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	414	CLA	C3B-C2B	-2.11	1.37	1.40
15	b3	407	CLA	CMC-C2C	-2.11	1.46	1.50
18	cI	102	BCR	C34-C9	-2.11	1.46	1.50
18	aL	205	BCR	C30-C25	-2.11	1.50	1.53
18	cA	849	BCR	C33-C5	-2.11	1.47	1.50
15	a5	404	CLA	MG-ND	-2.11	2.01	2.05
15	aB	829	CLA	C4B-CHC	-2.11	1.35	1.41
15	cA	825	CLA	C3B-CAB	-2.11	1.43	1.47
15	c6	415	CLA	CMD-C2D	-2.11	1.46	1.50
15	b3	416	CLA	C1C-NC	-2.11	1.34	1.37
15	cB	816	CLA	MG-ND	-2.11	2.01	2.05
15	b5	413	CLA	MG-ND	-2.11	2.01	2.05
15	c3	404	CLA	C3B-C2B	-2.11	1.37	1.40
15	a3	416	CLA	C1C-NC	-2.11	1.34	1.37
15	b3	410	CLA	C3C-C2C	2.11	1.41	1.36
15	aA	823	CLA	C3B-C2B	-2.11	1.37	1.40
15	bA	823	CLA	C3B-C2B	-2.11	1.37	1.40
15	b3	404	CLA	C3B-C2B	-2.11	1.37	1.40
15	bA	807	CLA	CAC-C3C	-2.11	1.45	1.51
15	cB	816	CLA	CMC-C2C	-2.11	1.46	1.50
15	b1	414	CLA	CMD-C2D	-2.11	1.46	1.50
15	cA	832	CLA	CMC-C2C	-2.11	1.46	1.50
15	aA	802	CLA	C5-C3	-2.11	1.46	1.51
15	cA	823	CLA	C3B-C2B	-2.11	1.37	1.40
15	a5	403	CLA	MG-ND	-2.11	2.01	2.05
18	aA	851	BCR	C10-C9	-2.11	1.33	1.35
15	b2	411	CLA	CMD-C2D	-2.11	1.46	1.50
15	cB	822	CLA	CMD-C2D	-2.11	1.46	1.50
15	bB	830	CLA	C1B-NB	-2.11	1.33	1.35
15	aB	816	CLA	MG-ND	-2.11	2.01	2.05
15	aA	837	CLA	CMC-C2C	-2.11	1.46	1.50
15	c6	416	CLA	C3B-C2B	-2.11	1.37	1.40
15	bB	819	CLA	C3B-CAB	-2.11	1.43	1.47
15	a1	413	CLA	CMC-C2C	-2.11	1.46	1.50
15	aA	803	CLA	CAC-C3C	-2.11	1.45	1.51
15	c3	416	CLA	C1C-NC	-2.11	1.34	1.37
15	aA	844	CLA	CMD-C2D	-2.11	1.46	1.50
15	bB	816	CLA	CMD-C2D	-2.11	1.46	1.50
15	bB	826	CLA	CMC-C2C	-2.11	1.46	1.50
15	c3	412	CLA	CMD-C2D	-2.11	1.46	1.50
15	aA	816	CLA	MG-ND	-2.11	2.01	2.05
18	b6	401	BCR	C4-C5	-2.11	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	412	CLA	CMD-C2D	-2.11	1.46	1.50
15	b6	410	CLA	CMD-C2D	-2.11	1.46	1.50
15	c5	403	CLA	MG-ND	-2.11	2.01	2.05
15	cA	803	CLA	CAC-C3C	-2.11	1.45	1.51
15	cB	810	CLA	C3B-CAB	-2.11	1.43	1.47
15	c6	418	CLA	C4D-ND	-2.11	1.34	1.37
15	aA	818	CLA	C3B-C2B	-2.11	1.37	1.40
15	c4	415	CLA	C3B-C2B	-2.11	1.37	1.40
15	b2	413	CLA	CMD-C2D	-2.11	1.46	1.50
15	c3	414	CLA	CMC-C2C	-2.11	1.46	1.50
15	aA	824	CLA	MG-ND	-2.11	2.01	2.05
15	a5	407	CLA	MG-ND	-2.11	2.01	2.05
15	cK	102	CLA	CMC-C2C	-2.11	1.46	1.50
19	bA	855	LHG	O8-C6	-2.11	1.40	1.45
15	bA	807	CLA	C1D-ND	2.10	1.40	1.37
15	aB	815	CLA	C3B-CAB	-2.10	1.43	1.47
15	cB	835	CLA	C3B-CAB	-2.10	1.43	1.47
18	bI	102	BCR	C34-C9	-2.10	1.46	1.50
15	a1	416	CLA	C4D-ND	-2.10	1.34	1.37
15	a4	404	CLA	MG-ND	-2.10	2.01	2.05
15	c4	404	CLA	MG-ND	-2.10	2.01	2.05
15	a3	405	CLA	CMD-C2D	-2.10	1.46	1.50
15	a6	422	CLA	CMC-C2C	-2.10	1.46	1.50
15	b4	413	CLA	MG-ND	-2.10	2.01	2.05
15	aB	816	CLA	CMD-C2D	-2.10	1.46	1.50
15	b3	406	CLA	CMD-C2D	-2.10	1.46	1.50
15	a1	401	CLA	CMD-C2D	-2.10	1.46	1.50
18	bA	848	BCR	C33-C5	-2.10	1.47	1.50
15	c6	416	CLA	MG-ND	-2.10	2.01	2.05
15	bA	832	CLA	CMC-C2C	-2.10	1.46	1.50
15	cL	203	CLA	C3B-CAB	-2.10	1.43	1.47
15	a1	413	CLA	CMD-C2D	-2.10	1.46	1.50
15	c5	406	CLA	CMC-C2C	-2.10	1.46	1.50
15	b4	415	CLA	C3B-C2B	-2.10	1.37	1.40
15	aA	831	CLA	C3B-CAB	-2.10	1.43	1.47
15	bB	815	CLA	C3B-CAB	-2.10	1.43	1.47
15	cX	102	CLA	CMC-C2C	-2.10	1.46	1.50
15	aA	838	CLA	C3B-C2B	-2.10	1.37	1.40
15	bA	821	CLA	CMD-C2D	-2.10	1.46	1.50
15	cA	817	CLA	C3B-CAB	-2.10	1.43	1.47
15	a5	408	CLA	MG-ND	-2.10	2.01	2.05
15	aB	809	CLA	C4B-CHC	-2.10	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	407	CLA	CMC-C2C	-2.10	1.46	1.50
15	a4	410	CLA	C3B-C2B	-2.10	1.37	1.40
15	a5	413	CLA	MG-ND	-2.10	2.01	2.05
15	b1	411	CLA	CMC-C2C	-2.10	1.46	1.50
15	b5	414	CLA	CMC-C2C	-2.10	1.46	1.50
15	c1	407	CLA	CMD-C2D	-2.10	1.46	1.50
15	aA	845	CLA	MG-ND	-2.10	2.01	2.05
15	bA	805	CLA	C3B-C2B	-2.10	1.37	1.40
15	a3	410	CLA	C3C-C2C	2.10	1.41	1.36
15	cA	805	CLA	C3B-CAB	-2.10	1.43	1.47
15	cA	843	CLA	CMD-C2D	-2.10	1.46	1.50
15	c2	413	CLA	CMD-C2D	-2.10	1.46	1.50
15	bA	838	CLA	C3B-C2B	-2.10	1.37	1.40
15	bA	845	CLA	MG-ND	-2.10	2.01	2.05
15	a1	407	CLA	CMC-C2C	-2.10	1.46	1.50
15	bA	824	CLA	MG-ND	-2.10	2.01	2.05
15	aA	805	CLA	C3B-C2B	-2.10	1.37	1.40
15	c3	417	CLA	CMC-C2C	-2.10	1.46	1.50
15	bB	816	CLA	MG-ND	-2.10	2.01	2.05
15	b4	414	CLA	CMC-C2C	-2.10	1.46	1.50
15	a2	408	CLA	MG-ND	-2.10	2.01	2.05
18	a6	401	BCR	C4-C5	-2.10	1.46	1.51
15	bB	829	CLA	C4B-CHC	-2.10	1.35	1.41
18	aB	845	BCR	C38-C26	-2.10	1.47	1.50
15	c1	411	CLA	CMD-C2D	-2.09	1.46	1.50
15	c3	421	CLA	CMC-C2C	-2.09	1.46	1.50
15	a1	414	CLA	C3B-C2B	-2.09	1.37	1.40
15	c6	415	CLA	CMC-C2C	-2.09	1.46	1.50
18	aB	844	BCR	C33-C5	-2.09	1.47	1.50
15	cB	834	CLA	C3B-CAB	-2.09	1.43	1.47
15	c2	414	CLA	C3B-C2B	-2.09	1.37	1.40
15	aB	818	CLA	MG-ND	-2.09	2.01	2.05
15	a3	421	CLA	CMC-C2C	-2.09	1.46	1.50
15	c3	407	CLA	CMC-C2C	-2.09	1.46	1.50
18	b1	401	BCR	C4-C5	-2.09	1.46	1.51
18	cB	848	BCR	C38-C26	-2.09	1.47	1.50
15	b2	422	CLA	C3B-CAB	-2.09	1.43	1.47
15	b6	416	CLA	MG-ND	-2.09	2.01	2.05
15	cA	803	CLA	C3B-CAB	-2.09	1.43	1.47
18	bB	845	BCR	C38-C26	-2.09	1.47	1.50
15	a5	402	CLA	CMC-C2C	-2.09	1.46	1.50
15	a6	418	CLA	CMC-C2C	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	415	CLA	CMD-C2D	-2.09	1.46	1.50
18	b2	401	BCR	C4-C5	-2.09	1.46	1.51
15	b5	404	CLA	CMD-C2D	-2.09	1.46	1.50
15	c1	411	CLA	CMC-C2C	-2.09	1.46	1.50
15	c6	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	b6	414	CLA	CAC-C3C	-2.09	1.45	1.51
15	a2	413	CLA	CMD-C2D	-2.09	1.46	1.50
15	bA	803	CLA	C3B-CAB	-2.09	1.43	1.47
15	cB	815	CLA	C3B-CAB	-2.09	1.43	1.47
15	a4	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	aL	201	CLA	CMC-C2C	-2.09	1.46	1.50
15	cB	838	CLA	CMC-C2C	-2.09	1.46	1.50
15	c1	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	cA	812	CLA	C4B-CHC	-2.09	1.35	1.41
15	c2	408	CLA	CMC-C2C	-2.09	1.46	1.50
15	c5	405	CLA	CMD-C2D	-2.09	1.46	1.50
15	a2	422	CLA	C3B-CAB	-2.09	1.43	1.47
15	a5	414	CLA	CMD-C2D	-2.09	1.46	1.50
15	c4	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	aA	822	CLA	C4B-CHC	-2.09	1.35	1.41
15	bA	817	CLA	C3B-CAB	-2.09	1.43	1.47
15	bB	832	CLA	C4B-CHC	-2.09	1.35	1.41
15	bA	837	CLA	CMC-C2C	-2.09	1.46	1.50
15	c1	416	CLA	C1C-NC	-2.09	1.34	1.37
15	a4	414	CLA	CMC-C2C	-2.09	1.46	1.50
15	b5	403	CLA	MG-ND	-2.09	2.01	2.05
15	cA	820	CLA	C3B-CAB	-2.09	1.43	1.47
15	bB	809	CLA	C4B-CHC	-2.09	1.35	1.41
15	bA	802	CLA	C5-C3	-2.09	1.46	1.51
18	c6	401	BCR	C4-C5	-2.09	1.46	1.51
15	c5	420	CLA	C3B-C2B	-2.09	1.37	1.40
15	a2	415	CLA	CMD-C2D	-2.09	1.46	1.50
15	bB	831	CLA	C4B-CHC	-2.09	1.35	1.41
15	cA	806	CLA	C4B-CHC	-2.09	1.35	1.41
18	b5	401	BCR	C4-C5	-2.09	1.46	1.51
15	b3	414	CLA	CMC-C2C	-2.09	1.46	1.50
15	a5	404	CLA	CMD-C2D	-2.09	1.46	1.50
15	a6	413	CLA	CMD-C2D	-2.09	1.46	1.50
19	bA	854	LHG	O6-C4	-2.09	1.36	1.44
15	bA	803	CLA	C1D-ND	2.09	1.40	1.37
15	c4	414	CLA	CMC-C2C	-2.09	1.46	1.50
15	b6	416	CLA	C3B-C2B	-2.09	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c5	420	CLA	C2A-C1A	2.09	1.56	1.52
15	cB	809	CLA	C4B-CHC	-2.09	1.35	1.41
15	c4	403	CLA	MG-ND	-2.09	2.01	2.05
15	bA	810	CLA	CMC-C2C	-2.09	1.46	1.50
15	b6	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	c4	417	CLA	CMD-C2D	-2.08	1.46	1.50
15	bB	824	CLA	C3B-C2B	-2.08	1.37	1.40
15	aB	835	CLA	C3B-CAB	-2.08	1.43	1.47
15	bA	828	CLA	C3B-CAB	-2.08	1.43	1.47
15	aB	805	CLA	MG-ND	-2.08	2.01	2.05
18	cK	101	BCR	C33-C5	-2.08	1.47	1.50
15	c1	410	CLA	C3B-C2B	-2.08	1.37	1.40
15	a6	422	CLA	C4D-CHA	2.08	1.45	1.38
15	cA	815	CLA	MG-ND	-2.08	2.01	2.05
15	b6	418	CLA	CMC-C2C	-2.08	1.46	1.50
15	c5	407	CLA	CMD-C2D	-2.08	1.46	1.50
15	c6	413	CLA	CMD-C2D	-2.08	1.46	1.50
15	aA	819	CLA	MG-ND	-2.08	2.01	2.05
15	bB	811	CLA	CAC-C3C	-2.08	1.45	1.51
15	aB	816	CLA	C4B-CHC	-2.08	1.35	1.41
15	bB	835	CLA	C3B-CAB	-2.08	1.43	1.47
15	b4	417	CLA	CMD-C2D	-2.08	1.46	1.50
16	bB	843	PQN	C9-C10	-2.08	1.36	1.39
15	bA	814	CLA	C3B-CAB	-2.08	1.43	1.47
15	bB	805	CLA	C3B-CAB	-2.08	1.43	1.47
15	aA	806	CLA	C4B-CHC	-2.08	1.35	1.41
15	c2	418	CLA	C3B-CAB	-2.08	1.43	1.47
15	aA	811	CLA	MG-ND	-2.08	2.01	2.05
15	cA	844	CLA	MG-ND	-2.08	2.01	2.05
15	bA	815	CLA	MG-ND	-2.08	2.01	2.05
15	a3	405	CLA	C4B-CHC	-2.08	1.35	1.41
15	aB	824	CLA	C3B-C2B	-2.08	1.37	1.40
15	bA	819	CLA	MG-ND	-2.08	2.01	2.05
15	a5	409	CLA	CMC-C2C	-2.08	1.46	1.50
15	cA	810	CLA	CMC-C2C	-2.08	1.46	1.50
15	c3	415	CLA	O2A-CGA	2.08	1.37	1.30
15	b5	420	CLA	C3B-C2B	-2.08	1.37	1.40
19	cA	852	LHG	O6-C4	-2.08	1.36	1.44
18	bB	844	BCR	C33-C5	-2.08	1.47	1.50
15	cA	824	CLA	MG-ND	-2.08	2.01	2.05
15	cB	811	CLA	CAC-C3C	-2.08	1.45	1.51
15	a4	417	CLA	CMD-C2D	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	409	CLA	MG-ND	-2.08	2.01	2.05
15	aA	840	CLA	CMC-C2C	-2.08	1.46	1.50
15	c3	405	CLA	C4B-CHC	-2.08	1.35	1.41
15	c1	404	CLA	C3B-C2B	-2.08	1.37	1.40
15	aB	826	CLA	CMC-C2C	-2.08	1.46	1.50
15	bA	806	CLA	C4B-CHC	-2.08	1.35	1.41
15	a2	407	CLA	CMD-C2D	-2.08	1.46	1.50
15	b2	407	CLA	CMD-C2D	-2.07	1.46	1.50
15	cB	833	CLA	C1D-ND	2.07	1.40	1.37
15	aA	811	CLA	C3B-CAB	-2.07	1.43	1.47
19	aA	853	LHG	O6-C4	-2.07	1.36	1.44
15	c3	412	CLA	C4B-CHC	-2.07	1.35	1.41
15	b6	407	CLA	CMC-C2C	-2.07	1.46	1.50
19	aA	854	LHG	O8-C6	-2.07	1.40	1.45
15	a1	411	CLA	CHC-C1C	2.07	1.40	1.35
15	a5	407	CLA	CMD-C2D	-2.07	1.46	1.50
15	c5	407	CLA	MG-ND	-2.07	2.01	2.05
15	b3	412	CLA	C4B-CHC	-2.07	1.35	1.41
15	aA	838	CLA	C1C-NC	-2.07	1.34	1.37
15	aA	833	CLA	CAC-C3C	-2.07	1.45	1.51
15	aX	102	CLA	CMC-C2C	-2.07	1.46	1.50
15	c6	418	CLA	CMC-C2C	-2.07	1.46	1.50
15	aA	843	CLA	C3B-CAB	-2.07	1.43	1.47
15	a5	406	CLA	CMC-C2C	-2.07	1.46	1.50
15	b6	407	CLA	CMD-C2D	-2.07	1.46	1.50
15	aA	828	CLA	C3B-CAB	-2.07	1.43	1.47
15	b6	418	CLA	C4D-ND	-2.07	1.34	1.37
15	c2	404	CLA	CMC-C2C	-2.07	1.46	1.50
15	cA	825	CLA	C3B-C2B	-2.07	1.37	1.40
15	a6	418	CLA	C4D-ND	-2.07	1.34	1.37
15	b1	417	CLA	C4D-ND	-2.07	1.34	1.37
15	aB	805	CLA	C3B-CAB	-2.07	1.43	1.47
15	b5	407	CLA	MG-ND	-2.07	2.01	2.05
15	aA	803	CLA	C3B-CAB	-2.07	1.43	1.47
15	b6	405	CLA	MG-ND	-2.07	2.01	2.05
15	b3	421	CLA	CMC-C2C	-2.07	1.46	1.50
18	aB	848	BCR	C38-C26	-2.07	1.47	1.50
15	a1	403	CLA	C3B-C2B	-2.07	1.37	1.40
15	b5	406	CLA	CMC-C2C	-2.07	1.46	1.50
15	a3	413	CLA	CMD-C2D	-2.07	1.46	1.50
15	c1	413	CLA	CMD-C2D	-2.07	1.46	1.50
15	cB	805	CLA	C3B-CAB	-2.07	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	aA	848	BCR	C38-C26	-2.07	1.47	1.50
15	bA	805	CLA	C3B-CAB	-2.07	1.43	1.47
15	a2	412	CLA	CMD-C2D	-2.07	1.46	1.50
15	b6	408	CLA	MG-ND	-2.07	2.01	2.05
15	aA	805	CLA	C3B-CAB	-2.07	1.43	1.47
15	bK	101	CLA	CMC-C2C	-2.07	1.46	1.50
15	b3	406	CLA	CMC-C2C	-2.07	1.46	1.50
15	a6	414	CLA	CMD-C2D	-2.07	1.46	1.50
15	bA	825	CLA	CMC-C2C	-2.07	1.46	1.50
18	aK	101	BCR	C33-C5	-2.07	1.47	1.50
18	cF	205	BCR	C38-C26	-2.07	1.47	1.50
15	bX	102	CLA	CMC-C2C	-2.07	1.46	1.50
15	cB	826	CLA	C3B-C2B	-2.07	1.37	1.40
15	a3	404	CLA	MG-ND	-2.07	2.01	2.05
15	aB	834	CLA	C3B-CAB	-2.07	1.43	1.47
15	bA	825	CLA	C3B-C2B	-2.07	1.37	1.40
15	b6	422	CLA	CMC-C2C	-2.07	1.46	1.50
15	c5	413	CLA	MG-ND	-2.07	2.01	2.05
15	c5	414	CLA	CMC-C2C	-2.07	1.46	1.50
15	cA	802	CLA	C1D-ND	2.07	1.40	1.37
18	aF	203	BCR	C33-C5	-2.07	1.47	1.50
15	aA	845	CLA	CMC-C2C	-2.07	1.46	1.50
15	a6	412	CLA	CMD-C2D	-2.07	1.46	1.50
15	aB	811	CLA	CAC-C3C	-2.07	1.45	1.51
15	aA	820	CLA	C3B-CAB	-2.06	1.43	1.47
18	c5	401	BCR	C4-C5	-2.06	1.46	1.51
15	cA	828	CLA	C3B-CAB	-2.06	1.43	1.47
15	aA	812	CLA	C4B-CHC	-2.06	1.35	1.41
15	bB	826	CLA	C3B-C2B	-2.06	1.37	1.40
15	b3	409	CLA	CMC-C2C	-2.06	1.46	1.50
15	b4	406	CLA	CMC-C2C	-2.06	1.46	1.50
15	cA	844	CLA	CMC-C2C	-2.06	1.46	1.50
15	b2	409	CLA	MG-ND	-2.06	2.01	2.05
15	aB	807	CLA	CAC-C3C	-2.06	1.45	1.51
18	cA	850	BCR	C10-C9	-2.06	1.33	1.35
15	aA	817	CLA	C3B-CAB	-2.06	1.43	1.47
15	b6	409	CLA	MG-ND	-2.06	2.01	2.05
15	cB	801	CLA	C4B-CHC	-2.06	1.35	1.41
15	aJ	202	CLA	MG-ND	-2.06	2.01	2.05
18	cF	202	BCR	C38-C26	-2.06	1.47	1.50
15	bJ	101	CLA	CMC-C2C	-2.06	1.46	1.50
15	b1	411	CLA	CMD-C2D	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	411	CLA	CMD-C2D	-2.06	1.46	1.50
15	c3	406	CLA	CMD-C2D	-2.06	1.46	1.50
15	cA	834	CLA	CAA-C2A	-2.06	1.50	1.54
18	bA	849	BCR	C38-C26	-2.06	1.47	1.50
15	aJ	202	CLA	CMC-C2C	-2.06	1.46	1.50
15	c6	407	CLA	CMC-C2C	-2.06	1.46	1.50
15	aA	823	CLA	C3B-CAB	-2.06	1.43	1.47
15	a6	409	CLA	MG-ND	-2.06	2.01	2.05
15	b4	404	CLA	MG-ND	-2.06	2.01	2.05
15	aA	830	CLA	C3B-C2B	-2.06	1.37	1.40
15	c2	416	CLA	O2A-CGA	2.06	1.37	1.30
15	b5	408	CLA	MG-ND	-2.06	2.01	2.05
15	a5	412	CLA	C4B-CHC	-2.06	1.35	1.41
18	bA	852	BCR	C33-C5	-2.06	1.47	1.50
15	bA	835	CLA	C4B-CHC	-2.06	1.35	1.41
15	a4	415	CLA	C3B-C2B	-2.06	1.37	1.40
15	c3	405	CLA	MG-ND	-2.06	2.01	2.05
15	cA	811	CLA	C3B-CAB	-2.06	1.43	1.47
15	c2	409	CLA	MG-ND	-2.06	2.01	2.05
18	bA	851	BCR	C33-C5	-2.06	1.47	1.50
15	cA	838	CLA	C1C-NC	-2.06	1.34	1.37
15	c2	412	CLA	CMD-C2D	-2.06	1.46	1.50
15	aA	815	CLA	MG-ND	-2.06	2.01	2.05
15	c1	407	CLA	MG-ND	-2.06	2.01	2.05
15	b1	412	CLA	CMD-C2D	-2.06	1.46	1.50
15	c2	407	CLA	CMD-C2D	-2.06	1.46	1.50
15	c2	411	CLA	CMD-C2D	-2.06	1.46	1.50
15	c4	406	CLA	CMC-C2C	-2.06	1.46	1.50
15	a4	406	CLA	CMC-C2C	-2.06	1.46	1.50
15	b5	405	CLA	CMD-C2D	-2.06	1.46	1.50
15	c1	402	CLA	CMC-C2C	-2.06	1.46	1.50
18	aA	851	BCR	C33-C5	-2.06	1.47	1.50
15	a3	409	CLA	CMC-C2C	-2.06	1.46	1.50
15	b6	411	CLA	CMD-C2D	-2.06	1.46	1.50
15	c4	421	CLA	CMC-C2C	-2.06	1.46	1.50
15	c5	405	CLA	CMC-C2C	-2.06	1.46	1.50
15	aJ	203	CLA	MG-ND	-2.06	2.01	2.05
15	a1	406	CLA	CMD-C2D	-2.06	1.46	1.50
15	a4	407	CLA	CMC-C2C	-2.06	1.46	1.50
15	b2	408	CLA	CMC-C2C	-2.06	1.46	1.50
15	a2	412	CLA	O2A-CGA	2.06	1.37	1.30
15	b6	413	CLA	CMD-C2D	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	416	CLA	MG-ND	-2.06	2.01	2.05
15	c4	421	CLA	C4D-CHA	2.06	1.45	1.38
15	bA	812	CLA	C4B-CHC	-2.06	1.35	1.41
15	aB	826	CLA	C3B-C2B	-2.06	1.37	1.40
15	a6	407	CLA	CMC-C2C	-2.06	1.46	1.50
15	b4	404	CLA	CMC-C2C	-2.05	1.46	1.50
15	c2	415	CLA	CMD-C2D	-2.05	1.46	1.50
15	cA	814	CLA	C3B-CAB	-2.05	1.43	1.47
15	cJ	101	CLA	CMC-C2C	-2.05	1.46	1.50
15	cB	818	CLA	MG-ND	-2.05	2.01	2.05
15	c1	411	CLA	MG-ND	-2.05	2.01	2.05
15	bA	812	CLA	MG-ND	-2.05	2.01	2.05
15	aB	801	CLA	C3B-CAB	-2.05	1.43	1.47
15	bA	840	CLA	CMC-C2C	-2.05	1.46	1.50
15	a4	421	CLA	O2D-CGD	2.05	1.38	1.33
15	b3	415	CLA	C4B-CHC	-2.05	1.35	1.41
15	cA	827	CLA	C3B-C2B	-2.05	1.37	1.40
15	bA	844	CLA	CBD-CAD	2.05	1.56	1.51
18	bJ	103	BCR	C33-C5	-2.05	1.47	1.50
15	bB	834	CLA	C3B-CAB	-2.05	1.43	1.47
15	aA	810	CLA	CMC-C2C	-2.05	1.46	1.50
15	aA	829	CLA	C3B-C2B	-2.05	1.37	1.40
15	cA	830	CLA	C3B-C2B	-2.05	1.37	1.40
15	a3	414	CLA	CMC-C2C	-2.05	1.46	1.50
15	b5	402	CLA	CMC-C2C	-2.05	1.46	1.50
15	a4	413	CLA	MG-ND	-2.05	2.01	2.05
15	aA	802	CLA	C1D-ND	2.05	1.40	1.37
15	a3	415	CLA	C3B-C2B	-2.05	1.37	1.40
15	c4	407	CLA	CMC-C2C	-2.05	1.46	1.50
15	a3	412	CLA	C4B-CHC	-2.05	1.35	1.41
15	b1	414	CLA	CMC-C2C	-2.05	1.46	1.50
15	b2	412	CLA	O2A-CGA	2.05	1.37	1.30
15	a2	408	CLA	CMC-C2C	-2.05	1.46	1.50
15	b2	416	CLA	O2A-CGA	2.05	1.37	1.30
16	aB	843	PQN	C9-C10	-2.05	1.36	1.39
15	a1	410	CLA	MG-ND	-2.05	2.01	2.05
15	b4	417	CLA	C3B-CAB	-2.05	1.43	1.47
15	a6	413	CLA	C4B-CHC	-2.05	1.35	1.41
18	cA	847	BCR	C38-C26	-2.05	1.47	1.50
15	cJ	102	CLA	MG-ND	-2.05	2.01	2.05
15	b4	421	CLA	CMC-C2C	-2.05	1.46	1.50
15	bB	818	CLA	MG-ND	-2.05	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	812	CLA	MG-ND	-2.05	2.01	2.05
15	cA	833	CLA	C1D-ND	2.05	1.40	1.37
15	aA	827	CLA	C4B-CHC	-2.05	1.35	1.41
18	aA	852	BCR	C38-C26	-2.05	1.47	1.50
15	c3	415	CLA	C4B-CHC	-2.05	1.35	1.41
15	a1	403	CLA	CMD-C2D	-2.05	1.46	1.50
15	b5	420	CLA	C2A-C1A	2.05	1.56	1.52
15	a4	404	CLA	CMC-C2C	-2.05	1.46	1.50
15	cA	811	CLA	MG-ND	-2.05	2.01	2.05
15	c4	408	CLA	MG-ND	-2.05	2.01	2.05
15	c3	414	CLA	C3B-C2B	-2.05	1.37	1.40
15	a2	415	CLA	CMC-C2C	-2.05	1.46	1.50
15	bA	833	CLA	C1D-ND	2.05	1.40	1.37
15	a6	405	CLA	MG-ND	-2.05	2.01	2.05
15	c6	409	CLA	MG-ND	-2.05	2.01	2.05
15	b5	405	CLA	CMC-C2C	-2.05	1.46	1.50
15	cA	815	CLA	CMC-C2C	-2.05	1.46	1.50
18	aJ	204	BCR	C33-C5	-2.05	1.47	1.50
15	aA	825	CLA	C3B-CAB	-2.05	1.43	1.47
15	b1	407	CLA	MG-ND	-2.04	2.01	2.05
15	a2	414	CLA	C4B-CHC	-2.04	1.35	1.41
16	cB	843	PQN	C9-C10	-2.04	1.36	1.39
18	bA	852	BCR	C10-C9	-2.04	1.33	1.35
15	a3	405	CLA	CMC-C2C	-2.04	1.46	1.50
15	c3	402	CLA	CMC-C2C	-2.04	1.46	1.50
15	a4	421	CLA	C4D-CHA	2.04	1.45	1.38
15	a2	411	CLA	CMD-C2D	-2.04	1.46	1.50
15	c4	414	CLA	C3B-C2B	-2.04	1.37	1.40
15	aB	801	CLA	C4B-CHC	-2.04	1.35	1.41
15	aA	815	CLA	CMC-C2C	-2.04	1.46	1.50
15	c5	402	CLA	CMC-C2C	-2.04	1.46	1.50
15	c2	412	CLA	O2A-CGA	2.04	1.37	1.30
15	cA	819	CLA	MG-ND	-2.04	2.01	2.05
15	a1	406	CLA	CMC-C2C	-2.04	1.46	1.50
15	a1	410	CLA	CMD-C2D	-2.04	1.46	1.50
15	b4	421	CLA	C4D-CHA	2.04	1.45	1.38
15	a1	412	CLA	CMD-C2D	-2.04	1.46	1.50
15	b3	413	CLA	C4B-CHC	-2.04	1.35	1.41
15	a5	420	CLA	C2A-C1A	2.04	1.56	1.52
15	a3	409	CLA	C3B-CAB	-2.04	1.43	1.47
15	bA	815	CLA	CMC-C2C	-2.04	1.46	1.50
15	aA	834	CLA	CAA-C2A	-2.04	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	416	CLA	O2A-CGA	2.04	1.37	1.30
18	bB	849	BCR	C38-C26	-2.04	1.47	1.50
18	bJ	105	BCR	C33-C5	-2.04	1.47	1.50
18	cB	845	BCR	C38-C26	-2.04	1.47	1.50
15	c2	405	CLA	CMC-C2C	-2.04	1.46	1.50
15	c3	413	CLA	CMD-C2D	-2.04	1.46	1.50
15	c4	404	CLA	CMC-C2C	-2.04	1.46	1.50
15	b6	422	CLA	CAA-C2A	2.04	1.57	1.54
15	aA	812	CLA	MG-ND	-2.04	2.01	2.05
15	cA	832	CLA	MG-ND	-2.04	2.01	2.05
15	bB	806	CLA	CMA-C3A	-2.04	1.48	1.53
15	a1	416	CLA	C3B-CAB	-2.04	1.43	1.47
18	aJ	205	BCR	C33-C5	-2.04	1.47	1.50
15	bA	811	CLA	MG-ND	-2.04	2.01	2.05
15	a1	414	CLA	O2A-CGA	2.04	1.37	1.30
15	aB	812	CLA	CMC-C2C	-2.04	1.46	1.50
15	a1	401	CLA	CMC-C2C	-2.04	1.46	1.50
18	aJ	205	BCR	C38-C26	-2.04	1.47	1.50
15	aA	835	CLA	CAC-C3C	-2.04	1.45	1.51
15	a6	416	CLA	C3B-C2B	-2.04	1.37	1.40
15	b4	421	CLA	O2D-CGD	2.04	1.38	1.33
15	b4	407	CLA	CMC-C2C	-2.04	1.46	1.50
15	cA	840	CLA	CMC-C2C	-2.04	1.46	1.50
15	cB	807	CLA	CAC-C3C	-2.04	1.45	1.51
18	bI	102	BCR	C17-C18	-2.04	1.33	1.35
15	bA	830	CLA	C3B-C2B	-2.04	1.37	1.40
15	bB	824	CLA	CMC-C2C	-2.04	1.46	1.50
15	c3	414	CLA	CMD-C2D	-2.04	1.46	1.50
15	cB	801	CLA	C3B-CAB	-2.04	1.43	1.47
15	cA	802	CLA	C5-C3	-2.04	1.47	1.51
18	b1	420	BCR	C31-C1	-2.04	1.49	1.53
15	aA	803	CLA	C1D-ND	2.04	1.40	1.37
15	a5	412	CLA	CMD-C2D	-2.04	1.46	1.50
15	bA	833	CLA	CAC-C3C	-2.04	1.45	1.51
15	a3	415	CLA	C4B-CHC	-2.04	1.35	1.41
15	bA	838	CLA	C1C-NC	-2.04	1.34	1.37
15	b4	414	CLA	MG-ND	-2.04	2.01	2.05
15	bB	807	CLA	CAC-C3C	-2.04	1.45	1.51
18	aF	203	BCR	C38-C26	-2.04	1.47	1.50
15	a1	422	CLA	CMC-C2C	-2.04	1.46	1.50
15	bB	801	CLA	C3B-CAB	-2.04	1.43	1.47
15	c4	414	CLA	MG-ND	-2.03	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	405	CLA	CMD-C2D	-2.03	1.46	1.50
15	b2	418	CLA	C3B-CAB	-2.03	1.43	1.47
15	bB	801	CLA	C4B-CHC	-2.03	1.35	1.41
15	c6	405	CLA	MG-ND	-2.03	2.01	2.05
18	aB	849	BCR	C36-C18	-2.03	1.46	1.50
15	b3	415	CLA	O2A-CGA	2.03	1.37	1.30
15	bA	845	CLA	CMC-C2C	-2.03	1.46	1.50
15	b1	413	CLA	CMD-C2D	-2.03	1.46	1.50
15	c3	413	CLA	C4B-CHC	-2.03	1.35	1.41
15	b2	411	CLA	C3B-C2B	-2.03	1.37	1.40
15	cB	806	CLA	C3B-C2B	-2.03	1.37	1.40
15	bA	802	CLA	C1D-ND	2.03	1.40	1.37
15	a2	404	CLA	CMC-C2C	-2.03	1.46	1.50
15	cA	805	CLA	C3B-C2B	-2.03	1.37	1.40
15	aB	808	CLA	C4B-CHC	-2.03	1.35	1.41
15	aL	202	CLA	C1D-ND	2.03	1.40	1.37
15	b5	412	CLA	C4B-CHC	-2.03	1.35	1.41
15	c2	414	CLA	C4B-CHC	-2.03	1.35	1.41
15	bA	823	CLA	CMC-C2C	-2.03	1.46	1.50
20	aB	850	LMG	O4-C4	-2.03	1.38	1.43
18	bJ	104	BCR	C38-C26	-2.03	1.47	1.50
18	cJ	104	BCR	C38-C26	-2.03	1.47	1.50
15	bA	827	CLA	C4B-CHC	-2.03	1.35	1.41
15	cA	843	CLA	CBD-CAD	2.03	1.56	1.51
15	a5	415	CLA	O2A-CGA	2.03	1.37	1.30
15	b3	405	CLA	C4B-CHC	-2.03	1.35	1.41
18	cA	851	BCR	C38-C26	-2.03	1.47	1.50
15	aA	825	CLA	CMC-C2C	-2.03	1.46	1.50
15	aB	839	CLA	MG-ND	-2.03	2.01	2.05
15	a4	414	CLA	MG-ND	-2.03	2.01	2.05
15	cA	829	CLA	C3B-C2B	-2.03	1.37	1.40
15	bA	834	CLA	CAA-C2A	-2.03	1.50	1.54
15	b2	415	CLA	CMC-C2C	-2.03	1.46	1.50
18	a5	401	BCR	C4-C5	-2.03	1.47	1.51
15	bJ	102	CLA	MG-ND	-2.03	2.01	2.05
15	c3	404	CLA	MG-ND	-2.03	2.01	2.05
15	a4	421	CLA	CMC-C2C	-2.03	1.46	1.50
15	b3	413	CLA	CMD-C2D	-2.03	1.46	1.50
15	cB	824	CLA	CMC-C2C	-2.03	1.46	1.50
18	bJ	105	BCR	C36-C18	-2.03	1.46	1.50
15	bA	823	CLA	MG-ND	-2.03	2.01	2.05
15	bA	832	CLA	MG-ND	-2.03	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	bB	848	BCR	C38-C26	-2.03	1.47	1.50
15	b5	413	CLA	CMC-C2C	-2.03	1.46	1.50
15	cB	830	CLA	C1B-NB	-2.03	1.33	1.35
15	cB	802	CLA	CAC-C3C	-2.03	1.45	1.51
15	c6	413	CLA	C4B-CHC	-2.03	1.35	1.41
18	aB	846	BCR	C38-C26	-2.03	1.47	1.50
15	a3	413	CLA	C4B-CHC	-2.03	1.35	1.41
14	aA	801	CL0	CMD-C2D	-2.03	1.46	1.50
15	a5	417	CLA	CMD-C2D	-2.03	1.46	1.50
15	a1	422	CLA	CAA-C2A	2.03	1.57	1.54
15	aA	841	CLA	C3B-CAB	-2.03	1.43	1.47
15	c3	409	CLA	C3B-CAB	-2.03	1.43	1.47
15	b5	409	CLA	CMC-C2C	-2.03	1.46	1.50
15	b5	411	CLA	CMD-C2D	-2.03	1.46	1.50
15	cB	839	CLA	MG-ND	-2.03	2.01	2.05
15	a5	411	CLA	CMD-C2D	-2.03	1.46	1.50
15	b6	405	CLA	CMC-C2C	-2.03	1.46	1.50
18	bB	850	BCR	C36-C18	-2.03	1.46	1.50
18	a5	418	BCR	C27-C26	-2.03	1.47	1.51
15	cA	825	CLA	CMC-C2C	-2.03	1.46	1.50
18	cF	205	BCR	C33-C5	-2.03	1.47	1.50
15	b1	404	CLA	CMD-C2D	-2.03	1.46	1.50
15	a3	415	CLA	O2A-CGA	2.03	1.37	1.30
15	aB	808	CLA	C3B-CAB	-2.03	1.43	1.47
14	cA	801	CL0	CMD-C2D	-2.03	1.46	1.50
15	c6	405	CLA	CMC-C2C	-2.03	1.46	1.50
15	a1	422	CLA	C4D-CHA	2.03	1.45	1.38
15	aA	814	CLA	C3B-C2B	-2.03	1.37	1.40
18	bL	206	BCR	C33-C5	-2.02	1.47	1.50
15	cA	823	CLA	C3B-CAB	-2.02	1.43	1.47
15	a5	413	CLA	CMC-C2C	-2.02	1.46	1.50
15	bA	802	CLA	C4B-CHC	-2.02	1.35	1.41
18	bJ	105	BCR	C38-C26	-2.02	1.47	1.50
15	c1	407	CLA	CMC-C2C	-2.02	1.46	1.50
15	aA	814	CLA	C3B-CAB	-2.02	1.43	1.47
15	aA	833	CLA	C1D-ND	2.02	1.40	1.37
15	aA	830	CLA	C4B-CHC	-2.02	1.35	1.41
15	bA	842	CLA	CMC-C2C	-2.02	1.46	1.50
15	a6	411	CLA	CMD-C2D	-2.02	1.46	1.50
15	c5	413	CLA	CMD-C2D	-2.02	1.46	1.50
15	b2	414	CLA	C4B-CHC	-2.02	1.35	1.41
15	aB	831	CLA	C3B-CAB	-2.02	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	811	CLA	C3B-CAB	-2.02	1.43	1.47
14	bA	801	CL0	C1B-CHB	2.02	1.46	1.41
15	c4	410	CLA	C3B-C2B	-2.02	1.37	1.40
15	cA	803	CLA	C1D-ND	2.02	1.40	1.37
15	bA	823	CLA	C3B-CAB	-2.02	1.43	1.47
15	cA	833	CLA	CAC-C3C	-2.02	1.45	1.51
18	bB	846	BCR	C38-C26	-2.02	1.47	1.50
15	cA	823	CLA	MG-ND	-2.02	2.01	2.05
15	b2	412	CLA	CMC-C2C	-2.02	1.46	1.50
15	c2	414	CLA	CMD-C2D	-2.02	1.46	1.50
15	cB	818	CLA	C3B-CAB	-2.02	1.43	1.47
15	c4	417	CLA	C3B-CAB	-2.02	1.43	1.47
15	aA	835	CLA	C4B-CHC	-2.02	1.35	1.41
15	a1	407	CLA	MG-ND	-2.02	2.01	2.05
15	bB	808	CLA	C4B-CHC	-2.02	1.35	1.41
15	bF	201	CLA	C4B-CHC	-2.02	1.35	1.41
15	cA	835	CLA	C4B-CHC	-2.02	1.35	1.41
15	a3	402	CLA	CMC-C2C	-2.02	1.46	1.50
15	a2	418	CLA	C3B-CAB	-2.02	1.43	1.47
18	cJ	103	BCR	C33-C5	-2.02	1.47	1.50
15	a4	402	CLA	CMC-C2C	-2.02	1.46	1.50
15	b3	414	CLA	CMD-C2D	-2.02	1.46	1.50
15	a5	420	CLA	C3B-C2B	-2.02	1.37	1.40
15	bA	843	CLA	C3B-CAB	-2.02	1.43	1.47
15	aA	823	CLA	CMC-C2C	-2.02	1.46	1.50
15	aB	811	CLA	MG-ND	-2.02	2.01	2.05
15	bL	203	CLA	C1D-ND	2.02	1.40	1.37
18	cA	850	BCR	C33-C5	-2.02	1.47	1.50
15	c4	405	CLA	C4B-CHC	-2.02	1.35	1.41
18	bL	201	BCR	C33-C5	-2.02	1.47	1.50
14	aA	801	CL0	C1B-CHB	2.02	1.46	1.41
15	aB	824	CLA	CMC-C2C	-2.02	1.46	1.50
15	a3	406	CLA	CMD-C2D	-2.02	1.46	1.50
15	aB	838	CLA	C4B-CHC	-2.02	1.35	1.41
18	aL	205	BCR	C33-C5	-2.02	1.47	1.50
15	b5	413	CLA	C3B-CAB	-2.02	1.43	1.47
15	cA	842	CLA	C3B-CAB	-2.02	1.43	1.47
15	c2	412	CLA	CMC-C2C	-2.01	1.46	1.50
15	c3	406	CLA	CMC-C2C	-2.01	1.46	1.50
15	a2	406	CLA	C3B-C2B	-2.01	1.37	1.40
15	aA	832	CLA	MG-ND	-2.01	2.01	2.05
15	a1	404	CLA	C4B-CHC	-2.01	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	823	CLA	CMC-C2C	-2.01	1.46	1.50
18	c1	420	BCR	C35-C13	-2.01	1.46	1.50
15	bB	839	CLA	MG-ND	-2.01	2.01	2.05
15	cA	824	CLA	C3B-CAB	-2.01	1.43	1.47
15	b5	412	CLA	CMD-C2D	-2.01	1.46	1.50
15	c6	406	CLA	CMD-C2D	-2.01	1.46	1.50
15	cA	830	CLA	C4B-CHC	-2.01	1.35	1.41
18	cF	205	BCR	C36-C18	-2.01	1.46	1.50
15	c1	415	CLA	O2A-CGA	2.01	1.37	1.30
15	bB	811	CLA	MG-ND	-2.01	2.01	2.05
15	c2	404	CLA	C3B-CAB	-2.01	1.43	1.47
15	c1	405	CLA	C4B-CHC	-2.01	1.35	1.41
18	b1	420	BCR	C35-C13	-2.01	1.46	1.50
15	bB	812	CLA	CMC-C2C	-2.01	1.46	1.50
15	c2	415	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	802	CLA	O2D-CED	-2.01	1.40	1.45
15	a5	413	CLA	C4B-CHC	-2.01	1.35	1.41
15	b4	415	CLA	O2A-CGA	2.01	1.37	1.30
15	bA	814	CLA	C4B-CHC	-2.01	1.35	1.41
15	c1	408	CLA	MG-ND	-2.01	2.01	2.05
14	bA	801	CL0	CMD-C2D	-2.01	1.46	1.50
15	c5	413	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	824	CLA	C3B-CAB	-2.01	1.43	1.47
18	aI	102	BCR	C33-C5	-2.01	1.47	1.50
18	bJ	104	BCR	C33-C5	-2.01	1.47	1.50
15	aA	824	CLA	C3B-CAB	-2.01	1.43	1.47
15	cA	841	CLA	C3B-CAB	-2.01	1.43	1.47
15	bB	835	CLA	MG-ND	-2.01	2.01	2.05
15	cF	201	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	805	CLA	CAA-C2A	-2.01	1.50	1.54
15	aJ	202	CLA	O2A-CGA	2.01	1.37	1.30
15	aA	833	CLA	C4B-CHC	-2.01	1.35	1.41
15	a6	405	CLA	CMC-C2C	-2.01	1.46	1.50
15	a1	404	CLA	C3B-CAB	-2.01	1.43	1.47
15	a4	408	CLA	MG-ND	-2.01	2.01	2.05
15	a6	412	CLA	CMC-C2C	-2.01	1.46	1.50
15	c5	412	CLA	C4B-CHC	-2.01	1.35	1.41
15	bJ	102	CLA	C3B-CAB	-2.01	1.43	1.47
15	cB	808	CLA	C3B-CAB	-2.01	1.43	1.47
15	c5	415	CLA	O2A-CGA	2.01	1.37	1.30
18	cB	849	BCR	C36-C18	-2.01	1.46	1.50
15	aJ	203	CLA	C4B-CHC	-2.01	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	806	CLA	C3B-C2B	-2.01	1.37	1.40
15	bJ	101	CLA	O2A-CGA	2.01	1.37	1.30
15	cB	806	CLA	CMA-C3A	-2.01	1.48	1.53
15	cA	827	CLA	C4B-CHC	-2.01	1.35	1.41
15	cF	203	CLA	C4B-CHC	-2.01	1.35	1.41
15	a5	405	CLA	CMC-C2C	-2.01	1.46	1.50
15	b4	405	CLA	C4B-CHC	-2.01	1.35	1.41
15	b3	414	CLA	MG-ND	-2.01	2.01	2.05
15	a1	404	CLA	CMC-C2C	-2.01	1.46	1.50
15	aB	806	CLA	CMA-C3A	-2.01	1.48	1.53
15	b4	402	CLA	CMC-C2C	-2.01	1.46	1.50
15	c5	404	CLA	CMC-C2C	-2.01	1.46	1.50
15	cA	833	CLA	C4B-CHC	-2.00	1.35	1.41
15	b3	417	CLA	CMB-C2B	-2.00	1.47	1.51
15	cA	838	CLA	C3B-CAB	-2.00	1.43	1.47
14	cA	801	CL0	C1B-CHB	2.00	1.46	1.41
15	c6	405	CLA	C3B-CAB	-2.00	1.43	1.47
15	aB	835	CLA	MG-ND	-2.00	2.01	2.05
15	bA	818	CLA	MG-ND	-2.00	2.01	2.05
15	a4	417	CLA	C3B-CAB	-2.00	1.43	1.47
15	b2	404	CLA	C3B-CAB	-2.00	1.43	1.47
18	a1	419	BCR	C35-C13	-2.00	1.46	1.50
15	a2	412	CLA	CMC-C2C	-2.00	1.46	1.50
15	b6	410	CLA	MG-ND	-2.00	2.01	2.05
15	bA	841	CLA	C3B-CAB	-2.00	1.43	1.47
15	b6	413	CLA	C4B-CHC	-2.00	1.35	1.41
15	cA	802	CLA	C4B-CHC	-2.00	1.35	1.41
15	cA	805	CLA	CAA-C2A	-2.00	1.50	1.54
15	a3	414	CLA	CMD-C2D	-2.00	1.46	1.50
15	bA	835	CLA	CAC-C3C	-2.00	1.46	1.51
15	cL	202	CLA	C1D-ND	2.00	1.40	1.37
18	b4	418	BCR	C27-C26	-2.00	1.47	1.51
15	a3	414	CLA	MG-ND	-2.00	2.01	2.05
15	b4	408	CLA	MG-ND	-2.00	2.01	2.05
15	aA	844	CLA	CBD-CAD	2.00	1.56	1.51
18	c3	418	BCR	C27-C26	-2.00	1.47	1.51
15	c5	413	CLA	C3B-CAB	-2.00	1.43	1.47
15	c5	409	CLA	CMC-C2C	-2.00	1.46	1.50
15	b5	415	CLA	O2A-CGA	2.00	1.37	1.30
15	c4	405	CLA	MG-ND	-2.00	2.01	2.05
15	a4	405	CLA	C4B-CHC	-2.00	1.35	1.41
15	bA	842	CLA	C3B-CAB	-2.00	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	404	CLA	CMC-C2C	-2.00	1.46	1.50
15	cB	841	CLA	MG-ND	-2.00	2.01	2.05
15	bB	827	CLA	C4B-CHC	-2.00	1.35	1.41
15	bJ	102	CLA	C4B-CHC	-2.00	1.35	1.41
15	a3	413	CLA	CMC-C2C	-2.00	1.46	1.50
15	aA	814	CLA	C4B-CHC	-2.00	1.35	1.41

All (7393) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	bB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	aB	804	CLA	C4A-NA-C1A	10.44	111.40	106.71
15	aA	803	CLA	C4A-NA-C1A	9.96	111.19	106.71
15	cA	803	CLA	C4A-NA-C1A	9.91	111.16	106.71
15	bA	803	CLA	C4A-NA-C1A	9.83	111.13	106.71
15	cB	840	CLA	C4A-NA-C1A	9.66	111.05	106.71
15	bB	811	CLA	C4A-NA-C1A	9.63	111.04	106.71
15	cB	811	CLA	C4A-NA-C1A	9.60	111.02	106.71
15	aB	840	CLA	C4A-NA-C1A	9.58	111.01	106.71
15	bB	840	CLA	C4A-NA-C1A	9.55	111.00	106.71
15	aB	811	CLA	C4A-NA-C1A	9.50	110.97	106.71
15	a1	416	CLA	CMB-C2B-C1B	-9.27	114.22	128.46
15	b1	417	CLA	CMB-C2B-C1B	-9.23	114.28	128.46
15	c1	417	CLA	CMB-C2B-C1B	-9.22	114.30	128.46
15	a5	417	CLA	CMB-C2B-C1B	-9.20	114.32	128.46
15	b5	417	CLA	CMB-C2B-C1B	-9.18	114.35	128.46
15	b3	417	CLA	CMB-C2B-C1B	-9.18	114.36	128.46
15	c5	417	CLA	CMB-C2B-C1B	-9.17	114.37	128.46
15	c3	417	CLA	CMB-C2B-C1B	-9.16	114.38	128.46
15	a4	417	CLA	CMB-C2B-C1B	-9.16	114.38	128.46
15	a3	417	CLA	CMB-C2B-C1B	-9.15	114.41	128.46
15	c4	417	CLA	CMB-C2B-C1B	-9.13	114.43	128.46
15	b4	417	CLA	CMB-C2B-C1B	-9.12	114.45	128.46
15	bB	809	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	cA	840	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	aA	840	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	cA	806	CLA	C4A-NA-C1A	9.04	110.77	106.71
15	cB	809	CLA	C4A-NA-C1A	9.03	110.76	106.71
15	bA	806	CLA	C4A-NA-C1A	9.02	110.76	106.71
15	c2	418	CLA	CMB-C2B-C1B	-9.01	114.61	128.46
15	bA	840	CLA	C4A-NA-C1A	9.01	110.75	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	806	CLA	C4A-NA-C1A	9.00	110.75	106.71
15	a2	418	CLA	CMB-C2B-C1B	-8.99	114.64	128.46
15	b6	418	CLA	CMB-C2B-C1B	-8.99	114.65	128.46
15	b2	418	CLA	CMB-C2B-C1B	-8.98	114.67	128.46
15	aB	809	CLA	C4A-NA-C1A	8.97	110.74	106.71
15	a6	418	CLA	CMB-C2B-C1B	-8.96	114.70	128.46
15	c6	418	CLA	CMB-C2B-C1B	-8.94	114.73	128.46
15	c5	420	CLA	C4A-NA-C1A	8.79	110.66	106.71
15	bL	203	CLA	C4A-NA-C1A	8.73	110.63	106.71
15	cL	202	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	b5	420	CLA	C4A-NA-C1A	8.70	110.62	106.71
15	aL	202	CLA	C4A-NA-C1A	8.70	110.62	106.71
14	cA	801	CL0	C1D-ND-C4D	-8.66	100.19	106.33
15	a5	420	CLA	C4A-NA-C1A	8.64	110.59	106.71
15	aA	843	CLA	C4A-NA-C1A	8.62	110.58	106.71
14	bA	801	CL0	C1D-ND-C4D	-8.60	100.22	106.33
15	cA	832	CLA	C4A-NA-C1A	8.56	110.56	106.71
14	aA	801	CL0	C1D-ND-C4D	-8.55	100.26	106.33
15	cA	842	CLA	C4A-NA-C1A	8.55	110.55	106.71
15	bA	832	CLA	C4A-NA-C1A	8.53	110.54	106.71
15	aA	832	CLA	C4A-NA-C1A	8.53	110.54	106.71
15	aA	834	CLA	C4A-NA-C1A	8.51	110.53	106.71
15	aA	818	CLA	C4A-NA-C1A	8.47	110.52	106.71
15	bA	843	CLA	C4A-NA-C1A	8.47	110.51	106.71
15	bB	816	CLA	C4A-NA-C1A	8.43	110.50	106.71
15	bA	818	CLA	C4A-NA-C1A	8.40	110.48	106.71
15	c2	406	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	a2	406	CLA	C4A-NA-C1A	8.34	110.46	106.71
15	cB	823	CLA	C4A-NA-C1A	8.34	110.46	106.71
15	bB	823	CLA	C4A-NA-C1A	8.32	110.44	106.71
15	bA	834	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	aB	823	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	cA	834	CLA	C4A-NA-C1A	8.30	110.44	106.71
15	aB	816	CLA	C4A-NA-C1A	8.30	110.44	106.71
15	cA	818	CLA	C4A-NA-C1A	8.29	110.43	106.71
15	cB	822	CLA	C4A-NA-C1A	8.29	110.43	106.71
15	bB	808	CLA	C4A-NA-C1A	8.27	110.42	106.71
15	cA	810	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	aB	808	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	cA	816	CLA	C4A-NA-C1A	8.25	110.42	106.71
15	aA	810	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	aB	822	CLA	C4A-NA-C1A	8.23	110.41	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	822	CLA	C4A-NA-C1A	8.23	110.40	106.71
15	cB	816	CLA	C4A-NA-C1A	8.23	110.40	106.71
15	cB	828	CLA	C4A-NA-C1A	8.22	110.40	106.71
15	bA	810	CLA	C4A-NA-C1A	8.21	110.40	106.71
15	cB	808	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	b2	406	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	bB	835	CLA	C4A-NA-C1A	8.17	110.38	106.71
15	aA	816	CLA	C4A-NA-C1A	8.17	110.38	106.71
15	bA	816	CLA	C4A-NA-C1A	8.15	110.37	106.71
15	aA	844	CLA	C4A-NA-C1A	8.13	110.36	106.71
15	bB	805	CLA	C4A-NA-C1A	8.12	110.36	106.71
15	b6	422	CLA	C4A-NA-C1A	8.11	110.35	106.71
15	cB	835	CLA	C4A-NA-C1A	8.09	110.34	106.71
15	aB	835	CLA	C4A-NA-C1A	8.08	110.34	106.71
15	aB	838	CLA	C4A-NA-C1A	8.08	110.34	106.71
15	bJ	101	CLA	C4A-NA-C1A	8.07	110.34	106.71
15	aB	821	CLA	C4A-NA-C1A	8.07	110.33	106.71
15	bB	828	CLA	C4A-NA-C1A	8.06	110.33	106.71
15	bA	844	CLA	C4A-NA-C1A	8.05	110.33	106.71
15	aB	805	CLA	C4A-NA-C1A	8.05	110.33	106.71
15	aB	828	CLA	C4A-NA-C1A	8.05	110.32	106.71
15	cB	805	CLA	C4A-NA-C1A	8.04	110.32	106.71
15	cB	838	CLA	C4A-NA-C1A	8.04	110.32	106.71
15	cA	843	CLA	C4A-NA-C1A	8.03	110.31	106.71
15	a1	422	CLA	C4A-NA-C1A	8.00	110.30	106.71
15	a2	422	CLA	C4A-NA-C1A	8.00	110.30	106.71
15	a4	415	CLA	C4A-NA-C1A	7.99	110.30	106.71
15	a2	417	CLA	CMB-C2B-C1B	-7.99	116.19	128.46
15	cB	806	CLA	C4A-NA-C1A	7.97	110.29	106.71
15	c2	422	CLA	C4A-NA-C1A	7.96	110.29	106.71
15	bB	806	CLA	C4A-NA-C1A	7.96	110.28	106.71
15	c2	417	CLA	CMB-C2B-C1B	-7.95	116.24	128.46
15	bA	826	CLA	C4A-NA-C1A	7.95	110.28	106.71
15	aJ	202	CLA	C4A-NA-C1A	7.94	110.28	106.71
15	cJ	101	CLA	C4A-NA-C1A	7.94	110.27	106.71
15	b4	415	CLA	C4A-NA-C1A	7.93	110.27	106.71
15	cB	821	CLA	C4A-NA-C1A	7.93	110.27	106.71
15	c4	415	CLA	C4A-NA-C1A	7.93	110.27	106.71
15	bB	819	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	bB	821	CLA	C4A-NA-C1A	7.91	110.26	106.71
15	b2	422	CLA	C4A-NA-C1A	7.91	110.26	106.71
15	aB	802	CLA	C4A-NA-C1A	7.90	110.26	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	838	CLA	C4A-NA-C1A	7.90	110.26	106.71
15	a6	422	CLA	C4A-NA-C1A	7.89	110.25	106.71
15	a5	415	CLA	C4A-NA-C1A	7.88	110.25	106.71
15	cB	802	CLA	C4A-NA-C1A	7.87	110.25	106.71
15	aB	807	CLA	C4A-NA-C1A	7.87	110.24	106.71
15	c4	416	CLA	CMB-C2B-C1B	-7.86	116.38	128.46
15	b2	415	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	aA	826	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	b5	415	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	cB	819	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	b4	416	CLA	CMB-C2B-C1B	-7.84	116.42	128.46
15	cB	831	CLA	C4A-NA-C1A	7.83	110.23	106.71
15	c5	415	CLA	C4A-NA-C1A	7.82	110.22	106.71
15	aB	819	CLA	C4A-NA-C1A	7.81	110.22	106.71
15	bB	802	CLA	C4A-NA-C1A	7.81	110.22	106.71
15	cB	807	CLA	C4A-NA-C1A	7.81	110.22	106.71
15	a4	416	CLA	CMB-C2B-C1B	-7.80	116.48	128.46
15	aB	827	CLA	C4A-NA-C1A	7.79	110.21	106.71
15	cA	826	CLA	C4A-NA-C1A	7.79	110.21	106.71
15	b2	417	CLA	CMB-C2B-C1B	-7.79	116.50	128.46
15	aB	806	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	a2	415	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	bB	807	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	bB	831	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	aB	831	CLA	C4A-NA-C1A	7.77	110.20	106.71
15	c2	415	CLA	C4A-NA-C1A	7.76	110.20	106.71
15	bB	827	CLA	C4A-NA-C1A	7.74	110.19	106.71
15	a5	416	CLA	CMB-C2B-C1B	-7.73	116.58	128.46
15	b6	416	CLA	C4A-NA-C1A	7.73	110.18	106.71
15	cB	810	CLA	C4A-NA-C1A	7.72	110.18	106.71
15	bB	813	CLA	C4A-NA-C1A	7.72	110.18	106.71
15	aB	810	CLA	C4A-NA-C1A	7.71	110.17	106.71
15	c5	416	CLA	CMB-C2B-C1B	-7.71	116.62	128.46
15	c6	416	CLA	C4A-NA-C1A	7.69	110.16	106.71
15	b5	416	CLA	CMB-C2B-C1B	-7.68	116.66	128.46
15	cB	827	CLA	C4A-NA-C1A	7.67	110.16	106.71
15	b6	415	CLA	C4A-NA-C1A	7.67	110.16	106.71
15	cB	813	CLA	C4A-NA-C1A	7.66	110.15	106.71
15	bA	845	CLA	C4A-NA-C1A	7.65	110.14	106.71
15	a6	415	CLA	C4A-NA-C1A	7.64	110.14	106.71
15	bB	810	CLA	C4A-NA-C1A	7.62	110.13	106.71
15	b5	414	CLA	C4A-NA-C1A	7.62	110.13	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	414	CLA	C4A-NA-C1A	7.61	110.13	106.71
15	b4	414	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	b3	403	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	aA	845	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	c1	415	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	cA	837	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	c6	415	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	c3	403	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	c5	414	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	aB	813	CLA	C4A-NA-C1A	7.57	110.11	106.71
15	cX	102	CLA	C4A-NA-C1A	7.56	110.10	106.71
15	c4	414	CLA	C4A-NA-C1A	7.55	110.10	106.71
15	cA	844	CLA	C4A-NA-C1A	7.55	110.10	106.71
15	bA	837	CLA	C4A-NA-C1A	7.55	110.10	106.71
15	a3	415	CLA	C4A-NA-C1A	7.54	110.10	106.71
15	bX	102	CLA	C4A-NA-C1A	7.53	110.09	106.71
15	aA	829	CLA	C4A-NA-C1A	7.52	110.09	106.71
15	a1	414	CLA	C4A-NA-C1A	7.52	110.09	106.71
15	c3	414	CLA	C4A-NA-C1A	7.52	110.08	106.71
15	a6	416	CLA	C4A-NA-C1A	7.51	110.08	106.71
15	bA	829	CLA	C4A-NA-C1A	7.50	110.08	106.71
15	c6	417	CLA	CMB-C2B-C1B	-7.49	116.94	128.46
15	aA	837	CLA	C4A-NA-C1A	7.49	110.07	106.71
15	a2	403	CLA	C4A-NA-C1A	7.49	110.07	106.71
15	b6	417	CLA	CMB-C2B-C1B	-7.47	116.98	128.46
15	a6	417	CLA	CMB-C2B-C1B	-7.47	116.98	128.46
15	aX	102	CLA	C4A-NA-C1A	7.46	110.06	106.71
15	b1	403	CLA	C4A-NA-C1A	7.44	110.05	106.71
15	b3	415	CLA	C4A-NA-C1A	7.43	110.05	106.71
15	c5	403	CLA	C4A-NA-C1A	7.43	110.05	106.71
15	a5	403	CLA	C4A-NA-C1A	7.42	110.04	106.71
15	b3	414	CLA	C4A-NA-C1A	7.42	110.04	106.71
15	cA	829	CLA	C4A-NA-C1A	7.41	110.04	106.71
15	cJ	102	CLA	C4A-NA-C1A	7.40	110.03	106.71
15	a3	403	CLA	C4A-NA-C1A	7.40	110.03	106.71
15	a5	414	CLA	C4A-NA-C1A	7.40	110.03	106.71
15	b6	404	CLA	C4A-NA-C1A	7.39	110.03	106.71
15	a5	404	CLA	C4A-NA-C1A	7.39	110.03	106.71
15	c4	416	CLA	C4A-NA-C1A	7.39	110.03	106.71
15	c2	403	CLA	C4A-NA-C1A	7.38	110.02	106.71
15	b1	416	CLA	C4A-NA-C1A	7.38	110.02	106.71
15	aJ	203	CLA	C4A-NA-C1A	7.37	110.02	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	403	CLA	C4A-NA-C1A	7.37	110.02	106.71
15	b2	416	CLA	C4A-NA-C1A	7.37	110.02	106.71
15	a6	404	CLA	C4A-NA-C1A	7.36	110.02	106.71
15	c6	404	CLA	C4A-NA-C1A	7.36	110.01	106.71
15	aB	830	CLA	CMB-C2B-C1B	-7.36	117.16	128.46
15	bB	830	CLA	CMB-C2B-C1B	-7.35	117.16	128.46
15	c3	415	CLA	C4A-NA-C1A	7.35	110.01	106.71
15	c2	416	CLA	C4A-NA-C1A	7.34	110.01	106.71
15	bA	839	CLA	C4A-NA-C1A	7.34	110.01	106.71
15	cB	830	CLA	CMB-C2B-C1B	-7.34	117.18	128.46
15	a1	402	CLA	C4A-NA-C1A	7.34	110.00	106.71
15	c4	403	CLA	C4A-NA-C1A	7.33	110.00	106.71
15	a4	416	CLA	C4A-NA-C1A	7.32	110.00	106.71
15	a3	414	CLA	C4A-NA-C1A	7.32	110.00	106.71
15	a1	403	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	cA	839	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	c1	414	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	b2	403	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	aA	839	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	c1	403	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b1	404	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b4	403	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b4	416	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b1	415	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	cA	821	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	b6	417	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	cA	824	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	c5	404	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	c6	417	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	a2	417	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	a1	413	CLA	C4A-NA-C1A	7.27	109.98	106.71
15	a6	417	CLA	C4A-NA-C1A	7.27	109.98	106.71
15	a2	404	CLA	C4A-NA-C1A	7.27	109.97	106.71
15	c1	416	CLA	C4A-NA-C1A	7.27	109.97	106.71
15	a3	404	CLA	C4A-NA-C1A	7.26	109.97	106.71
15	bA	824	CLA	C4A-NA-C1A	7.26	109.97	106.71
15	c6	405	CLA	C4A-NA-C1A	7.25	109.96	106.71
15	bA	821	CLA	C4A-NA-C1A	7.24	109.96	106.71
15	a4	403	CLA	C4A-NA-C1A	7.24	109.96	106.71
15	b2	417	CLA	C4A-NA-C1A	7.23	109.96	106.71
15	b4	411	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	a1	415	CLA	C4A-NA-C1A	7.22	109.95	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	416	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	b1	407	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	b2	404	CLA	C4A-NA-C1A	7.21	109.95	106.71
15	b5	404	CLA	C4A-NA-C1A	7.21	109.95	106.71
15	aA	824	CLA	C4A-NA-C1A	7.20	109.94	106.71
15	c1	416	CLA	CMB-C2B-C1B	-7.20	117.39	128.46
15	bJ	102	CLA	C4A-NA-C1A	7.20	109.94	106.71
15	b4	421	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	b5	416	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	aA	821	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	a1	406	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	c4	421	CLA	C4A-NA-C1A	7.18	109.94	106.71
15	c1	407	CLA	C4A-NA-C1A	7.18	109.93	106.71
15	c2	404	CLA	C4A-NA-C1A	7.18	109.93	106.71
15	a1	410	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	cA	831	CLA	CMB-C2B-C1B	-7.17	117.45	128.46
15	bA	835	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	b6	412	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	aA	835	CLA	C4A-NA-C1A	7.16	109.92	106.71
15	c3	416	CLA	C4A-NA-C1A	7.16	109.92	106.71
15	b1	402	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	a2	416	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	a5	402	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	a5	416	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	c1	404	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	c3	404	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	b3	404	CLA	C4A-NA-C1A	7.14	109.92	106.71
15	bA	831	CLA	CMB-C2B-C1B	-7.14	117.49	128.46
15	a3	416	CLA	CMB-C2B-C1B	-7.14	117.49	128.46
15	b3	416	CLA	CMB-C2B-C1B	-7.14	117.50	128.46
15	b1	416	CLA	CMB-C2B-C1B	-7.13	117.50	128.46
15	c2	417	CLA	C4A-NA-C1A	7.13	109.91	106.71
15	b3	416	CLA	C4A-NA-C1A	7.13	109.91	106.71
15	a1	401	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	aA	831	CLA	CMB-C2B-C1B	-7.12	117.52	128.46
15	b6	405	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	a4	421	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	a1	415	CLA	CMB-C2B-C1B	-7.11	117.53	128.46
15	a3	411	CLA	C4A-NA-C1A	7.11	109.90	106.71
15	b1	411	CLA	C4A-NA-C1A	7.11	109.90	106.71
15	aA	823	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	b1	414	CLA	C4A-NA-C1A	7.10	109.90	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	829	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	c1	411	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	cA	801	CL0	C2D-C1D-ND	7.09	115.33	110.10
15	c3	416	CLA	CMB-C2B-C1B	-7.09	117.56	128.46
15	a6	405	CLA	C4A-NA-C1A	7.09	109.89	106.71
15	c5	416	CLA	C4A-NA-C1A	7.09	109.89	106.71
15	cA	823	CLA	C4A-NA-C1A	7.09	109.89	106.71
15	b5	402	CLA	C4A-NA-C1A	7.08	109.89	106.71
15	b3	411	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	c6	412	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	a4	411	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	cA	836	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	b2	412	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	bA	801	CL0	C2D-C1D-ND	7.05	115.30	110.10
15	a2	412	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	b5	411	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	aA	808	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	cA	838	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	aA	801	CL0	C2D-C1D-ND	7.03	115.29	110.10
15	a1	416	CLA	CMB-C2B-C3B	7.03	137.83	124.68
15	a6	412	CLA	C4A-NA-C1A	7.02	109.86	106.71
15	bA	808	CLA	C4A-NA-C1A	7.02	109.86	106.71
15	bB	829	CLA	C4A-NA-C1A	7.02	109.86	106.71
15	a6	410	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	a3	402	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	cA	835	CLA	C4A-NA-C1A	7.00	109.86	106.71
15	aA	836	CLA	C4A-NA-C1A	7.00	109.85	106.71
15	aB	829	CLA	C4A-NA-C1A	7.00	109.85	106.71
15	bA	838	CLA	C4A-NA-C1A	7.00	109.85	106.71
15	cA	808	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	bA	823	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	bB	839	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	c4	411	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	c6	403	CLA	C4A-NA-C1A	6.98	109.85	106.71
15	c4	402	CLA	C4A-NA-C1A	6.98	109.84	106.71
15	cB	837	CLA	C4A-NA-C1A	6.98	109.84	106.71
15	bB	834	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	aA	838	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	a5	411	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	cB	839	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	bB	837	CLA	C4A-NA-C1A	6.96	109.84	106.71
15	c5	411	CLA	C4A-NA-C1A	6.96	109.84	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	402	CLA	C4A-NA-C1A	6.96	109.83	106.71
15	cA	822	CLA	C4A-NA-C1A	6.96	109.83	106.71
15	b4	402	CLA	C4A-NA-C1A	6.95	109.83	106.71
15	a6	422	CLA	CAA-CBA-CGA	-6.95	92.94	113.25
15	c4	404	CLA	C4A-NA-C1A	6.95	109.83	106.71
15	aB	839	CLA	C4A-NA-C1A	6.94	109.83	106.71
15	bA	836	CLA	C4A-NA-C1A	6.94	109.82	106.71
15	a6	403	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	b4	406	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	b6	403	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	aB	834	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	aB	837	CLA	C4A-NA-C1A	6.92	109.82	106.71
15	c3	411	CLA	C4A-NA-C1A	6.92	109.82	106.71
15	b5	407	CLA	C4A-NA-C1A	6.92	109.82	106.71
15	a4	404	CLA	C4A-NA-C1A	6.92	109.81	106.71
15	c4	406	CLA	C4A-NA-C1A	6.91	109.81	106.71
15	c1	417	CLA	CMB-C2B-C3B	6.91	137.60	124.68
15	bA	809	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	bB	842	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	aA	827	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	aB	842	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	b4	404	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	a5	407	CLA	C4A-NA-C1A	6.89	109.81	106.71
15	b1	417	CLA	CMB-C2B-C3B	6.89	137.57	124.68
15	b6	408	CLA	C4A-NA-C1A	6.89	109.80	106.71
15	bA	827	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	cA	809	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	c2	412	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	cB	842	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	cB	834	CLA	C4A-NA-C1A	6.87	109.79	106.71
15	aA	822	CLA	C4A-NA-C1A	6.86	109.79	106.71
15	bA	822	CLA	C4A-NA-C1A	6.85	109.79	106.71
15	b6	410	CLA	C4A-NA-C1A	6.85	109.78	106.71
15	c5	402	CLA	C4A-NA-C1A	6.85	109.78	106.71
15	aA	809	CLA	C4A-NA-C1A	6.84	109.78	106.71
15	cA	827	CLA	C4A-NA-C1A	6.84	109.78	106.71
15	c5	407	CLA	C4A-NA-C1A	6.84	109.78	106.71
15	a5	409	CLA	C4A-NA-C1A	6.83	109.78	106.71
15	a4	406	CLA	C4A-NA-C1A	6.83	109.78	106.71
15	b3	406	CLA	C4A-NA-C1A	6.83	109.78	106.71
15	c6	410	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	a6	408	CLA	C4A-NA-C1A	6.82	109.77	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c5	406	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	a5	417	CLA	CMB-C2B-C3B	6.81	137.43	124.68
15	cA	841	CLA	C4A-NA-C1A	6.81	109.77	106.71
15	b3	409	CLA	C4A-NA-C1A	6.80	109.76	106.71
15	b3	407	CLA	C4A-NA-C1A	6.80	109.76	106.71
15	a5	406	CLA	C4A-NA-C1A	6.79	109.76	106.71
15	b5	406	CLA	C4A-NA-C1A	6.78	109.76	106.71
15	c4	407	CLA	C4A-NA-C1A	6.78	109.75	106.71
15	a5	416	CLA	CMB-C2B-C3B	6.78	137.36	124.68
15	c3	402	CLA	C4A-NA-C1A	6.78	109.75	106.71
15	a3	407	CLA	C4A-NA-C1A	6.77	109.75	106.71
15	c3	406	CLA	C4A-NA-C1A	6.77	109.75	106.71
15	c2	418	CLA	CMB-C2B-C3B	6.77	137.35	124.68
15	a2	418	CLA	CMB-C2B-C3B	6.77	137.35	124.68
15	c5	417	CLA	CMB-C2B-C3B	6.76	137.33	124.68
15	b2	418	CLA	CMB-C2B-C3B	6.76	137.32	124.68
15	aA	841	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	a4	402	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	b5	417	CLA	CMB-C2B-C3B	6.76	137.32	124.68
15	bA	811	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	b5	409	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	c5	416	CLA	CMB-C2B-C3B	6.75	137.31	124.68
15	b5	416	CLA	CMB-C2B-C3B	6.75	137.30	124.68
15	c4	416	CLA	CMB-C2B-C3B	6.75	137.30	124.68
15	c3	407	CLA	C4A-NA-C1A	6.74	109.74	106.71
15	aA	811	CLA	C4A-NA-C1A	6.74	109.73	106.71
15	bA	805	CLA	C4A-NA-C1A	6.73	109.73	106.71
15	a4	417	CLA	CMB-C2B-C3B	6.73	137.26	124.68
15	a4	416	CLA	CMB-C2B-C3B	6.72	137.26	124.68
15	b4	416	CLA	CMB-C2B-C3B	6.72	137.26	124.68
15	c4	417	CLA	CMB-C2B-C3B	6.72	137.25	124.68
15	b4	407	CLA	C4A-NA-C1A	6.72	109.73	106.71
15	c6	418	CLA	CMB-C2B-C3B	6.72	137.25	124.68
15	bA	841	CLA	C4A-NA-C1A	6.71	109.72	106.71
15	b6	418	CLA	CMB-C2B-C3B	6.71	137.23	124.68
15	aA	807	CLA	C4A-NA-C1A	6.70	109.72	106.71
15	b4	417	CLA	CMB-C2B-C3B	6.70	137.22	124.68
15	aA	805	CLA	C4A-NA-C1A	6.70	109.72	106.71
15	a3	417	CLA	CMB-C2B-C3B	6.69	137.20	124.68
15	a6	418	CLA	CMB-C2B-C3B	6.69	137.20	124.68
15	a3	409	CLA	C4A-NA-C1A	6.69	109.71	106.71
15	b3	402	CLA	C4A-NA-C1A	6.69	109.71	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c6	408	CLA	C4A-NA-C1A	6.69	109.71	106.71
15	bA	807	CLA	C4A-NA-C1A	6.68	109.71	106.71
15	c3	409	CLA	C4A-NA-C1A	6.68	109.71	106.71
15	a3	406	CLA	C4A-NA-C1A	6.68	109.71	106.71
15	a4	407	CLA	C4A-NA-C1A	6.67	109.71	106.71
15	b3	417	CLA	CMB-C2B-C3B	6.67	137.16	124.68
15	b2	407	CLA	C4A-NA-C1A	6.67	109.70	106.71
15	cA	811	CLA	C4A-NA-C1A	6.67	109.70	106.71
15	c3	417	CLA	CMB-C2B-C3B	6.66	137.15	124.68
15	b6	407	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	cA	805	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	a2	408	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	c5	409	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	c6	407	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	aB	841	CLA	C4A-NA-C1A	6.65	109.69	106.71
15	bB	841	CLA	C4A-NA-C1A	6.64	109.69	106.71
15	a2	410	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	c2	407	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	b2	410	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	c1	416	CLA	CMC-C2C-C1C	-6.62	114.96	125.04
15	aB	820	CLA	C4A-NA-C1A	6.62	109.68	106.71
15	a2	407	CLA	C4A-NA-C1A	6.61	109.68	106.71
15	b2	408	CLA	C4A-NA-C1A	6.61	109.68	106.71
15	a2	417	CLA	CMB-C2B-C3B	6.60	137.02	124.68
15	a6	407	CLA	C4A-NA-C1A	6.59	109.67	106.71
15	c2	417	CLA	CMB-C2B-C3B	6.59	137.01	124.68
15	bA	833	CLA	C4A-NA-C1A	6.59	109.67	106.71
15	c4	416	CLA	CMC-C2C-C1C	-6.59	115.01	125.04
15	cA	807	CLA	C4A-NA-C1A	6.58	109.67	106.71
15	b4	416	CLA	CMC-C2C-C1C	-6.58	115.02	125.04
15	c2	408	CLA	C4A-NA-C1A	6.58	109.66	106.71
15	aA	802	CLA	CMB-C2B-C1B	-6.57	118.37	128.46
15	a4	416	CLA	CMC-C2C-C1C	-6.56	115.05	125.04
15	cA	802	CLA	CMB-C2B-C1B	-6.56	118.38	128.46
15	bA	830	CLA	C4A-NA-C1A	6.56	109.65	106.71
15	a1	408	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	cA	833	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	b2	414	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	b1	416	CLA	CMC-C2C-C1C	-6.55	115.07	125.04
15	cB	820	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	bA	802	CLA	CMB-C2B-C1B	-6.54	118.42	128.46
15	b2	402	CLA	C4A-NA-C1A	6.53	109.64	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	820	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	aA	830	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	cB	841	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	cB	815	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	c2	402	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	c2	410	CLA	C4A-NA-C1A	6.50	109.63	106.71
15	cA	830	CLA	C4A-NA-C1A	6.49	109.62	106.71
15	aB	815	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	aA	833	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	a2	414	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	aA	828	CLA	C4A-NA-C1A	6.47	109.62	106.71
15	a2	402	CLA	C4A-NA-C1A	6.47	109.62	106.71
15	b1	406	CLA	C4A-NA-C1A	6.47	109.61	106.71
15	cA	828	CLA	C4A-NA-C1A	6.47	109.61	106.71
15	b1	409	CLA	C4A-NA-C1A	6.47	109.61	106.71
14	aA	801	CL0	O2D-CGD-CBD	6.46	122.74	111.27
15	b5	416	CLA	CMC-C2C-C1C	-6.45	115.22	125.04
14	bA	801	CL0	O2D-CGD-CBD	6.45	122.73	111.27
14	cA	801	CL0	O2D-CGD-CBD	6.45	122.73	111.27
15	bB	815	CLA	C4A-NA-C1A	6.45	109.61	106.71
15	a4	409	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	cA	814	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	cA	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	c4	409	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	aB	826	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	bA	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	a1	415	CLA	CMC-C2C-C1C	-6.44	115.24	125.04
15	bB	826	CLA	C4A-NA-C1A	6.43	109.60	106.71
15	a5	416	CLA	CMC-C2C-C1C	-6.43	115.25	125.04
15	c2	414	CLA	C4A-NA-C1A	6.42	109.59	106.71
15	aA	814	CLA	C4A-NA-C1A	6.41	109.59	106.71
15	c5	416	CLA	CMC-C2C-C1C	-6.41	115.28	125.04
15	b2	417	CLA	CMB-C2B-C3B	6.40	136.65	124.68
15	bK	101	CLA	C4A-NA-C1A	6.40	109.58	106.71
15	a3	416	CLA	CMC-C2C-C1C	-6.39	115.31	125.04
15	aA	820	CLA	C4A-NA-C1A	6.39	109.58	106.71
15	bA	814	CLA	C4A-NA-C1A	6.39	109.58	106.71
15	b3	416	CLA	CMC-C2C-C1C	-6.37	115.33	125.04
15	b6	417	CLA	CMC-C2C-C1C	-6.36	115.35	125.04
15	c3	416	CLA	CMC-C2C-C1C	-6.36	115.35	125.04
15	a6	417	CLA	CMC-C2C-C1C	-6.36	115.36	125.04
15	cB	826	CLA	C4A-NA-C1A	6.35	109.56	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	405	CLA	C4A-NA-C1A	6.35	109.56	106.71
15	c6	417	CLA	CMC-C2C-C1C	-6.34	115.38	125.04
15	b4	409	CLA	C4A-NA-C1A	6.34	109.56	106.71
15	c6	417	CLA	CMB-C2B-C3B	6.34	136.53	124.68
15	c1	409	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	a6	417	CLA	CMB-C2B-C3B	6.33	136.53	124.68
15	cA	815	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	bA	815	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	bA	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	cA	819	CLA	C4A-NA-C1A	6.32	109.55	106.71
15	b6	414	CLA	C4A-NA-C1A	6.31	109.54	106.71
15	aA	815	CLA	C4A-NA-C1A	6.30	109.54	106.71
15	b6	417	CLA	CMB-C2B-C3B	6.30	136.46	124.68
15	c1	406	CLA	C4A-NA-C1A	6.28	109.53	106.71
15	aK	102	CLA	C4A-NA-C1A	6.28	109.53	106.71
15	aJ	201	CLA	C4A-NA-C1A	6.28	109.53	106.71
15	b3	413	CLA	C4A-NA-C1A	6.27	109.53	106.71
15	bF	201	CLA	C4A-NA-C1A	6.27	109.52	106.71
15	cK	102	CLA	C4A-NA-C1A	6.26	109.52	106.71
15	b5	411	CLA	CMB-C2B-C1B	-6.25	118.86	128.46
15	c3	421	CLA	C4A-NA-C1A	6.24	109.51	106.71
15	a3	421	CLA	C4A-NA-C1A	6.24	109.51	106.71
15	bB	825	CLA	C4A-NA-C1A	6.23	109.51	106.71
15	cF	203	CLA	C4A-NA-C1A	6.23	109.51	106.71
15	aB	825	CLA	C4A-NA-C1A	6.22	109.50	106.71
15	c5	411	CLA	CMB-C2B-C1B	-6.21	118.92	128.46
15	a3	413	CLA	C4A-NA-C1A	6.19	109.49	106.71
15	bA	819	CLA	C4A-NA-C1A	6.19	109.49	106.71
15	a5	411	CLA	CMB-C2B-C1B	-6.19	118.96	128.46
15	c1	416	CLA	CMB-C2B-C3B	6.19	136.25	124.68
15	bB	818	CLA	C4A-NA-C1A	6.18	109.48	106.71
15	c2	412	CLA	CMB-C2B-C1B	-6.18	118.97	128.46
15	c5	413	CLA	C4A-NA-C1A	6.18	109.48	106.71
15	a2	412	CLA	CMB-C2B-C1B	-6.18	118.97	128.46
15	aA	845	CLA	CAC-C3C-C4C	-6.17	116.80	124.81
15	cA	844	CLA	CAC-C3C-C4C	-6.17	116.81	124.81
15	bA	845	CLA	CAC-C3C-C4C	-6.16	116.81	124.81
15	b2	412	CLA	CMB-C2B-C1B	-6.16	118.99	128.46
15	c4	411	CLA	CMB-C2B-C1B	-6.16	119.00	128.46
15	cA	812	CLA	C4A-NA-C1A	6.15	109.47	106.71
15	aB	818	CLA	C4A-NA-C1A	6.15	109.47	106.71
15	c3	413	CLA	C4A-NA-C1A	6.15	109.47	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	411	CLA	CMB-C2B-C1B	-6.15	119.02	128.46
15	b2	417	CLA	CMC-C2C-C1C	-6.14	115.68	125.04
15	bA	817	CLA	C4A-NA-C1A	6.14	109.47	106.71
15	c2	417	CLA	CMC-C2C-C1C	-6.14	115.69	125.04
15	cB	818	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	aA	804	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	aA	819	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	a2	417	CLA	CMC-C2C-C1C	-6.13	115.71	125.04
15	aA	817	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	cA	817	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	b1	416	CLA	CMB-C2B-C3B	6.13	136.14	124.68
15	cB	825	CLA	C4A-NA-C1A	6.12	109.46	106.71
15	a1	415	CLA	CMB-C2B-C3B	6.11	136.11	124.68
15	a1	412	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	aA	812	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	b3	421	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	a1	410	CLA	CMB-C2B-C1B	-6.10	119.09	128.46
15	bA	812	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	b4	408	CLA	C4A-NA-C1A	6.09	109.44	106.71
15	a6	414	CLA	C4A-NA-C1A	6.09	109.44	106.71
15	c1	411	CLA	CMB-C2B-C1B	-6.08	119.12	128.46
15	a5	413	CLA	C4A-NA-C1A	6.07	109.44	106.71
15	a4	411	CLA	CMB-C2B-C1B	-6.07	119.13	128.46
15	bA	804	CLA	C4A-NA-C1A	6.06	109.43	106.71
15	a3	416	CLA	CMB-C2B-C3B	6.06	136.01	124.68
15	b4	411	CLA	CMB-C2B-C1B	-6.05	119.16	128.46
15	cA	804	CLA	C4A-NA-C1A	6.05	109.43	106.71
15	b3	416	CLA	CMB-C2B-C3B	6.04	135.97	124.68
15	c4	413	CLA	C4A-NA-C1A	6.03	109.42	106.71
15	c6	414	CLA	C4A-NA-C1A	6.03	109.42	106.71
15	bA	820	CLA	CMB-C2B-C1B	-6.03	119.19	128.46
15	a4	413	CLA	C4A-NA-C1A	6.02	109.41	106.71
15	c1	413	CLA	C4A-NA-C1A	6.02	109.41	106.71
15	aA	820	CLA	CMB-C2B-C1B	-6.02	119.21	128.46
15	c3	411	CLA	CMB-C2B-C1B	-6.02	119.21	128.46
15	c3	416	CLA	CMB-C2B-C3B	6.02	135.94	124.68
15	b5	408	CLA	C4A-NA-C1A	6.01	109.41	106.71
15	b5	413	CLA	C4A-NA-C1A	5.98	109.40	106.71
15	cA	820	CLA	CMB-C2B-C1B	-5.98	119.28	128.46
18	c2	401	BCR	C11-C10-C9	-5.98	118.78	127.31
15	aB	836	CLA	C4A-NA-C1A	5.97	109.39	106.71
15	b4	413	CLA	C4A-NA-C1A	5.96	109.39	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	aA	801	CL0	CHD-C4C-C3C	-5.96	116.08	124.84
14	bA	801	CL0	CHD-C4C-C3C	-5.96	116.08	124.84
15	aA	805	CLA	CMB-C2B-C1B	-5.95	119.31	128.46
18	a2	401	BCR	C11-C10-C9	-5.95	118.81	127.31
15	c6	418	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	a3	411	CLA	CMB-C2B-C1B	-5.95	119.32	128.46
15	a5	408	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	bB	836	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	b1	410	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	cA	801	CL0	CHD-C4C-C3C	-5.94	116.10	124.84
15	c3	410	CLA	C4A-NA-C1A	5.94	109.38	106.71
15	bA	805	CLA	CMB-C2B-C1B	-5.94	119.34	128.46
15	cB	803	CLA	CMB-C2B-C1B	-5.93	119.35	128.46
15	cA	805	CLA	CMB-C2B-C1B	-5.93	119.35	128.46
15	cB	836	CLA	C4A-NA-C1A	5.93	109.37	106.71
15	b3	410	CLA	C4A-NA-C1A	5.93	109.37	106.71
15	b1	413	CLA	C4A-NA-C1A	5.92	109.37	106.71
15	b3	411	CLA	CMB-C2B-C1B	-5.92	119.37	128.46
15	c2	411	CLA	C4A-NA-C1A	5.92	109.37	106.71
15	a6	412	CLA	CMB-C2B-C1B	-5.91	119.37	128.46
15	bB	830	CLA	C4A-NA-C1A	5.91	109.36	106.71
15	aB	803	CLA	CMB-C2B-C1B	-5.91	119.38	128.46
15	bB	803	CLA	CMB-C2B-C1B	-5.91	119.39	128.46
15	c6	412	CLA	CMB-C2B-C1B	-5.90	119.40	128.46
15	a4	408	CLA	C4A-NA-C1A	5.89	109.35	106.71
15	b6	412	CLA	CMB-C2B-C1B	-5.89	119.42	128.46
15	a2	411	CLA	C4A-NA-C1A	5.88	109.35	106.71
15	c2	418	CLA	C4A-NA-C1A	5.87	109.35	106.71
15	c5	408	CLA	C4A-NA-C1A	5.87	109.35	106.71
15	a6	409	CLA	C4A-NA-C1A	5.87	109.34	106.71
15	a1	409	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	b2	418	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	b4	410	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	cB	801	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	aB	801	CLA	C4A-NA-C1A	5.85	109.34	106.71
15	bB	801	CLA	C4A-NA-C1A	5.85	109.34	106.71
18	a1	421	BCR	C11-C10-C9	-5.84	118.98	127.31
15	b2	409	CLA	C4A-NA-C1A	5.84	109.33	106.71
15	bB	804	CLA	CMB-C2B-C1B	-5.82	119.51	128.46
15	cB	804	CLA	CMB-C2B-C1B	-5.82	119.52	128.46
15	c6	409	CLA	CMB-C2B-C1B	-5.81	119.53	128.46
15	aB	833	CLA	C4A-NA-C1A	5.81	109.32	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	409	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	c2	409	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	c4	408	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	cB	830	CLA	C4A-NA-C1A	5.79	109.31	106.71
15	aB	804	CLA	CMB-C2B-C1B	-5.79	119.57	128.46
15	aB	832	CLA	C4A-NA-C1A	5.78	109.31	106.71
15	cB	832	CLA	C4A-NA-C1A	5.77	109.30	106.71
15	a1	416	CLA	C4A-NA-C1A	5.76	109.30	106.71
15	b6	409	CLA	CMB-C2B-C1B	-5.76	119.61	128.46
15	a6	409	CLA	CMB-C2B-C1B	-5.76	119.62	128.46
15	a4	410	CLA	C4A-NA-C1A	5.75	109.29	106.71
18	b2	401	BCR	C11-C10-C9	-5.75	119.11	127.31
15	a3	410	CLA	C4A-NA-C1A	5.74	109.29	106.71
15	b6	418	CLA	C4A-NA-C1A	5.74	109.29	106.71
15	cB	833	CLA	C4A-NA-C1A	5.73	109.28	106.71
15	c1	410	CLA	C4A-NA-C1A	5.73	109.28	106.71
15	b1	408	CLA	C4A-NA-C1A	5.73	109.28	106.71
15	c1	417	CLA	C4A-NA-C1A	5.72	109.28	106.71
15	b6	409	CLA	C4A-NA-C1A	5.71	109.28	106.71
15	aB	830	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	a6	418	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	bB	833	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	b1	417	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	b3	417	CLA	C4A-NA-C1A	5.70	109.27	106.71
14	cA	801	CL0	C2C-C1C-NC	5.70	115.31	109.97
14	bA	801	CL0	C2C-C1C-NC	5.69	115.31	109.97
15	a3	408	CLA	C4A-NA-C1A	5.69	109.27	106.71
15	bA	845	CLA	CAC-C3C-C2C	5.69	137.26	127.53
15	bB	832	CLA	C4A-NA-C1A	5.68	109.26	106.71
15	c4	410	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	aA	801	CL0	C2C-C1C-NC	5.68	115.29	109.97
15	cA	844	CLA	CAC-C3C-C2C	5.67	137.23	127.53
15	aA	845	CLA	CAC-C3C-C2C	5.67	137.23	127.53
15	bB	812	CLA	C4A-NA-C1A	5.67	109.25	106.71
15	b2	411	CLA	C4A-NA-C1A	5.67	109.25	106.71
15	bA	803	CLA	CMB-C2B-C1B	-5.65	119.78	128.46
15	a2	418	CLA	C4A-NA-C1A	5.65	109.25	106.71
15	cA	803	CLA	CMB-C2B-C1B	-5.64	119.79	128.46
15	c6	409	CLA	C4A-NA-C1A	5.64	109.24	106.71
15	cL	201	CLA	C4A-NA-C1A	5.63	109.23	106.71
15	cB	812	CLA	C4A-NA-C1A	5.62	109.23	106.71
15	bL	202	CLA	C4A-NA-C1A	5.62	109.23	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	408	CLA	C4A-NA-C1A	5.62	109.23	106.71
15	b3	408	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	a5	410	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	aA	830	CLA	CMB-C2B-C1B	-5.61	119.84	128.46
15	c3	417	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	a3	417	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	aL	201	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	cA	830	CLA	CMB-C2B-C1B	-5.60	119.85	128.46
15	aA	803	CLA	CMB-C2B-C1B	-5.59	119.87	128.46
15	bA	830	CLA	CMB-C2B-C1B	-5.59	119.88	128.46
15	bA	838	CLA	CMB-C2B-C1B	-5.57	119.90	128.46
15	cA	838	CLA	CMB-C2B-C1B	-5.57	119.90	128.46
15	aA	842	CLA	C4A-NA-C1A	5.56	109.21	106.71
15	aA	838	CLA	CMB-C2B-C1B	-5.55	119.93	128.46
15	aB	812	CLA	C4A-NA-C1A	5.55	109.20	106.71
15	c5	410	CLA	C4A-NA-C1A	5.54	109.20	106.71
15	a1	407	CLA	C4A-NA-C1A	5.54	109.20	106.71
15	aB	803	CLA	C4A-NA-C1A	5.54	109.20	106.71
15	c1	408	CLA	C4A-NA-C1A	5.54	109.19	106.71
15	bA	842	CLA	C4A-NA-C1A	5.53	109.19	106.71
15	b5	410	CLA	C4A-NA-C1A	5.53	109.19	106.71
15	bB	803	CLA	C4A-NA-C1A	5.51	109.19	106.71
15	aB	817	CLA	CMB-C2B-C3B	5.51	134.99	124.68
15	bB	817	CLA	CMB-C2B-C3B	5.51	134.99	124.68
18	b3	401	BCR	C3-C4-C5	-5.51	104.25	114.08
15	cB	803	CLA	C4A-NA-C1A	5.49	109.17	106.71
15	a6	422	CLA	C2A-C1A-CHA	5.49	133.46	123.86
18	a3	401	BCR	C3-C4-C5	-5.49	104.28	114.08
15	cB	817	CLA	CMB-C2B-C3B	5.48	134.93	124.68
15	a5	408	CLA	CMB-C2B-C1B	-5.48	120.04	128.46
15	cF	201	CLA	C4A-NA-C1A	5.48	109.17	106.71
15	b5	408	CLA	CMB-C2B-C1B	-5.45	120.08	128.46
18	c3	401	BCR	C3-C4-C5	-5.45	104.34	114.08
15	a3	403	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
15	c5	408	CLA	CMB-C2B-C1B	-5.44	120.11	128.46
15	c5	417	CLA	C4A-NA-C1A	5.43	109.14	106.71
15	b3	403	CLA	CMB-C2B-C1B	-5.42	120.13	128.46
15	c4	408	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
15	a1	407	CLA	CMB-C2B-C1B	-5.40	120.16	128.46
15	c4	417	CLA	C4A-NA-C1A	5.40	109.13	106.71
15	cL	203	CLA	C4A-NA-C1A	5.40	109.13	106.71
15	c1	408	CLA	CMB-C2B-C1B	-5.39	120.17	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	408	CLA	CMB-C2B-C1B	-5.37	120.21	128.46
15	bL	204	CLA	C4A-NA-C1A	5.37	109.12	106.71
15	aL	203	CLA	C4A-NA-C1A	5.37	109.12	106.71
15	a4	408	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
15	c3	403	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
15	aB	814	CLA	CMB-C2B-C1B	-5.35	120.24	128.46
15	a1	415	CLA	CMC-C2C-C3C	5.35	140.64	126.12
15	bB	814	CLA	CMB-C2B-C1B	-5.34	120.26	128.46
15	b4	408	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
15	cB	814	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
15	c2	417	CLA	CMC-C2C-C3C	5.33	140.59	126.12
15	bA	831	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	bA	813	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	a5	403	CLA	CMB-C2B-C1B	-5.32	120.28	128.46
15	a5	417	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	a2	417	CLA	CMC-C2C-C3C	5.32	140.56	126.12
15	cA	813	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	cF	203	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
15	aA	813	CLA	C4A-NA-C1A	5.31	109.09	106.71
15	a1	414	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
15	aA	831	CLA	C4A-NA-C1A	5.31	109.09	106.71
15	b1	403	CLA	CMB-C2B-C1B	-5.29	120.34	128.46
15	b2	417	CLA	CMC-C2C-C3C	5.29	140.47	126.12
15	aJ	201	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
15	c1	416	CLA	CMC-C2C-C3C	5.28	140.46	126.12
15	b5	403	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
15	bA	825	CLA	C4A-NA-C1A	5.28	109.08	106.71
15	bF	201	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
15	c5	403	CLA	CMB-C2B-C1B	-5.27	120.36	128.46
15	aB	818	CLA	CMB-C2B-C1B	-5.27	120.36	128.46
15	a4	417	CLA	C4A-NA-C1A	5.27	109.07	106.71
15	cB	818	CLA	CMB-C2B-C1B	-5.27	120.37	128.46
15	a1	402	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
15	c1	403	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
15	cA	825	CLA	C4A-NA-C1A	5.26	109.07	106.71
15	bB	818	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
15	a3	408	CLA	CMB-C2B-C1B	-5.26	120.39	128.46
15	b3	408	CLA	CMB-C2B-C1B	-5.25	120.40	128.46
15	a2	417	CLA	C2C-C1C-NC	5.25	114.89	109.97
15	cA	831	CLA	C4A-NA-C1A	5.24	109.06	106.71
15	c6	404	CLA	CMB-C2B-C1B	-5.23	120.42	128.46
15	a5	416	CLA	CMC-C2C-C3C	5.23	140.31	126.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	416	CLA	CMC-C2C-C3C	5.23	140.30	126.12
15	b4	417	CLA	C4A-NA-C1A	5.22	109.05	106.71
15	cB	803	CLA	CMB-C2B-C3B	5.22	134.45	124.68
15	bB	803	CLA	CMB-C2B-C3B	5.22	134.44	124.68
15	b1	416	CLA	CMC-C2C-C3C	5.22	140.28	126.12
15	b6	417	CLA	CMC-C2C-C3C	5.22	140.28	126.12
18	a6	402	BCR	C11-C10-C9	-5.22	119.87	127.31
15	c1	415	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
15	c3	416	CLA	CMC-C2C-C3C	5.21	140.27	126.12
18	a3	401	BCR	C11-C10-C9	-5.21	119.87	127.31
15	c5	416	CLA	CMC-C2C-C3C	5.21	140.26	126.12
15	a3	416	CLA	CMC-C2C-C3C	5.21	140.26	126.12
15	b3	416	CLA	CMC-C2C-C3C	5.21	140.25	126.12
15	b5	417	CLA	C4A-NA-C1A	5.20	109.05	106.71
15	a6	417	CLA	CMC-C2C-C3C	5.20	140.25	126.12
15	aA	825	CLA	C4A-NA-C1A	5.20	109.05	106.71
15	c4	416	CLA	CMC-C2C-C3C	5.20	140.24	126.12
15	aB	803	CLA	CMB-C2B-C3B	5.20	134.41	124.68
15	c3	408	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
18	c3	401	BCR	C11-C10-C9	-5.20	119.89	127.31
15	c6	417	CLA	CMC-C2C-C3C	5.20	140.22	126.12
15	a4	416	CLA	CMC-C2C-C3C	5.19	140.22	126.12
15	b4	416	CLA	CMC-C2C-C3C	5.19	140.21	126.12
15	c2	416	CLA	CMB-C2B-C1B	-5.19	120.48	128.46
15	b2	409	CLA	CMB-C2B-C1B	-5.18	120.50	128.46
15	a2	416	CLA	CMB-C2B-C1B	-5.18	120.50	128.46
18	b3	401	BCR	C11-C10-C9	-5.18	119.92	127.31
15	b1	415	CLA	CMB-C2B-C1B	-5.18	120.50	128.46
15	a6	404	CLA	CMB-C2B-C1B	-5.18	120.51	128.46
15	c2	417	CLA	C2C-C1C-NC	5.17	114.82	109.97
15	aB	817	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
15	c6	416	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
15	cB	817	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
15	b4	405	CLA	C4A-NA-C1A	5.16	109.03	106.71
15	b2	416	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
15	b4	415	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
15	a4	405	CLA	C4A-NA-C1A	5.16	109.02	106.71
15	c4	405	CLA	C4A-NA-C1A	5.16	109.02	106.71
15	b6	404	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
15	bB	817	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
18	b6	402	BCR	C11-C10-C9	-5.15	119.96	127.31
15	b6	416	CLA	CMB-C2B-C1B	-5.15	120.55	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	832	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
18	c6	402	BCR	C11-C10-C9	-5.13	119.98	127.31
15	c5	405	CLA	CAC-C3C-C4C	5.13	131.47	124.81
15	b6	422	CLA	CBA-CAA-C2A	5.12	128.99	113.86
15	c6	411	CLA	C4A-NA-C1A	5.12	109.01	106.71
15	aB	832	CLA	CMB-C2B-C1B	-5.12	120.59	128.46
15	a6	411	CLA	C4A-NA-C1A	5.12	109.01	106.71
15	a6	416	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
15	b3	415	CLA	CMB-C2B-C1B	-5.11	120.60	128.46
18	a6	421	BCR	C11-C10-C9	-5.11	120.01	127.31
15	b6	411	CLA	C4A-NA-C1A	5.11	109.00	106.71
15	b5	405	CLA	CAC-C3C-C4C	5.11	131.44	124.81
15	bA	816	CLA	CMB-C2B-C1B	-5.10	120.62	128.46
15	c6	406	CLA	CAC-C3C-C4C	5.10	131.43	124.81
18	a6	402	BCR	C3-C4-C5	-5.10	104.97	114.08
15	cA	816	CLA	CMB-C2B-C1B	-5.10	120.62	128.46
15	b6	406	CLA	CAC-C3C-C4C	5.10	131.42	124.81
18	c6	402	BCR	C3-C4-C5	-5.10	104.98	114.08
15	a3	405	CLA	C4A-NA-C1A	5.09	109.00	106.71
15	aA	816	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
15	bB	832	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
15	c3	405	CLA	C4A-NA-C1A	5.09	108.99	106.71
15	c3	415	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
15	a6	406	CLA	CAC-C3C-C4C	5.09	131.41	124.81
18	b6	402	BCR	C3-C4-C5	-5.09	105.00	114.08
15	cB	805	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
15	a3	415	CLA	CMB-C2B-C1B	-5.08	120.65	128.46
15	bB	805	CLA	CMB-C2B-C1B	-5.07	120.66	128.46
15	a2	409	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
15	bB	830	CLA	O2D-CGD-CBD	5.06	120.25	111.27
15	c2	409	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
15	cB	830	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	aB	830	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	aB	805	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
15	a4	415	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
15	a5	405	CLA	CAC-C3C-C4C	5.04	131.35	124.81
15	aB	827	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
15	cA	802	CLA	C4A-NA-C1A	5.02	108.96	106.71
15	c4	403	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
15	b2	405	CLA	CAC-C3C-C4C	5.01	131.31	124.81
15	cB	825	CLA	CMB-C2B-C1B	-5.01	120.76	128.46
15	c4	415	CLA	CMB-C2B-C1B	-5.00	120.77	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	825	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
15	aB	825	CLA	CMB-C2B-C1B	-5.00	120.79	128.46
15	b2	403	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
15	b2	417	CLA	C2C-C1C-NC	4.99	114.65	109.97
15	b4	403	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
15	a5	405	CLA	C4A-NA-C1A	4.99	108.95	106.71
15	a2	405	CLA	CAC-C3C-C4C	4.99	131.28	124.81
15	bB	827	CLA	CMB-C2B-C1B	-4.99	120.80	128.46
15	b5	415	CLA	CMB-C2B-C1B	-4.99	120.80	128.46
15	cA	827	CLA	CMB-C2B-C1B	-4.98	120.81	128.46
15	cB	827	CLA	CMB-C2B-C1B	-4.98	120.81	128.46
15	cA	829	CLA	CMB-C2B-C1B	-4.98	120.82	128.46
15	a4	403	CLA	CMB-C2B-C1B	-4.97	120.82	128.46
15	a2	403	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
15	bA	827	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
15	bA	802	CLA	C4A-NA-C1A	4.96	108.94	106.71
15	cA	830	CLA	CMB-C2B-C3B	4.96	133.96	124.68
15	c2	405	CLA	CAC-C3C-C4C	4.96	131.24	124.81
15	bA	830	CLA	CMB-C2B-C3B	4.95	133.94	124.68
18	b6	421	BCR	C11-C10-C9	-4.95	120.25	127.31
15	aA	830	CLA	CMB-C2B-C3B	4.95	133.94	124.68
18	a2	401	BCR	C3-C4-C5	-4.95	105.24	114.08
15	bA	829	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
15	a5	415	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
15	aA	829	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
15	c3	405	CLA	CAC-C3C-C4C	4.94	131.22	124.81
15	aA	827	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
18	b1	419	BCR	C11-C10-C9	-4.94	120.26	127.31
15	aB	804	CLA	CMB-C2B-C3B	4.94	133.92	124.68
18	c1	419	BCR	C11-C10-C9	-4.94	120.27	127.31
18	a1	418	BCR	C11-C10-C9	-4.94	120.27	127.31
15	b3	405	CLA	CAC-C3C-C4C	4.93	131.20	124.81
15	bA	822	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
15	bB	804	CLA	CMB-C2B-C3B	4.92	133.89	124.68
15	a1	404	CLA	C4A-NA-C1A	4.92	108.92	106.71
15	cB	804	CLA	CMB-C2B-C3B	4.92	133.88	124.68
15	aA	822	CLA	CMB-C2B-C1B	-4.91	120.91	128.46
15	bA	813	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
15	cA	826	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
18	c2	401	BCR	C3-C4-C5	-4.91	105.32	114.08
15	c5	415	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
15	bA	826	CLA	CMB-C2B-C1B	-4.90	120.93	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	802	CLA	C4A-NA-C1A	4.90	108.91	106.71
15	a1	422	CLA	C2A-C1A-CHA	4.89	132.42	123.86
15	cB	826	CLA	CMB-C2B-C1B	-4.89	120.94	128.46
15	aA	826	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
15	b1	405	CLA	CAC-C3C-C4C	4.89	131.15	124.81
18	b2	401	BCR	C3-C4-C5	-4.89	105.35	114.08
15	a3	405	CLA	CAC-C3C-C4C	4.88	131.15	124.81
15	aA	813	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
15	c5	410	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
15	cA	813	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
15	c2	403	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
15	bB	826	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
15	aB	826	CLA	CMB-C2B-C1B	-4.87	120.97	128.46
15	cA	822	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
15	b1	412	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
15	b3	405	CLA	C4A-NA-C1A	4.85	108.89	106.71
15	cB	814	CLA	CBC-CAC-C3C	4.84	125.78	112.43
15	bB	814	CLA	CBC-CAC-C3C	4.84	125.78	112.43
15	b5	405	CLA	C4A-NA-C1A	4.84	108.88	106.71
15	aB	814	CLA	CBC-CAC-C3C	4.84	125.77	112.43
15	a4	417	CLA	O2D-CGD-O1D	-4.83	114.39	123.84
15	bA	838	CLA	CMB-C2B-C3B	4.83	133.71	124.68
15	b5	410	CLA	CMB-C2B-C1B	-4.82	121.05	128.46
15	a5	410	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
15	a1	411	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
15	b1	411	CLA	CMB-C2B-C3B	4.82	133.69	124.68
15	c5	411	CLA	CMB-C2B-C3B	4.81	133.68	124.68
15	b5	411	CLA	CMB-C2B-C3B	4.81	133.68	124.68
15	aA	838	CLA	CMB-C2B-C3B	4.80	133.67	124.68
15	aB	818	CLA	CMB-C2B-C3B	4.80	133.66	124.68
15	cB	818	CLA	CMB-C2B-C3B	4.80	133.66	124.68
15	bB	818	CLA	CMB-C2B-C3B	4.80	133.65	124.68
15	cA	838	CLA	CMB-C2B-C3B	4.79	133.65	124.68
15	b2	405	CLA	C4A-NA-C1A	4.79	108.86	106.71
15	c5	405	CLA	C4A-NA-C1A	4.79	108.86	106.71
15	c3	410	CLA	CBC-CAC-C3C	4.79	125.64	112.43
18	b2	419	BCR	C29-C30-C25	4.79	117.86	110.48
15	a2	405	CLA	C4A-NA-C1A	4.79	108.86	106.71
15	cA	833	CLA	CMB-C2B-C1B	-4.79	121.11	128.46
15	b2	406	CLA	C1-C2-C3	-4.79	117.77	126.04
15	b3	410	CLA	CBC-CAC-C3C	4.78	125.61	112.43
15	bA	818	CLA	CMB-C2B-C1B	-4.78	121.12	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b6	422	CLA	C2A-C1A-CHA	4.77	132.20	123.86
15	aA	833	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
15	c1	405	CLA	C4A-NA-C1A	4.77	108.85	106.71
15	bB	814	CLA	CMB-C2B-C3B	4.77	133.60	124.68
15	cA	818	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
15	c2	406	CLA	C1-C2-C3	-4.76	117.80	126.04
15	a3	410	CLA	CBC-CAC-C3C	4.76	125.56	112.43
15	a2	412	CLA	CMB-C2B-C3B	4.76	133.59	124.68
15	a5	411	CLA	CMB-C2B-C3B	4.76	133.59	124.68
15	b5	412	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
15	cB	814	CLA	CMB-C2B-C3B	4.76	133.58	124.68
15	c4	405	CLA	CAC-C3C-C4C	4.76	130.99	124.81
15	a2	406	CLA	C1-C2-C3	-4.76	117.81	126.04
15	c4	417	CLA	O2D-CGD-O1D	-4.76	114.54	123.84
14	aA	801	CL0	CAA-C2A-C3A	-4.76	99.75	112.78
15	c2	405	CLA	C4A-NA-C1A	4.76	108.84	106.71
15	b2	413	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
14	bA	801	CL0	CAA-C2A-C3A	-4.75	99.76	112.78
15	c4	411	CLA	CMB-C2B-C3B	4.75	133.57	124.68
15	aA	818	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
15	c5	412	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
15	c1	405	CLA	CAC-C3C-C4C	4.75	130.97	124.81
15	c2	412	CLA	CMB-C2B-C3B	4.75	133.56	124.68
15	cB	813	CLA	CMB-C2B-C1B	-4.75	121.17	128.46
14	cA	801	CL0	CAA-C2A-C3A	-4.75	99.78	112.78
15	b3	403	CLA	CMB-C2B-C3B	4.75	133.56	124.68
15	aB	816	CLA	CMB-C2B-C1B	-4.75	121.17	128.46
15	aB	814	CLA	CMB-C2B-C3B	4.75	133.56	124.68
18	a2	419	BCR	C29-C30-C25	4.74	117.78	110.48
15	b4	417	CLA	O2D-CGD-O1D	-4.74	114.56	123.84
15	bA	833	CLA	CMB-C2B-C1B	-4.74	121.17	128.46
15	a2	413	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
15	c6	406	CLA	C4A-NA-C1A	4.74	108.84	106.71
15	a4	412	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
18	a4	418	BCR	C29-C30-C25	4.74	117.78	110.48
15	aB	813	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
15	b2	412	CLA	CMB-C2B-C3B	4.74	133.54	124.68
15	a3	403	CLA	CMB-C2B-C3B	4.73	133.54	124.68
18	c2	419	BCR	C29-C30-C25	4.73	117.77	110.48
15	bA	820	CLA	CMB-C2B-C3B	4.73	133.53	124.68
15	a5	412	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
15	b4	405	CLA	CAC-C3C-C4C	4.73	130.94	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	813	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
15	cB	816	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
15	cB	804	CLA	CAC-C3C-C4C	4.73	130.94	124.81
15	cA	829	CLA	CMB-C2B-C3B	4.73	133.52	124.68
15	a1	410	CLA	CMB-C2B-C3B	4.72	133.52	124.68
15	bB	816	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
15	bB	804	CLA	CAC-C3C-C4C	4.72	130.93	124.81
15	c6	409	CLA	CMB-C2B-C3B	4.72	133.50	124.68
15	b1	410	CLA	CBC-CAC-C3C	4.72	125.43	112.43
15	b6	411	CLA	CMB-C2B-C1B	-4.72	121.22	128.46
15	a6	412	CLA	CMB-C2B-C3B	4.71	133.50	124.68
15	cA	820	CLA	CMB-C2B-C3B	4.71	133.50	124.68
15	bA	829	CLA	CMB-C2B-C3B	4.71	133.50	124.68
15	aA	829	CLA	CMB-C2B-C3B	4.71	133.49	124.68
15	c5	420	CLA	C2A-C1A-CHA	4.71	132.09	123.86
15	cB	838	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
15	c6	411	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
15	aA	820	CLA	CMB-C2B-C3B	4.70	133.48	124.68
18	b3	418	BCR	C29-C30-C25	4.70	117.72	110.48
15	a1	422	CLA	CBA-CAA-C2A	4.70	127.74	113.86
15	aB	804	CLA	CAC-C3C-C4C	4.70	130.91	124.81
15	a4	405	CLA	CAC-C3C-C4C	4.70	130.91	124.81
15	c2	413	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
15	bB	819	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
15	bB	838	CLA	CMB-C2B-C1B	-4.70	121.25	128.46
15	b6	409	CLA	CMB-C2B-C3B	4.70	133.46	124.68
15	c3	403	CLA	CMB-C2B-C3B	4.70	133.46	124.68
15	a1	404	CLA	CAC-C3C-C4C	4.70	130.90	124.81
15	aB	819	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
15	b1	410	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
15	a5	420	CLA	C2A-C1A-CHA	4.69	132.07	123.86
15	bA	835	CLA	O2D-CGD-O1D	-4.69	114.67	123.84
15	c1	411	CLA	CMB-C2B-C3B	4.68	133.44	124.68
15	c1	412	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
15	c6	412	CLA	CMB-C2B-C3B	4.68	133.44	124.68
15	aA	840	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
15	cB	819	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
15	c1	410	CLA	CBC-CAC-C3C	4.68	125.33	112.43
15	bA	840	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
15	cA	835	CLA	O2D-CGD-O1D	-4.68	114.69	123.84
15	aB	838	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
15	c3	412	CLA	CMB-C2B-C1B	-4.67	121.28	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a6	409	CLA	CMB-C2B-C3B	4.67	133.42	124.68
15	b1	405	CLA	C4A-NA-C1A	4.67	108.81	106.71
15	cB	823	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
18	c3	418	BCR	C29-C30-C25	4.67	117.67	110.48
15	b5	420	CLA	C2A-C1A-CHA	4.67	132.02	123.86
15	cB	810	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
18	b4	418	BCR	C29-C30-C25	4.67	117.67	110.48
15	cA	840	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
18	a3	418	BCR	C29-C30-C25	4.67	117.67	110.48
15	bB	823	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
15	aA	835	CLA	O2D-CGD-O1D	-4.66	114.72	123.84
20	cB	850	LMG	O1-C1-C2	-4.66	101.03	108.30
15	a1	409	CLA	CBC-CAC-C3C	4.66	125.28	112.43
15	a6	411	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
20	bB	851	LMG	O1-C1-C2	-4.66	101.03	108.30
15	b5	410	CLA	CBC-CAC-C3C	4.66	125.27	112.43
20	aB	850	LMG	O1-C1-C2	-4.66	101.03	108.30
15	a4	411	CLA	CMB-C2B-C3B	4.65	133.39	124.68
15	a6	422	CLA	CAA-C2A-C1A	4.65	127.22	111.97
18	a6	419	BCR	C29-C30-C25	4.65	117.64	110.48
18	c6	419	BCR	C29-C30-C25	4.65	117.64	110.48
15	b6	406	CLA	C4A-NA-C1A	4.65	108.80	106.71
15	a5	410	CLA	CBC-CAC-C3C	4.65	125.25	112.43
15	aB	823	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
15	b6	412	CLA	CMB-C2B-C3B	4.65	133.37	124.68
15	bB	810	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
15	a1	409	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
15	a6	422	CLA	CED-O2D-CGD	4.64	126.44	115.94
18	a1	417	BCR	C29-C30-C25	4.64	117.63	110.48
15	b4	411	CLA	CMB-C2B-C3B	4.64	133.36	124.68
15	b4	412	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
18	b6	419	BCR	C29-C30-C25	4.64	117.62	110.48
15	cL	202	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
18	c4	418	BCR	C29-C30-C25	4.63	117.61	110.48
15	c3	411	CLA	CMB-C2B-C3B	4.63	133.34	124.68
15	aB	810	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
15	c4	412	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
15	a6	406	CLA	C4A-NA-C1A	4.62	108.78	106.71
15	a3	412	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
15	b3	412	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
18	b1	418	BCR	C29-C30-C25	4.62	117.59	110.48
15	cA	807	CLA	CMB-C2B-C1B	-4.61	121.37	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c5	410	CLA	CBC-CAC-C3C	4.61	125.15	112.43
15	b2	411	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
15	aL	202	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
15	b4	410	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
15	a2	411	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
15	a4	410	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
15	c1	410	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
15	a6	411	CLA	CBC-CAC-C3C	4.59	125.09	112.43
15	aA	807	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
15	bL	203	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
15	c6	404	CLA	CMB-C2B-C3B	4.58	133.25	124.68
15	a3	410	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
15	c2	411	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
15	c4	409	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
15	bA	807	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
15	a5	403	CLA	CMB-C2B-C3B	4.58	133.24	124.68
15	b4	409	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
15	c6	411	CLA	CBC-CAC-C3C	4.57	125.03	112.43
15	b3	410	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
19	aA	854	LHG	O4-P-O5	4.57	134.82	112.24
15	c1	408	CLA	CMB-C2B-C3B	4.56	133.22	124.68
19	cA	853	LHG	O4-P-O5	4.56	134.80	112.24
15	c4	410	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
15	a4	410	CLA	CBC-CAC-C3C	4.56	125.01	112.43
15	b6	411	CLA	CBC-CAC-C3C	4.56	125.00	112.43
15	a6	404	CLA	CMB-C2B-C3B	4.56	133.21	124.68
19	bA	855	LHG	O4-P-O5	4.56	134.77	112.24
15	cB	814	CLA	C4A-NA-C1A	4.56	108.75	106.71
15	c2	417	CLA	CBC-CAC-C3C	-4.56	99.87	112.43
15	b2	411	CLA	CBC-CAC-C3C	4.55	124.98	112.43
15	c4	421	CLA	C2A-C1A-CHA	4.55	131.82	123.86
18	b1	420	BCR	C2-C1-C6	4.55	117.49	110.48
15	c1	403	CLA	CMB-C2B-C3B	4.55	133.19	124.68
15	b5	403	CLA	CMB-C2B-C3B	4.55	133.19	124.68
15	b4	421	CLA	C2A-C1A-CHA	4.55	131.81	123.86
15	a1	407	CLA	CMB-C2B-C3B	4.54	133.18	124.68
18	c1	418	BCR	C29-C30-C25	4.54	117.48	110.48
15	bA	845	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
15	b5	405	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
15	b1	406	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
15	a2	411	CLA	CBC-CAC-C3C	4.54	124.94	112.43
15	a1	402	CLA	CMB-C2B-C3B	4.54	133.17	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	844	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
15	b2	409	CLA	CMB-C2B-C3B	4.54	133.17	124.68
15	aA	805	CLA	CMB-C2B-C3B	4.54	133.17	124.68
15	c4	410	CLA	CBC-CAC-C3C	4.54	124.94	112.43
15	cA	805	CLA	CMB-C2B-C3B	4.53	133.16	124.68
15	aB	837	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
18	c5	418	BCR	C29-C30-C25	4.53	117.46	110.48
15	a1	411	CLA	C4A-NA-C1A	4.53	108.74	106.71
15	cB	807	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
15	b3	411	CLA	CMB-C2B-C3B	4.53	133.15	124.68
15	b6	404	CLA	CMB-C2B-C3B	4.53	133.15	124.68
15	a4	409	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
15	b1	408	CLA	CMB-C2B-C3B	4.53	133.15	124.68
15	bA	805	CLA	CMB-C2B-C3B	4.52	133.14	124.68
15	bB	837	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
15	aA	845	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
15	b2	417	CLA	CBC-CAC-C3C	-4.52	99.97	112.43
18	a5	418	BCR	C29-C30-C25	4.52	117.44	110.48
15	a4	421	CLA	C2A-C1A-CHA	4.52	131.76	123.86
15	c6	406	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
15	a5	405	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
18	b5	418	BCR	C29-C30-C25	4.52	117.43	110.48
15	b1	403	CLA	CMB-C2B-C3B	4.51	133.12	124.68
15	a1	415	CLA	C2C-C1C-NC	4.51	114.20	109.97
15	c5	403	CLA	CMB-C2B-C3B	4.51	133.12	124.68
15	c2	411	CLA	CBC-CAC-C3C	4.51	124.86	112.43
15	a6	406	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
15	cB	837	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
15	a3	411	CLA	CMB-C2B-C3B	4.51	133.11	124.68
15	b4	410	CLA	CBC-CAC-C3C	4.51	124.86	112.43
15	b2	410	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
15	bB	815	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
15	c3	410	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
15	c5	405	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
15	c3	408	CLA	CMB-C2B-C3B	4.50	133.09	124.68
15	bB	814	CLA	C4A-NA-C1A	4.49	108.73	106.71
15	aB	830	CLA	CMB-C2B-C3B	4.49	133.08	124.68
15	aB	814	CLA	C4A-NA-C1A	4.49	108.72	106.71
15	aB	815	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
15	c1	412	CLA	C4A-NA-C1A	4.49	108.72	106.71
15	aA	825	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
15	bB	807	CLA	CMB-C2B-C1B	-4.48	121.57	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	412	CLA	C4A-NA-C1A	4.48	108.72	106.71
15	aB	825	CLA	CMB-C2B-C3B	4.48	133.06	124.68
15	a3	408	CLA	CMB-C2B-C3B	4.48	133.06	124.68
15	c3	409	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
15	c4	408	CLA	CMB-C2B-C3B	4.48	133.06	124.68
15	b3	408	CLA	CMB-C2B-C3B	4.48	133.06	124.68
15	cA	825	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
15	b6	422	CLA	CAA-C2A-C1A	4.48	126.64	111.97
15	cB	825	CLA	CMB-C2B-C3B	4.48	133.05	124.68
15	b6	406	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
15	a2	417	CLA	CBC-CAC-C3C	-4.47	100.11	112.43
15	aB	806	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
15	bB	830	CLA	CMB-C2B-C3B	4.47	133.04	124.68
15	cB	830	CLA	CMB-C2B-C3B	4.47	133.03	124.68
15	c2	410	CLA	CMB-C2B-C1B	-4.46	121.60	128.46
15	cB	815	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
15	aB	807	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
18	cF	202	BCR	C2-C1-C6	4.45	117.34	110.48
15	bB	825	CLA	CMB-C2B-C3B	4.45	133.01	124.68
15	cB	822	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
15	a2	409	CLA	CMB-C2B-C3B	4.45	133.00	124.68
15	a2	410	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
18	c1	420	BCR	C2-C1-C6	4.44	117.32	110.48
15	cB	817	CLA	C4A-NA-C1A	4.44	108.70	106.71
15	aA	802	CLA	CMB-C2B-C3B	4.44	132.99	124.68
15	cB	824	CLA	C4A-NA-C1A	4.44	108.70	106.71
15	bB	806	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
15	aB	822	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
15	bA	825	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
18	aF	201	BCR	C2-C1-C6	4.44	117.31	110.48
15	a5	417	CLA	O2D-CGD-O1D	-4.44	115.17	123.84
18	bB	849	BCR	C2-C1-C6	4.43	117.31	110.48
15	bB	822	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
15	c2	409	CLA	CMB-C2B-C3B	4.43	132.97	124.68
15	cA	802	CLA	CMB-C2B-C3B	4.43	132.97	124.68
15	aA	834	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
15	bA	802	CLA	CMB-C2B-C3B	4.43	132.96	124.68
15	a5	408	CLA	CMB-C2B-C3B	4.43	132.96	124.68
15	b4	408	CLA	CMB-C2B-C3B	4.43	132.96	124.68
15	cB	806	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
15	c5	408	CLA	CMB-C2B-C3B	4.43	132.96	124.68
15	b5	417	CLA	O2D-CGD-O1D	-4.42	115.19	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	832	CLA	CMB-C2B-C3B	4.42	132.95	124.68
15	aB	832	CLA	CMB-C2B-C3B	4.42	132.95	124.68
15	a1	405	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
15	c5	417	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
15	bB	817	CLA	C4A-NA-C1A	4.41	108.69	106.71
15	bA	803	CLA	CMB-C2B-C3B	4.41	132.93	124.68
15	cA	834	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
15	c4	421	CLA	CAA-C2A-C1A	4.41	126.42	111.97
15	aB	824	CLA	C4A-NA-C1A	4.41	108.69	106.71
15	c1	406	CLA	CMB-C2B-C1B	-4.40	121.69	128.46
15	b5	408	CLA	CMB-C2B-C3B	4.40	132.91	124.68
15	bA	834	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
15	aA	819	CLA	CAC-C3C-C4C	4.40	130.52	124.81
15	cA	803	CLA	CMB-C2B-C3B	4.40	132.90	124.68
15	b6	413	CLA	CMB-C2B-C1B	-4.40	121.71	128.46
14	aA	801	CL0	C3C-C4C-NC	4.40	115.50	110.57
18	a1	419	BCR	C2-C1-C6	4.39	117.25	110.48
15	c6	413	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
15	b3	409	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
15	bB	824	CLA	C4A-NA-C1A	4.39	108.68	106.71
15	a4	408	CLA	CMB-C2B-C3B	4.39	132.90	124.68
15	cA	819	CLA	CAC-C3C-C4C	4.39	130.51	124.81
15	b4	403	CLA	CMB-C2B-C3B	4.39	132.89	124.68
15	bA	816	CLA	CMB-C2B-C3B	4.39	132.89	124.68
15	bB	832	CLA	CMB-C2B-C3B	4.39	132.89	124.68
15	b3	406	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
15	a2	405	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
15	a1	408	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
15	b4	421	CLA	CAA-C2A-C1A	4.39	126.35	111.97
15	aB	826	CLA	CMB-C2B-C3B	4.39	132.88	124.68
15	b3	415	CLA	CMB-C2B-C3B	4.39	132.88	124.68
15	c3	417	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
15	a6	422	CLA	CBA-CAA-C2A	4.38	126.80	113.86
15	b1	416	CLA	CBC-CAC-C3C	-4.38	100.35	112.43
15	a3	409	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
15	c3	407	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
15	a3	406	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
15	b4	415	CLA	CMB-C2B-C3B	4.38	132.87	124.68
15	a2	402	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
15	a4	405	CLA	C2D-C1D-ND	-4.38	106.88	110.10
15	c4	403	CLA	CMB-C2B-C3B	4.38	132.87	124.68
15	aA	803	CLA	CMB-C2B-C3B	4.38	132.87	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	405	CLA	CMB-C2B-C1B	-4.38	121.74	128.46
15	a6	413	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
15	a3	417	CLA	O2D-CGD-O1D	-4.37	115.29	123.84
15	bA	819	CLA	CAC-C3C-C4C	4.37	130.48	124.81
15	c3	406	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
15	a1	422	CLA	CAA-C2A-C1A	4.37	126.29	111.97
15	c2	422	CLA	C2A-C1A-CHA	4.37	131.49	123.86
14	cA	801	CL0	C3C-C4C-NC	4.37	115.47	110.57
15	cB	826	CLA	CMB-C2B-C3B	4.36	132.84	124.68
15	a4	421	CLA	CAA-C2A-C1A	4.36	126.26	111.97
15	aB	828	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
15	a4	403	CLA	CMB-C2B-C3B	4.36	132.83	124.68
15	cA	816	CLA	CMB-C2B-C3B	4.36	132.83	124.68
15	c2	416	CLA	CMB-C2B-C3B	4.36	132.83	124.68
15	aA	816	CLA	CMB-C2B-C3B	4.35	132.83	124.68
14	bA	801	CL0	C3C-C4C-NC	4.35	115.45	110.57
15	cB	824	CLA	CMB-C2B-C1B	-4.35	121.77	128.46
15	a2	416	CLA	CMB-C2B-C3B	4.35	132.82	124.68
15	c2	402	CLA	CMB-C2B-C1B	-4.35	121.77	128.46
14	bA	801	CL0	C1D-CHD-C4C	-4.35	116.67	126.06
15	aB	841	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
18	b5	401	BCR	C3-C4-C5	-4.35	106.31	114.08
15	bB	826	CLA	CMB-C2B-C3B	4.35	132.82	124.68
14	cA	801	CL0	C1D-CHD-C4C	-4.35	116.67	126.06
15	aA	806	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
15	aB	817	CLA	C4A-NA-C1A	4.35	108.66	106.71
15	a2	422	CLA	C2A-C1A-CHA	4.35	131.46	123.86
15	c1	409	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
15	bB	841	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
15	b3	417	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
15	b1	409	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
15	c5	420	CLA	CAA-C2A-C1A	4.34	126.21	111.97
18	c5	401	BCR	C3-C4-C5	-4.34	106.32	114.08
15	aB	824	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
15	cB	828	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
14	aA	801	CL0	C1D-CHD-C4C	-4.34	116.70	126.06
15	bB	824	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
15	b3	407	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
15	cA	806	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
15	cB	841	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
15	a3	407	CLA	CMB-C2B-C1B	-4.33	121.80	128.46
15	bB	828	CLA	O2D-CGD-O1D	-4.33	115.37	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	bA	854	LHG	O4-P-O5	4.33	133.65	112.24
15	c3	415	CLA	CMB-C2B-C3B	4.33	132.78	124.68
15	a3	415	CLA	CMB-C2B-C3B	4.33	132.77	124.68
15	c4	405	CLA	C2D-C1D-ND	-4.33	106.92	110.10
15	a5	406	CLA	CMB-C2B-C1B	-4.33	121.82	128.46
15	bA	806	CLA	CMB-C2B-C1B	-4.33	121.82	128.46
15	bB	828	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
19	cA	852	LHG	O4-P-O5	4.32	133.62	112.24
15	a6	413	CLA	C4A-NA-C1A	4.32	108.65	106.71
15	aB	828	CLA	O2D-CGD-O1D	-4.32	115.38	123.84
15	cB	828	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
15	c2	405	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
15	b2	403	CLA	CMB-C2B-C3B	4.32	132.76	124.68
18	a5	401	BCR	C3-C4-C5	-4.32	106.36	114.08
19	aA	853	LHG	O4-P-O5	4.32	133.58	112.24
15	a4	405	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
15	c4	402	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
15	a1	414	CLA	CMB-C2B-C3B	4.32	132.75	124.68
15	b5	406	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
15	c4	405	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
15	b2	408	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
15	b2	416	CLA	CMB-C2B-C3B	4.31	132.74	124.68
15	b5	420	CLA	CAA-C2A-C1A	4.31	126.09	111.97
15	aL	202	CLA	CMB-C2B-C3B	4.30	132.73	124.68
15	c1	415	CLA	CMB-C2B-C3B	4.30	132.73	124.68
15	a2	403	CLA	CMB-C2B-C3B	4.30	132.72	124.68
15	b2	422	CLA	C2A-C1A-CHA	4.30	131.38	123.86
15	b6	417	CLA	CBC-CAC-C3C	-4.30	100.58	112.43
15	cL	202	CLA	CMB-C2B-C3B	4.29	132.71	124.68
15	bL	203	CLA	CMB-C2B-C3B	4.29	132.71	124.68
15	a5	420	CLA	CAA-C2A-C1A	4.29	126.04	111.97
15	b3	405	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
15	c5	406	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
15	b4	405	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
15	aA	840	CLA	O2D-CGD-O1D	-4.28	115.46	123.84
15	a3	405	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
15	c6	408	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
15	bA	840	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
15	a5	407	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
15	a2	417	CLA	CHD-C4C-C3C	4.27	131.12	124.84
15	a4	402	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
15	b2	402	CLA	CMB-C2B-C1B	-4.27	121.91	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	416	CLA	CBC-CAC-C3C	-4.26	100.68	112.43
15	c3	410	CLA	CMC-C2C-C1C	-4.26	118.55	125.04
15	c2	417	CLA	CHD-C4C-C3C	4.26	131.10	124.84
15	b1	405	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
15	a3	402	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
15	a6	408	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
15	aB	801	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
15	c6	417	CLA	CBC-CAC-C3C	-4.26	100.70	112.43
15	b1	415	CLA	CMB-C2B-C3B	4.26	132.64	124.68
15	b5	407	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
15	a6	407	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
15	b6	408	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
15	b5	409	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
15	cB	819	CLA	CMB-C2B-C3B	4.25	132.63	124.68
15	cB	801	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
15	b3	402	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
15	c5	409	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
15	c4	406	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
15	cA	840	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
15	bB	812	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
15	aB	812	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
15	bL	204	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
15	aL	203	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
15	b5	412	CLA	C4A-NA-C1A	4.24	108.61	106.71
15	cB	812	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
15	c3	405	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
15	b4	405	CLA	C2D-C1D-ND	-4.24	106.98	110.10
15	a5	409	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
15	a4	406	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
15	a4	415	CLA	CMB-C2B-C3B	4.24	132.61	124.68
15	cB	816	CLA	CMB-C2B-C3B	4.24	132.61	124.68
15	b5	415	CLA	CMB-C2B-C3B	4.24	132.60	124.68
15	b4	410	CLA	CMC-C2C-C1C	-4.24	118.59	125.04
15	b4	402	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
15	a6	410	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
15	bB	816	CLA	CMB-C2B-C3B	4.23	132.59	124.68
15	aB	819	CLA	CMB-C2B-C3B	4.23	132.59	124.68
14	aA	801	CL0	C4A-NA-C1A	-4.23	104.81	106.71
15	a1	404	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
15	b6	410	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
20	bB	851	LMG	O1-C7-C8	-4.23	100.70	110.90
15	a4	417	CLA	O2D-CGD-CBD	4.23	118.78	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	405	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
15	c4	415	CLA	CMB-C2B-C3B	4.22	132.58	124.68
14	bA	801	CL0	C4A-NA-C1A	-4.22	104.81	106.71
14	cA	801	CL0	C4A-NA-C1A	-4.22	104.81	106.71
20	cB	850	LMG	O1-C7-C8	-4.22	100.71	110.90
15	b6	413	CLA	C4A-NA-C1A	4.22	108.60	106.71
19	bX	101	LHG	O4-P-O5	4.22	133.11	112.24
20	aB	850	LMG	O1-C7-C8	-4.22	100.71	110.90
15	b4	406	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
15	aB	816	CLA	CMB-C2B-C3B	4.22	132.57	124.68
15	bB	819	CLA	CMB-C2B-C3B	4.22	132.57	124.68
15	c3	402	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
15	b3	405	CLA	C2D-C1D-ND	-4.22	107.00	110.10
15	cL	203	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
15	b3	410	CLA	CMC-C2C-C1C	-4.22	118.62	125.04
19	aX	101	LHG	O4-P-O5	4.22	133.08	112.24
15	bB	801	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
15	c5	407	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
15	b6	407	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
15	b1	407	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
15	c6	403	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
15	a6	417	CLA	CBC-CAC-C3C	-4.21	100.82	112.43
19	cX	101	LHG	O4-P-O5	4.21	133.06	112.24
15	a1	416	CLA	O2D-CGD-O1D	-4.21	115.61	123.84
15	cF	203	CLA	CMB-C2B-C3B	4.21	132.55	124.68
15	bB	830	CLA	C2D-C1D-ND	-4.21	107.00	110.10
15	a1	415	CLA	CBC-CAC-C3C	-4.21	100.83	112.43
15	c6	407	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
15	c2	403	CLA	CMB-C2B-C3B	4.21	132.55	124.68
15	cB	830	CLA	C2D-C1D-ND	-4.20	107.01	110.10
15	c1	417	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
15	a5	405	CLA	C2D-C1D-ND	-4.20	107.01	110.10
15	c5	405	CLA	C2D-C1D-ND	-4.20	107.01	110.10
15	b6	403	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
15	c1	407	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
15	c4	410	CLA	CMC-C2C-C1C	-4.19	118.65	125.04
18	c4	420	BCR	C2-C1-C6	4.19	116.94	110.48
15	cB	838	CLA	CMB-C2B-C3B	4.19	132.52	124.68
15	a6	403	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
15	b2	417	CLA	CHD-C4C-C3C	4.19	131.00	124.84
15	c5	410	CLA	CMC-C2C-C1C	-4.19	118.66	125.04
15	a3	410	CLA	CMC-C2C-C1C	-4.19	118.66	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	406	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
15	a6	418	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
15	bX	102	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
15	b5	402	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
18	c3	420	BCR	C2-C1-C6	4.18	116.92	110.48
15	a2	408	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
15	a5	402	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
15	c6	410	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
15	a3	412	CLA	C4A-NA-C1A	4.18	108.58	106.71
15	b6	418	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
15	c6	418	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
15	aJ	201	CLA	CMB-C2B-C3B	4.18	132.49	124.68
15	bF	201	CLA	CMB-C2B-C3B	4.18	132.49	124.68
15	a1	409	CLA	CMC-C2C-C1C	-4.18	118.68	125.04
15	c1	402	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
15	b1	417	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
18	a3	420	BCR	C2-C1-C6	4.17	116.91	110.48
15	b4	417	CLA	O2D-CGD-CBD	4.17	118.68	111.27
15	a5	415	CLA	CMB-C2B-C3B	4.17	132.49	124.68
18	b4	420	BCR	C2-C1-C6	4.17	116.90	110.48
15	b2	406	CLA	C2A-C1A-CHA	4.17	131.15	123.86
18	a4	420	BCR	C2-C1-C6	4.17	116.90	110.48
15	c5	402	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
15	cX	102	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
18	b3	420	BCR	C2-C1-C6	4.17	116.90	110.48
15	c5	415	CLA	CMB-C2B-C3B	4.17	132.47	124.68
15	c2	408	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
15	c2	418	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
15	aB	830	CLA	C2D-C1D-ND	-4.16	107.04	110.10
15	a1	401	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
15	b5	416	CLA	CBC-CAC-C3C	-4.16	100.96	112.43
15	a2	405	CLA	C2D-C1D-ND	-4.16	107.04	110.10
15	c5	416	CLA	CBC-CAC-C3C	-4.16	100.97	112.43
15	c1	410	CLA	CMC-C2C-C1C	-4.16	118.71	125.04
15	bB	838	CLA	CMB-C2B-C3B	4.15	132.45	124.68
15	aB	838	CLA	CMB-C2B-C3B	4.15	132.45	124.68
15	b6	416	CLA	CMB-C2B-C3B	4.15	132.45	124.68
15	a6	416	CLA	CMB-C2B-C3B	4.15	132.44	124.68
15	aX	102	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
18	b2	421	BCR	C2-C1-C6	4.15	116.87	110.48
15	c3	416	CLA	C2C-C1C-NC	4.15	113.86	109.97
18	a2	421	BCR	C2-C1-C6	4.15	116.87	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	416	CLA	CHD-C4C-C3C	4.15	130.94	124.84
15	b2	407	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
15	c6	416	CLA	CMB-C2B-C3B	4.14	132.43	124.68
15	a5	416	CLA	CBC-CAC-C3C	-4.14	101.01	112.43
15	b1	410	CLA	CMC-C2C-C1C	-4.14	118.73	125.04
15	b5	405	CLA	C2D-C1D-ND	-4.14	107.05	110.10
15	c4	417	CLA	O2D-CGD-CBD	4.14	118.62	111.27
15	c3	405	CLA	C2D-C1D-ND	-4.14	107.06	110.10
15	b3	416	CLA	C2C-C1C-NC	4.14	113.85	109.97
15	a4	410	CLA	CMC-C2C-C1C	-4.13	118.75	125.04
15	a2	407	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
15	a3	416	CLA	C2C-C1C-NC	4.13	113.84	109.97
15	b2	405	CLA	C2D-C1D-ND	-4.12	107.07	110.10
15	b2	406	CLA	CAA-CBA-CGA	-4.12	101.21	113.25
15	a3	405	CLA	C2D-C1D-ND	-4.12	107.07	110.10
15	c2	407	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
15	a5	412	CLA	C4A-NA-C1A	4.11	108.56	106.71
15	cB	829	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
15	b2	411	CLA	CMC-C2C-C1C	-4.11	118.78	125.04
15	a2	411	CLA	CMC-C2C-C1C	-4.11	118.78	125.04
15	c2	405	CLA	C2D-C1D-ND	-4.11	107.08	110.10
15	c2	406	CLA	CAA-CBA-CGA	-4.11	101.24	113.25
15	cA	827	CLA	CMB-C2B-C3B	4.11	132.37	124.68
15	bA	827	CLA	CMB-C2B-C3B	4.10	132.36	124.68
18	c2	421	BCR	C2-C1-C6	4.10	116.80	110.48
15	aA	808	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
15	a2	418	CLA	O2D-CGD-O1D	-4.10	115.82	123.84
15	a1	415	CLA	CHD-C4C-C3C	4.10	130.86	124.84
15	a3	416	CLA	CHD-C4C-C3C	4.09	130.86	124.84
15	a5	410	CLA	CMC-C2C-C1C	-4.09	118.81	125.04
15	a6	417	CLA	CHD-C4C-C3C	4.09	130.85	124.84
15	b3	416	CLA	CHD-C4C-C3C	4.09	130.85	124.84
15	bA	808	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
15	bB	829	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
15	a2	406	CLA	CAA-CBA-CGA	-4.09	101.30	113.25
15	bA	826	CLA	CMB-C2B-C3B	4.09	132.32	124.68
15	aA	826	CLA	CMB-C2B-C3B	4.09	132.32	124.68
15	b5	410	CLA	CMC-C2C-C1C	-4.09	118.82	125.04
15	cA	808	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
14	cA	801	CL0	C3D-C4D-ND	4.08	116.84	110.24
15	b1	414	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
15	cA	833	CLA	CMB-C2B-C3B	4.08	132.32	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	406	CLA	C2A-C1A-CHA	4.08	131.00	123.86
15	aA	833	CLA	CMB-C2B-C3B	4.08	132.31	124.68
15	a2	406	CLA	C2A-C1A-CHA	4.08	130.99	123.86
18	cB	844	BCR	C24-C23-C22	-4.08	120.07	126.23
15	bB	828	CLA	O2D-CGD-CBD	4.08	118.52	111.27
15	c4	407	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
15	a6	417	CLA	C2C-C1C-NC	4.08	113.79	109.97
15	c6	417	CLA	CHD-C4C-C3C	4.08	130.83	124.84
15	b6	417	CLA	CHD-C4C-C3C	4.08	130.83	124.84
15	cA	826	CLA	CMB-C2B-C3B	4.07	132.30	124.68
15	a4	407	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
15	b4	407	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
15	c2	411	CLA	CMC-C2C-C1C	-4.07	118.84	125.04
18	aB	844	BCR	C24-C23-C22	-4.07	120.09	126.23
15	bB	830	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
15	b2	418	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
15	cB	828	CLA	O2D-CGD-CBD	4.07	118.49	111.27
15	bA	833	CLA	CMB-C2B-C3B	4.07	132.28	124.68
15	c6	413	CLA	C4A-NA-C1A	4.06	108.53	106.71
15	cA	831	CLA	CMB-C2B-C3B	4.06	132.27	124.68
14	bA	801	CL0	C3D-C4D-ND	4.06	116.80	110.24
15	aB	829	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
15	aB	827	CLA	CMB-C2B-C3B	4.06	132.27	124.68
15	a1	422	CLA	C1-C2-C3	-4.05	119.03	126.04
15	aB	828	CLA	O2D-CGD-CBD	4.05	118.47	111.27
15	aA	827	CLA	CMB-C2B-C3B	4.05	132.26	124.68
18	b5	419	BCR	C2-C1-C6	4.05	116.72	110.48
18	bB	844	BCR	C24-C23-C22	-4.05	120.12	126.23
15	c6	417	CLA	C2C-C1C-NC	4.05	113.76	109.97
18	c5	419	BCR	C2-C1-C6	4.04	116.71	110.48
15	b6	417	CLA	C2C-C1C-NC	4.04	113.76	109.97
15	aB	837	CLA	CMB-C2B-C3B	4.04	132.24	124.68
15	bA	831	CLA	CMB-C2B-C3B	4.04	132.24	124.68
18	a6	420	BCR	C2-C1-C6	4.04	116.70	110.48
15	cB	837	CLA	CMB-C2B-C3B	4.04	132.24	124.68
15	b1	402	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
15	aA	831	CLA	CMB-C2B-C3B	4.04	132.24	124.68
15	aB	830	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
14	aA	801	CL0	C3D-C4D-ND	4.04	116.77	110.24
15	cB	830	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
15	cB	827	CLA	CMB-C2B-C3B	4.04	132.23	124.68
15	bB	827	CLA	CMB-C2B-C3B	4.03	132.23	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	816	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
15	c5	416	CLA	CHD-C4C-C3C	4.03	130.76	124.84
15	a5	416	CLA	CHD-C4C-C3C	4.02	130.76	124.84
15	aB	816	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
15	a6	422	CLA	C1-C2-C3	-4.02	119.09	126.04
15	b3	416	CLA	CBC-CAC-C3C	-4.02	101.35	112.43
15	b2	413	CLA	C4A-NA-C1A	4.02	108.51	106.71
15	bB	837	CLA	CMB-C2B-C3B	4.02	132.19	124.68
15	c1	416	CLA	CHD-C4C-C3C	4.01	130.74	124.84
18	c6	420	BCR	C2-C1-C6	4.01	116.66	110.48
18	a5	419	BCR	C2-C1-C6	4.01	116.66	110.48
15	aB	828	CLA	CMB-C2B-C3B	4.01	132.18	124.68
15	b5	416	CLA	CHD-C4C-C3C	4.01	130.74	124.84
15	c3	416	CLA	CBC-CAC-C3C	-4.01	101.38	112.43
15	bB	828	CLA	CMB-C2B-C3B	4.01	132.18	124.68
15	a4	416	CLA	CHD-C4C-C3C	4.01	130.73	124.84
15	cB	828	CLA	CMB-C2B-C3B	4.00	132.17	124.68
15	c4	416	CLA	CHD-C4C-C3C	4.00	130.72	124.84
15	b4	415	CLA	C1B-CHB-C4A	-4.00	122.20	130.12
15	c3	412	CLA	C4A-NA-C1A	3.99	108.50	106.71
15	a4	415	CLA	C1B-CHB-C4A	-3.99	122.21	130.12
18	b6	420	BCR	C2-C1-C6	3.99	116.62	110.48
15	cA	809	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
15	bB	816	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
15	c1	415	CLA	C1B-CHB-C4A	-3.99	122.22	130.12
15	bB	820	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
15	cB	820	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
15	b4	416	CLA	CBC-CAC-C3C	-3.98	101.45	112.43
15	bA	818	CLA	CMB-C2B-C3B	3.98	132.13	124.68
15	bB	802	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
15	bB	839	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
15	cB	802	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
15	aB	802	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
15	cB	839	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
15	aB	839	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
15	aA	809	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
15	cB	836	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
15	c4	416	CLA	CBC-CAC-C3C	-3.97	101.49	112.43
15	b4	416	CLA	CHD-C4C-C3C	3.97	130.67	124.84
15	bA	809	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
15	a5	416	CLA	C2C-C1C-NC	3.97	113.69	109.97
15	c5	416	CLA	C2C-C1C-NC	3.96	113.69	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	818	CLA	CMB-C2B-C3B	3.96	132.09	124.68
15	aA	818	CLA	CMB-C2B-C3B	3.96	132.09	124.68
18	c6	401	BCR	C34-C9-C8	-3.96	111.84	118.08
15	aA	840	CLA	CMB-C2B-C3B	3.96	132.09	124.68
15	c5	412	CLA	C4A-NA-C1A	3.96	108.48	106.71
15	aA	845	CLA	CBC-CAC-C3C	3.95	123.33	112.43
15	aB	820	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
15	cA	844	CLA	CBC-CAC-C3C	3.95	123.33	112.43
15	cB	805	CLA	CMB-C2B-C3B	3.95	132.06	124.68
15	aB	805	CLA	CMB-C2B-C3B	3.95	132.06	124.68
15	a1	413	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
15	cA	838	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
15	cA	840	CLA	CMB-C2B-C3B	3.94	132.06	124.68
15	c6	411	CLA	CMC-C2C-C1C	-3.94	119.03	125.04
15	a5	420	CLA	C1-C2-C3	-3.94	119.22	126.04
15	b5	420	CLA	C1-C2-C3	-3.94	119.23	126.04
15	bB	805	CLA	CMB-C2B-C3B	3.94	132.05	124.68
15	b1	416	CLA	CHD-C4C-C3C	3.94	130.63	124.84
15	bB	836	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
15	bA	840	CLA	CMB-C2B-C3B	3.94	132.05	124.68
15	c1	414	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
15	a5	410	CLA	CMB-C2B-C3B	3.94	132.04	124.68
15	bA	838	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
15	a2	413	CLA	C4A-NA-C1A	3.94	108.48	106.71
15	a4	412	CLA	C4A-NA-C1A	3.94	108.48	106.71
15	a4	416	CLA	CBC-CAC-C3C	-3.93	101.58	112.43
15	c5	420	CLA	O2D-CGD-O1D	-3.93	116.14	123.84
15	c4	415	CLA	C1B-CHB-C4A	-3.93	122.33	130.12
15	c5	410	CLA	CMB-C2B-C3B	3.93	132.04	124.68
18	a6	401	BCR	C34-C9-C8	-3.93	111.88	118.08
15	bA	845	CLA	CBC-CAC-C3C	3.93	123.27	112.43
18	cL	204	BCR	C24-C23-C22	-3.93	120.30	126.23
15	a3	416	CLA	CBC-CAC-C3C	-3.93	101.59	112.43
15	aB	823	CLA	CMB-C2B-C3B	3.93	132.03	124.68
15	cB	823	CLA	CMB-C2B-C3B	3.93	132.03	124.68
15	a5	420	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
15	b6	411	CLA	CMC-C2C-C1C	-3.93	119.06	125.04
15	a5	417	CLA	O2D-CGD-CBD	3.93	118.25	111.27
15	b6	422	CLA	C1-C2-C3	-3.93	119.25	126.04
15	aA	838	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
15	bB	823	CLA	CMB-C2B-C3B	3.93	132.02	124.68
15	b5	416	CLA	C2C-C1C-NC	3.92	113.65	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	414	CLA	C1B-CHB-C4A	-3.92	122.35	130.12
15	aB	840	CLA	CAC-C3C-C4C	3.92	129.90	124.81
15	c5	420	CLA	C1-C2-C3	-3.92	119.27	126.04
15	c1	416	CLA	C2C-C1C-NC	3.92	113.64	109.97
18	b6	401	BCR	C34-C9-C8	-3.92	111.91	118.08
15	bB	840	CLA	CAC-C3C-C4C	3.91	129.88	124.81
15	b5	410	CLA	CMB-C2B-C3B	3.91	131.99	124.68
15	b1	415	CLA	C1B-CHB-C4A	-3.91	122.38	130.12
15	cB	840	CLA	CAC-C3C-C4C	3.91	129.88	124.81
15	cB	833	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
18	aI	103	BCR	C24-C23-C22	-3.91	120.33	126.23
15	cA	807	CLA	CMB-C2B-C3B	3.90	131.98	124.68
18	c1	401	BCR	C34-C9-C8	-3.90	111.93	118.08
15	a6	411	CLA	CMC-C2C-C1C	-3.90	119.10	125.04
15	b5	420	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
18	bL	205	BCR	C24-C23-C22	-3.89	120.35	126.23
15	aB	836	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
15	bB	833	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
15	aB	833	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
15	b4	412	CLA	C4A-NA-C1A	3.89	108.46	106.71
15	aJ	203	CLA	CAA-C2A-C3A	-3.89	107.02	116.10
15	c5	417	CLA	O2D-CGD-CBD	3.89	118.18	111.27
15	bJ	102	CLA	CAA-C2A-C3A	-3.89	107.03	116.10
15	b5	417	CLA	O2D-CGD-CBD	3.89	118.18	111.27
15	aA	825	CLA	CMB-C2B-C3B	3.89	131.95	124.68
15	b3	412	CLA	C4A-NA-C1A	3.89	108.45	106.71
15	a5	415	CLA	C1B-CHB-C4A	-3.89	122.42	130.12
15	cA	839	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
15	c3	415	CLA	C1B-CHB-C4A	-3.88	122.42	130.12
15	cB	806	CLA	CMB-C2B-C3B	3.88	131.94	124.68
15	aA	807	CLA	CMB-C2B-C3B	3.88	131.94	124.68
15	cA	817	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
15	aB	806	CLA	CMB-C2B-C3B	3.88	131.94	124.68
15	aA	817	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
15	bA	807	CLA	CMB-C2B-C3B	3.87	131.93	124.68
18	b6	421	BCR	C3-C4-C5	-3.87	107.16	114.08
15	aA	819	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
15	bA	839	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
15	bB	806	CLA	CMB-C2B-C3B	3.87	131.92	124.68
15	c4	409	CLA	CMB-C2B-C3B	3.87	131.91	124.68
14	aA	801	CL0	O2D-CGD-O1D	-3.87	116.28	123.84
15	c3	421	CLA	CAA-CBA-CGA	-3.86	101.96	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	839	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
15	cJ	102	CLA	CAA-C2A-C3A	-3.86	107.09	116.10
18	c4	401	BCR	C3-C4-C5	-3.86	107.19	114.08
15	cA	834	CLA	CMB-C2B-C3B	3.86	131.90	124.68
18	aA	851	BCR	C24-C23-C22	-3.86	120.41	126.23
15	bA	819	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
15	bA	817	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
18	a4	401	BCR	C2-C1-C6	3.85	116.41	110.48
18	b4	401	BCR	C3-C4-C5	-3.85	107.20	114.08
18	bA	852	BCR	C24-C23-C22	-3.85	120.41	126.23
15	cA	825	CLA	CMB-C2B-C3B	3.85	131.88	124.68
14	cA	801	CL0	O2D-CGD-O1D	-3.85	116.31	123.84
15	b6	406	CLA	C2D-C1D-ND	-3.85	107.27	110.10
14	bA	801	CL0	O2D-CGD-O1D	-3.85	116.31	123.84
18	c4	401	BCR	C2-C1-C6	3.85	116.40	110.48
15	bA	835	CLA	O2D-CGD-CBD	3.85	118.10	111.27
15	b3	415	CLA	C1B-CHB-C4A	-3.84	122.51	130.12
15	b5	415	CLA	C1B-CHB-C4A	-3.84	122.51	130.12
15	b6	422	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
15	cA	819	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
18	cA	850	BCR	C24-C23-C22	-3.84	120.43	126.23
15	aA	814	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
15	bA	834	CLA	CMB-C2B-C3B	3.84	131.86	124.68
15	c5	415	CLA	C1B-CHB-C4A	-3.84	122.52	130.12
15	b1	416	CLA	C2C-C1C-NC	3.84	113.56	109.97
18	a4	401	BCR	C3-C4-C5	-3.83	107.23	114.08
15	b1	405	CLA	C2D-C1D-ND	-3.83	107.28	110.10
15	a3	415	CLA	C1B-CHB-C4A	-3.83	122.53	130.12
15	bA	825	CLA	CMB-C2B-C3B	3.83	131.85	124.68
15	b4	409	CLA	CMB-C2B-C3B	3.83	131.85	124.68
15	cB	812	CLA	CMB-C2B-C3B	3.83	131.84	124.68
18	b4	401	BCR	C2-C1-C6	3.83	116.37	110.48
15	aB	812	CLA	CMB-C2B-C3B	3.83	131.84	124.68
15	aA	834	CLA	CMB-C2B-C3B	3.82	131.83	124.68
15	bA	814	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
15	aB	815	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
15	a3	421	CLA	CAA-CBA-CGA	-3.82	102.09	113.25
15	a4	409	CLA	CMB-C2B-C3B	3.82	131.82	124.68
15	cB	815	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
15	a1	404	CLA	C2D-C1D-ND	-3.81	107.30	110.10
15	cA	814	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
15	c6	416	CLA	C1B-CHB-C4A	-3.81	122.57	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	815	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
15	bB	812	CLA	CMB-C2B-C3B	3.81	131.80	124.68
15	cB	824	CLA	CMB-C2B-C3B	3.81	131.80	124.68
15	cA	835	CLA	O2D-CGD-CBD	3.81	118.03	111.27
15	b6	411	CLA	CMB-C2B-C3B	3.80	131.79	124.68
15	cA	803	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
15	b1	406	CLA	CMB-C2B-C3B	3.80	131.79	124.68
15	c1	413	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
15	aA	803	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
15	bA	803	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
15	b3	421	CLA	CAA-CBA-CGA	-3.79	102.18	113.25
15	c3	407	CLA	CMB-C2B-C3B	3.79	131.77	124.68
15	a6	416	CLA	C1B-CHB-C4A	-3.79	122.61	130.12
15	b6	416	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
15	a6	411	CLA	CMB-C2B-C3B	3.79	131.76	124.68
15	c2	416	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
15	cA	806	CLA	CMB-C2B-C3B	3.79	131.76	124.68
15	bB	824	CLA	CMB-C2B-C3B	3.79	131.76	124.68
15	a1	422	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
15	a3	407	CLA	CMB-C2B-C3B	3.78	131.76	124.68
15	a2	416	CLA	C1B-CHB-C4A	-3.78	122.63	130.12
15	aA	835	CLA	O2D-CGD-CBD	3.78	117.99	111.27
15	b3	407	CLA	CMB-C2B-C3B	3.78	131.75	124.68
15	cB	829	CLA	CMB-C2B-C3B	3.78	131.75	124.68
15	aA	806	CLA	CMB-C2B-C3B	3.78	131.75	124.68
15	bB	829	CLA	CMB-C2B-C3B	3.78	131.74	124.68
15	aA	811	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
15	aB	824	CLA	CMB-C2B-C3B	3.77	131.74	124.68
15	b2	404	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
15	bA	806	CLA	CMB-C2B-C3B	3.77	131.74	124.68
15	c2	413	CLA	C4A-NA-C1A	3.77	108.40	106.71
15	c3	409	CLA	CMB-C2B-C3B	3.77	131.73	124.68
15	c3	413	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
15	a3	414	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
15	a6	406	CLA	C2D-C1D-ND	-3.77	107.33	110.10
15	aB	829	CLA	CMB-C2B-C3B	3.76	131.72	124.68
15	c6	411	CLA	CMB-C2B-C3B	3.76	131.71	124.68
15	cB	835	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
15	b2	416	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
15	a5	414	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
15	cA	811	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
15	cB	822	CLA	CMB-C2B-C3B	3.75	131.70	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	404	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
15	c6	406	CLA	C2D-C1D-ND	-3.75	107.34	110.10
15	aL	202	CLA	CHB-C4A-NA	3.75	129.69	124.51
15	c5	405	CLA	CAC-C3C-C2C	-3.74	121.12	127.53
15	c5	404	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
15	bB	822	CLA	CMB-C2B-C3B	3.74	131.68	124.68
15	bA	845	CLA	CMB-C2B-C3B	3.74	131.68	124.68
15	c1	415	CLA	CHB-C4A-NA	3.74	129.68	124.51
15	aA	845	CLA	CMB-C2B-C3B	3.74	131.67	124.68
15	bB	835	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
15	aB	835	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
15	aA	804	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
15	aB	822	CLA	CMB-C2B-C3B	3.74	131.67	124.68
15	bA	811	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
15	c2	404	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
15	cA	844	CLA	CMB-C2B-C3B	3.73	131.66	124.68
15	bA	806	CLA	CAA-C2A-C3A	-3.73	102.56	112.78
18	b1	401	BCR	C11-C10-C9	-3.73	121.99	127.31
15	cA	806	CLA	CAA-C2A-C3A	-3.73	102.57	112.78
15	b5	405	CLA	CAC-C3C-C2C	-3.73	121.16	127.53
15	b3	409	CLA	CMB-C2B-C3B	3.72	131.64	124.68
15	b3	413	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
15	b2	408	CLA	CMB-C2B-C3B	3.72	131.63	124.68
15	c1	405	CLA	C2D-C1D-ND	-3.72	107.36	110.10
15	bA	804	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
15	cL	202	CLA	CHB-C4A-NA	3.72	129.65	124.51
15	aA	843	CLA	C1-O2A-CGA	3.72	126.19	116.44
15	a5	404	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
15	b1	410	CLA	CMB-C2B-C3B	3.71	131.62	124.68
15	aA	806	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
15	aB	815	CLA	CMB-C2B-C3B	3.71	131.62	124.68
15	a1	405	CLA	CMB-C2B-C3B	3.71	131.62	124.68
15	a3	413	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
15	a3	409	CLA	CMB-C2B-C3B	3.71	131.61	124.68
15	b2	410	CLA	CMB-C2B-C3B	3.71	131.61	124.68
15	bB	815	CLA	CMB-C2B-C3B	3.70	131.60	124.68
15	cA	842	CLA	C1-O2A-CGA	3.70	126.15	116.44
15	c1	406	CLA	CMB-C2B-C3B	3.70	131.60	124.68
15	bB	808	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
15	aK	102	CLA	CMB-C2B-C1B	-3.69	122.78	128.46
15	bL	203	CLA	CHB-C4A-NA	3.69	129.62	124.51
15	cB	815	CLA	CMB-C2B-C3B	3.69	131.59	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	804	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
15	a1	422	CLA	CAA-CBA-CGA	-3.69	102.47	113.25
15	a4	415	CLA	CHB-C4A-NA	3.69	129.62	124.51
15	cB	808	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
15	b5	404	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
15	b5	414	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
15	c4	413	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
15	a2	410	CLA	CMB-C2B-C3B	3.69	131.58	124.68
15	bA	843	CLA	C1-O2A-CGA	3.69	126.12	116.44
15	b1	413	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
15	c2	410	CLA	CMB-C2B-C3B	3.69	131.57	124.68
15	a4	404	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
14	cA	801	CL0	CMD-C2D-C1D	3.68	131.21	124.71
15	bA	832	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
15	c3	417	CLA	O2D-CGD-CBD	3.68	117.81	111.27
15	a5	415	CLA	CHB-C4A-NA	3.68	129.60	124.51
15	cB	807	CLA	CMB-C2B-C3B	3.68	131.56	124.68
15	b3	414	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
15	a1	414	CLA	CHB-C4A-NA	3.68	129.60	124.51
15	a5	405	CLA	CAC-C3C-C2C	-3.68	121.24	127.53
18	cB	848	BCR	C15-C16-C17	-3.67	115.95	123.47
15	a1	409	CLA	CMB-C2B-C3B	3.67	131.55	124.68
15	bK	101	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
15	aB	817	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
15	c5	414	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
15	b2	422	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
15	cA	832	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
18	aB	848	BCR	C15-C16-C17	-3.67	115.96	123.47
15	a2	422	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
15	b5	405	CLA	CMB-C2B-C3B	3.66	131.53	124.68
15	a3	417	CLA	O2D-CGD-CBD	3.66	117.78	111.27
15	b1	415	CLA	CHB-C4A-NA	3.66	129.58	124.51
15	b2	407	CLA	CMB-C2B-C3B	3.66	131.52	124.68
15	b6	418	CLA	O2D-CGD-CBD	3.66	117.77	111.27
15	a3	415	CLA	CHB-C4A-NA	3.66	129.57	124.51
15	aA	832	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
15	cK	102	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
15	a5	405	CLA	CMB-C2B-C3B	3.66	131.52	124.68
15	cB	817	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
15	aB	808	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
15	bB	817	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
15	c6	406	CLA	CAC-C3C-C2C	-3.66	121.28	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	407	CLA	CMB-C2B-C3B	3.65	131.51	124.68
15	c2	422	CLA	C1-C2-C3	-3.65	119.72	126.04
15	bX	102	CLA	CHB-C4A-NA	3.65	129.56	124.51
15	bL	204	CLA	CMB-C2B-C3B	3.65	131.51	124.68
15	a6	418	CLA	O2D-CGD-CBD	3.65	117.75	111.27
15	b4	404	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
15	c5	415	CLA	CHB-C4A-NA	3.65	129.56	124.51
15	b6	405	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
15	aX	102	CLA	CHB-C4A-NA	3.65	129.56	124.51
18	aA	850	BCR	C15-C16-C17	-3.65	116.01	123.47
18	bB	848	BCR	C15-C16-C17	-3.65	116.01	123.47
15	a2	407	CLA	CMB-C2B-C3B	3.65	131.50	124.68
15	bB	807	CLA	CMB-C2B-C3B	3.65	131.50	124.68
15	b4	415	CLA	CHB-C4A-NA	3.64	129.55	124.51
15	aL	203	CLA	CMB-C2B-C3B	3.64	131.50	124.68
15	cX	102	CLA	CHB-C4A-NA	3.64	129.55	124.51
15	a1	416	CLA	O2D-CGD-CBD	3.64	117.74	111.27
15	a4	416	CLA	C2C-C1C-NC	3.64	113.38	109.97
14	bA	801	CL0	CMD-C2D-C1D	3.64	131.13	124.71
15	aB	807	CLA	CMB-C2B-C3B	3.64	131.49	124.68
15	b4	416	CLA	C2C-C1C-NC	3.64	113.38	109.97
14	aA	801	CL0	CMD-C2D-C1D	3.64	131.13	124.71
15	c5	405	CLA	CMB-C2B-C3B	3.64	131.49	124.68
15	c1	417	CLA	O2D-CGD-CBD	3.64	117.73	111.27
15	b3	421	CLA	C2A-C1A-CHA	3.64	130.22	123.86
15	bA	823	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
18	a6	421	BCR	C3-C4-C5	-3.64	107.58	114.08
15	a1	408	CLA	CMB-C2B-C3B	3.64	131.48	124.68
15	a2	411	CLA	CMB-C2B-C3B	3.64	131.48	124.68
15	cL	203	CLA	CMB-C2B-C3B	3.63	131.48	124.68
15	b5	415	CLA	CHB-C4A-NA	3.63	129.53	124.51
15	a4	410	CLA	CMB-C2B-C3B	3.63	131.47	124.68
15	b2	411	CLA	CMB-C2B-C3B	3.63	131.47	124.68
15	cA	823	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
15	bB	806	CLA	CHB-C4A-NA	3.63	129.53	124.51
18	bA	851	BCR	C15-C16-C17	-3.63	116.05	123.47
15	aA	823	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
15	a6	405	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
15	b6	406	CLA	CAC-C3C-C2C	-3.62	121.33	127.53
15	c1	410	CLA	CMB-C2B-C3B	3.62	131.46	124.68
18	bA	848	BCR	C15-C16-C17	-3.62	116.05	123.47
15	aB	809	CLA	O2D-CGD-O1D	-3.62	116.75	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	404	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
15	cB	806	CLA	CHB-C4A-NA	3.62	129.52	124.51
18	cA	849	BCR	C15-C16-C17	-3.62	116.06	123.47
15	b6	415	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
15	c3	421	CLA	C2A-C1A-CHA	3.62	130.19	123.86
18	c1	418	BCR	C2-C1-C6	3.62	116.05	110.48
15	a3	421	CLA	C2A-C1A-CHA	3.62	130.19	123.86
15	c4	412	CLA	C4A-NA-C1A	3.62	108.33	106.71
15	b6	416	CLA	CHB-C4A-NA	3.62	129.52	124.51
15	bB	803	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
18	cK	101	BCR	C15-C16-C17	-3.62	116.06	123.47
15	aB	803	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
15	c4	410	CLA	CMB-C2B-C3B	3.62	131.44	124.68
15	c4	415	CLA	CHB-C4A-NA	3.61	129.51	124.51
15	c2	411	CLA	CMB-C2B-C3B	3.61	131.44	124.68
14	aA	801	CL0	CMA-C3A-C2A	-3.61	99.25	113.83
15	a2	408	CLA	CMB-C2B-C3B	3.61	131.44	124.68
15	a2	405	CLA	CAC-C3C-C2C	-3.61	121.35	127.53
15	aA	837	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
15	a6	422	CLA	C3A-C2A-C1A	3.61	106.75	101.34
15	aA	806	CLA	CHB-C4A-NA	3.61	129.50	124.51
18	a1	417	BCR	C2-C1-C6	3.61	116.03	110.48
14	bA	801	CL0	CMA-C3A-C2A	-3.61	99.27	113.83
15	c6	418	CLA	O2D-CGD-CBD	3.61	117.68	111.27
15	cA	806	CLA	CHB-C4A-NA	3.61	129.50	124.51
15	cB	803	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
15	b2	405	CLA	CAC-C3C-C2C	-3.61	121.36	127.53
15	aB	806	CLA	CHB-C4A-NA	3.60	129.50	124.51
15	b6	422	CLA	CED-O2D-CGD	3.60	124.08	115.94
15	bB	808	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
15	b4	410	CLA	CMB-C2B-C3B	3.60	131.41	124.68
15	bA	837	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
18	aK	101	BCR	C15-C16-C17	-3.60	116.10	123.47
15	a2	402	CLA	CMB-C2B-C3B	3.60	131.41	124.68
15	c4	416	CLA	C2C-C1C-NC	3.60	113.34	109.97
14	cA	801	CL0	CMA-C3A-C2A	-3.60	99.32	113.83
15	b1	417	CLA	O2D-CGD-CBD	3.60	117.66	111.27
15	b3	417	CLA	O2D-CGD-CBD	3.60	117.66	111.27
15	a3	404	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
15	c2	408	CLA	CMB-C2B-C3B	3.60	131.41	124.68
15	c4	404	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
15	c2	402	CLA	CMB-C2B-C3B	3.59	131.40	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	837	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
15	c6	405	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
15	cJ	101	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
15	cB	809	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
15	b3	402	CLA	CMB-C2B-C3B	3.59	131.40	124.68
18	a3	418	BCR	C30-C25-C26	-3.59	117.55	122.61
15	c3	415	CLA	CHB-C4A-NA	3.59	129.48	124.51
15	a6	415	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
15	bB	809	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
15	b1	409	CLA	CMB-C2B-C3B	3.59	131.39	124.68
15	b2	422	CLA	C1-C2-C3	-3.59	119.84	126.04
18	bB	844	BCR	C28-C27-C26	-3.59	107.67	114.08
15	a3	410	CLA	CMB-C2B-C3B	3.59	131.39	124.68
15	c6	416	CLA	CHB-C4A-NA	3.59	129.47	124.51
15	cB	808	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
15	a3	402	CLA	CMB-C2B-C3B	3.59	131.39	124.68
15	a2	422	CLA	C1-C2-C3	-3.59	119.84	126.04
15	a6	410	CLA	CMB-C2B-C3B	3.59	131.39	124.68
15	c3	405	CLA	CAC-C3C-C2C	-3.59	121.39	127.53
14	bA	801	CL0	C1C-C2C-C3C	-3.59	103.19	106.96
15	c3	414	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
15	bA	843	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
15	b6	408	CLA	CMB-C2B-C3B	3.58	131.38	124.68
15	c1	409	CLA	CMB-C2B-C3B	3.58	131.38	124.68
15	b3	405	CLA	CAC-C3C-C2C	-3.58	121.40	127.53
15	c2	405	CLA	CAC-C3C-C2C	-3.58	121.40	127.53
15	b4	413	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
14	cA	801	CL0	C1C-C2C-C3C	-3.58	103.19	106.96
15	c5	413	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
18	b3	418	BCR	C30-C25-C26	-3.58	117.57	122.61
18	bB	848	BCR	C24-C23-C22	-3.58	120.83	126.23
15	a6	416	CLA	CHB-C4A-NA	3.58	129.46	124.51
15	a6	406	CLA	CAC-C3C-C2C	-3.58	121.41	127.53
15	aJ	202	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
18	aB	848	BCR	C24-C23-C22	-3.58	120.83	126.23
18	aB	844	BCR	C28-C27-C26	-3.58	107.69	114.08
15	cB	836	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
15	c6	415	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
18	cB	844	BCR	C28-C27-C26	-3.57	107.70	114.08
15	bA	813	CLA	CMB-C2B-C3B	3.57	131.36	124.68
15	aB	836	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
15	bB	836	CLA	O2D-CGD-O1D	-3.57	116.86	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bJ	101	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
14	aA	801	CL0	C1C-C2C-C3C	-3.57	103.20	106.96
15	b5	407	CLA	CMB-C2B-C3B	3.57	131.35	124.68
14	bA	801	CL0	C3B-C4B-NB	3.57	113.82	109.21
18	aJ	205	BCR	C2-C1-C6	3.57	115.97	110.48
15	b5	406	CLA	CMB-C2B-C3B	3.57	131.35	124.68
15	a2	422	CLA	O2D-CGD-CBD	3.57	117.61	111.27
15	cA	813	CLA	CMB-C2B-C3B	3.57	131.35	124.68
15	aA	843	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
15	a6	422	CLA	CGD-CBD-CAD	-3.56	99.19	110.73
15	aA	813	CLA	CMB-C2B-C3B	3.56	131.35	124.68
15	bA	806	CLA	CHB-C4A-NA	3.56	129.44	124.51
18	b2	419	BCR	C2-C1-C6	3.56	115.97	110.48
15	bJ	101	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
18	cJ	104	BCR	C2-C1-C6	3.56	115.96	110.48
18	aA	850	BCR	C15-C14-C13	-3.56	122.23	127.31
18	bA	851	BCR	C15-C14-C13	-3.56	122.23	127.31
15	aB	808	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
15	c3	421	CLA	CAA-C2A-C1A	3.56	123.64	111.97
18	a1	421	BCR	C3-C4-C5	-3.56	107.72	114.08
18	cB	848	BCR	C24-C23-C22	-3.56	120.86	126.23
18	b2	401	BCR	C2-C1-C6	3.56	115.96	110.48
15	b3	415	CLA	CHB-C4A-NA	3.56	129.43	124.51
15	b3	410	CLA	CMB-C2B-C3B	3.56	131.34	124.68
15	b6	410	CLA	CMB-C2B-C3B	3.56	131.34	124.68
15	c6	410	CLA	CMB-C2B-C3B	3.56	131.34	124.68
15	b3	405	CLA	CMB-C2B-C3B	3.56	131.34	124.68
15	c6	406	CLA	CMB-C2B-C3B	3.56	131.34	124.68
15	c2	422	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
15	a6	406	CLA	CMB-C2B-C3B	3.56	131.34	124.68
15	cA	839	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
15	aJ	202	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
15	a6	408	CLA	CMB-C2B-C3B	3.56	131.33	124.68
15	a5	406	CLA	CMB-C2B-C3B	3.56	131.33	124.68
15	c6	408	CLA	CMB-C2B-C3B	3.56	131.33	124.68
15	a6	414	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
18	b1	418	BCR	C2-C1-C6	3.55	115.95	110.48
15	a4	413	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
15	cJ	101	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
15	a3	421	CLA	CAA-C2A-C1A	3.55	123.62	111.97
15	a5	407	CLA	CMB-C2B-C3B	3.55	131.32	124.68
15	a3	405	CLA	CAC-C3C-C2C	-3.55	121.45	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	412	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
15	c2	416	CLA	CHB-C4A-NA	3.55	129.42	124.51
18	bJ	104	BCR	C2-C1-C6	3.55	115.94	110.48
15	c2	418	CLA	O2D-CGD-CBD	3.55	117.58	111.27
15	c2	414	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
14	cA	801	CL0	C3B-C4B-NB	3.55	113.80	109.21
15	c3	404	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
15	b3	421	CLA	CAA-C2A-C1A	3.55	123.60	111.97
15	a2	418	CLA	O2D-CGD-CBD	3.55	117.57	111.27
18	cA	849	BCR	C15-C14-C13	-3.55	122.25	127.31
15	c3	402	CLA	CMB-C2B-C3B	3.55	131.31	124.68
15	bA	839	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
18	c2	401	BCR	C2-C1-C6	3.54	115.94	110.48
15	cA	840	CLA	CHB-C4A-NA	3.54	129.41	124.51
15	c3	405	CLA	CMB-C2B-C3B	3.54	131.31	124.68
15	b6	406	CLA	CMB-C2B-C3B	3.54	131.30	124.68
14	aA	801	CL0	C3B-C4B-NB	3.54	113.79	109.21
15	c4	405	CLA	CMB-C2B-C3B	3.54	131.30	124.68
15	c3	410	CLA	CMB-C2B-C3B	3.54	131.29	124.68
18	c2	419	BCR	C2-C1-C6	3.54	115.92	110.48
15	b4	405	CLA	CMB-C2B-C3B	3.54	131.29	124.68
15	aA	805	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
15	c5	406	CLA	CMB-C2B-C3B	3.53	131.28	124.68
15	cA	805	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
15	a3	405	CLA	CMB-C2B-C3B	3.53	131.28	124.68
18	a2	401	BCR	C2-C1-C6	3.53	115.91	110.48
15	bA	805	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
15	b1	407	CLA	CMB-C2B-C3B	3.53	131.28	124.68
15	a4	407	CLA	CMB-C2B-C3B	3.52	131.27	124.68
15	a3	406	CLA	CMB-C2B-C3B	3.52	131.27	124.68
15	bB	825	CLA	O2D-CGD-CBD	3.52	117.53	111.27
15	c4	402	CLA	CMB-C2B-C3B	3.52	131.27	124.68
18	a3	419	BCR	C2-C1-C6	3.52	115.90	110.48
18	bA	853	BCR	C40-C30-C25	3.52	116.01	110.30
15	a5	413	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
15	cA	842	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
15	b3	421	CLA	C1-C2-C3	-3.52	119.96	126.04
15	c3	421	CLA	C1-C2-C3	-3.52	119.96	126.04
15	aB	825	CLA	O2D-CGD-CBD	3.52	117.52	111.27
15	c5	407	CLA	CMB-C2B-C3B	3.52	131.26	124.68
18	b3	419	BCR	C2-C1-C6	3.52	115.89	110.48
18	c3	419	BCR	C2-C1-C6	3.52	115.89	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aA	852	BCR	C40-C30-C25	3.52	116.00	110.30
15	aA	839	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
15	a4	405	CLA	CMB-C2B-C3B	3.52	131.26	124.68
18	a2	419	BCR	C2-C1-C6	3.51	115.89	110.48
15	c5	409	CLA	CMB-C2B-C3B	3.51	131.25	124.68
15	cB	825	CLA	O2D-CGD-CBD	3.51	117.50	111.27
15	cB	826	CLA	CHB-C4A-NA	3.51	129.37	124.51
15	bA	840	CLA	CHB-C4A-NA	3.51	129.36	124.51
15	b5	409	CLA	CMB-C2B-C3B	3.51	131.24	124.68
15	aB	827	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
15	a5	409	CLA	CMB-C2B-C3B	3.51	131.24	124.68
15	aA	840	CLA	CHB-C4A-NA	3.50	129.36	124.51
15	aA	820	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
15	a2	416	CLA	CHB-C4A-NA	3.50	129.36	124.51
15	aA	824	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
18	c3	418	BCR	C30-C25-C26	-3.50	117.68	122.61
15	aB	810	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
15	c4	407	CLA	CMB-C2B-C3B	3.50	131.23	124.68
15	b5	413	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
15	c1	407	CLA	CMB-C2B-C3B	3.50	131.23	124.68
15	aA	812	CLA	CAA-CBA-CGA	3.50	123.48	113.25
15	bA	812	CLA	CAA-CBA-CGA	3.50	123.48	113.25
18	b5	401	BCR	C2-C1-C6	3.50	115.87	110.48
15	b2	416	CLA	CHB-C4A-NA	3.50	129.35	124.51
15	cB	840	CLA	CHB-C4A-NA	3.50	129.35	124.51
15	cB	827	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
18	cA	851	BCR	C40-C30-C25	3.50	115.97	110.30
15	bB	810	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
18	b2	419	BCR	C30-C25-C26	-3.50	117.69	122.61
15	b1	405	CLA	CMB-C2B-C3B	3.50	131.22	124.68
18	a1	420	BCR	C11-C10-C9	-3.49	122.32	127.31
18	b5	418	BCR	C2-C1-C6	3.49	115.86	110.48
15	cA	841	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
15	c6	414	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
18	b2	420	BCR	C11-C10-C9	-3.49	122.33	127.31
15	cA	824	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
18	c1	419	BCR	C34-C9-C10	-3.49	118.03	122.92
15	a2	406	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
15	bB	839	CLA	CMB-C2B-C3B	3.49	131.21	124.68
15	aA	812	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
15	c1	404	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
15	bB	827	CLA	O2D-CGD-O1D	-3.49	117.02	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	810	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
15	a6	407	CLA	CMB-C2B-C3B	3.49	131.20	124.68
15	bA	824	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
15	b5	420	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
15	bB	826	CLA	CHB-C4A-NA	3.49	129.33	124.51
18	c5	401	BCR	C2-C1-C6	3.49	115.85	110.48
15	a4	402	CLA	CMB-C2B-C3B	3.48	131.20	124.68
15	cA	812	CLA	CAA-CBA-CGA	3.48	123.43	113.25
15	bA	812	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
15	cA	812	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
18	b6	401	BCR	C2-C1-C6	3.48	115.84	110.48
15	aB	840	CLA	CHB-C4A-NA	3.48	129.33	124.51
15	aB	826	CLA	CHB-C4A-NA	3.48	129.32	124.51
15	a1	406	CLA	CMB-C2B-C3B	3.48	131.19	124.68
15	cA	820	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
15	cB	839	CLA	CMB-C2B-C3B	3.48	131.19	124.68
15	a1	422	CLA	C3A-C2A-C1A	3.48	106.55	101.34
18	a5	401	BCR	C2-C1-C6	3.48	115.83	110.48
15	b2	418	CLA	O2D-CGD-CBD	3.47	117.44	111.27
15	bA	841	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
14	cA	801	CL0	CMA-C3A-C4A	-3.47	102.44	111.77
18	a5	418	BCR	C2-C1-C6	3.47	115.83	110.48
15	bA	822	CLA	CMB-C2B-C3B	3.47	131.17	124.68
18	c6	419	BCR	C30-C25-C26	-3.47	117.72	122.61
14	bA	801	CL0	CMA-C3A-C4A	-3.47	102.44	111.77
18	c2	420	BCR	C11-C10-C9	-3.47	122.36	127.31
15	aA	841	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
15	a3	421	CLA	C1-C2-C3	-3.47	120.04	126.04
15	bA	820	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
18	c5	418	BCR	C2-C1-C6	3.47	115.82	110.48
15	b2	402	CLA	CMB-C2B-C3B	3.47	131.17	124.68
15	c4	421	CLA	C1-C2-C3	-3.47	120.04	126.04
15	a6	414	CLA	CAC-C3C-C4C	3.47	129.31	124.81
15	b4	405	CLA	CAC-C3C-C2C	-3.47	121.60	127.53
15	c3	406	CLA	CMB-C2B-C3B	3.47	131.16	124.68
18	b6	419	BCR	C30-C25-C26	-3.47	117.73	122.61
15	b6	407	CLA	CMB-C2B-C3B	3.47	131.16	124.68
15	b4	407	CLA	CMB-C2B-C3B	3.47	131.16	124.68
15	aB	804	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
18	b1	401	BCR	C2-C1-C6	3.47	115.82	110.48
15	b2	422	CLA	CAA-C2A-C1A	3.47	123.33	111.97
15	cA	841	CLA	C1B-CHB-C4A	-3.46	123.25	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a6	419	BCR	C30-C25-C26	-3.46	117.74	122.61
15	a4	414	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
18	a4	419	BCR	C2-C1-C6	3.46	115.81	110.48
15	bF	201	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
15	b2	414	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
15	c2	422	CLA	CAA-C2A-C1A	3.46	123.32	111.97
14	aA	801	CL0	CMA-C3A-C4A	-3.46	102.47	111.77
15	b6	414	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
15	cA	822	CLA	CMB-C2B-C3B	3.46	131.15	124.68
15	bA	841	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
15	b4	421	CLA	C1-C2-C3	-3.46	120.06	126.04
15	a5	420	CLA	C3A-C2A-C1A	3.46	106.52	101.34
18	a4	418	BCR	C30-C25-C26	-3.46	117.74	122.61
15	a4	405	CLA	CAC-C3C-C2C	-3.46	121.61	127.53
15	c1	405	CLA	CMB-C2B-C3B	3.46	131.15	124.68
15	cB	804	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
15	a2	422	CLA	CAA-C2A-C1A	3.46	123.31	111.97
15	b6	403	CLA	CMB-C2B-C3B	3.46	131.15	124.68
15	bB	840	CLA	CHB-C4A-NA	3.46	129.29	124.51
15	bB	804	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
18	a6	402	BCR	C2-C1-C6	3.46	115.80	110.48
15	c5	420	CLA	C3A-C2A-C1A	3.46	106.52	101.34
15	aB	839	CLA	CMB-C2B-C3B	3.46	131.14	124.68
18	c6	401	BCR	C2-C1-C6	3.46	115.80	110.48
15	b2	422	CLA	O2D-CGD-CBD	3.45	117.41	111.27
15	cB	838	CLA	CHB-C4A-NA	3.45	129.29	124.51
15	b2	405	CLA	CMB-C2B-C3B	3.45	131.14	124.68
18	c6	402	BCR	C2-C1-C6	3.45	115.80	110.48
15	a2	405	CLA	CMB-C2B-C3B	3.45	131.14	124.68
15	bA	810	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
15	aA	822	CLA	CMB-C2B-C3B	3.45	131.14	124.68
14	bA	801	CL0	C3D-C2D-C1D	-3.45	101.12	105.83
15	c4	414	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
15	b4	402	CLA	CMB-C2B-C3B	3.45	131.13	124.68
15	c6	407	CLA	CMB-C2B-C3B	3.45	131.13	124.68
14	cA	801	CL0	C3D-C2D-C1D	-3.45	101.12	105.83
15	a2	414	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
15	aJ	201	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
15	c6	403	CLA	CMB-C2B-C3B	3.45	131.13	124.68
18	c4	419	BCR	C2-C1-C6	3.45	115.79	110.48
18	b4	418	BCR	C30-C25-C26	-3.45	117.76	122.61
15	b3	406	CLA	CMB-C2B-C3B	3.45	131.12	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	420	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
15	aA	844	CLA	CHB-C4A-NA	3.44	129.28	124.51
18	a2	420	BCR	C11-C10-C9	-3.44	122.40	127.31
15	cA	810	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
15	a1	404	CLA	CMB-C2B-C3B	3.44	131.12	124.68
15	cF	203	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
18	bA	848	BCR	C15-C14-C13	-3.44	122.41	127.31
15	aL	201	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
15	c2	406	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	aK	101	BCR	C15-C14-C13	-3.43	122.41	127.31
18	aL	205	BCR	C2-C1-C6	3.43	115.77	110.48
15	aA	841	CLA	C1B-CHB-C4A	-3.43	123.32	130.12
18	b5	418	BCR	C30-C25-C26	-3.43	117.78	122.61
16	bA	846	PQN	C11-C12-C13	-3.43	121.08	126.79
18	c4	418	BCR	C30-C25-C26	-3.43	117.78	122.61
18	c5	401	BCR	C11-C10-C9	-3.43	122.41	127.31
18	bL	201	BCR	C2-C1-C6	3.43	115.76	110.48
15	c4	405	CLA	CAC-C3C-C2C	-3.43	121.66	127.53
15	c2	422	CLA	O2D-CGD-CBD	3.43	117.36	111.27
15	c5	420	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	b4	419	BCR	C2-C1-C6	3.43	115.76	110.48
15	bB	838	CLA	CHB-C4A-NA	3.43	129.25	124.51
18	bJ	103	BCR	C15-C16-C17	-3.43	116.45	123.47
18	b6	402	BCR	C2-C1-C6	3.43	115.76	110.48
15	bA	844	CLA	CHB-C4A-NA	3.43	129.25	124.51
18	cK	101	BCR	C15-C14-C13	-3.43	122.42	127.31
14	aA	801	CL0	C3D-C2D-C1D	-3.42	101.16	105.83
15	aB	838	CLA	CHB-C4A-NA	3.42	129.25	124.51
18	a6	401	BCR	C2-C1-C6	3.42	115.75	110.48
18	bA	849	BCR	C15-C16-C17	-3.42	116.47	123.47
15	a1	403	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
18	bL	206	BCR	C2-C1-C6	3.42	115.74	110.48
15	aA	814	CLA	CMB-C2B-C3B	3.42	131.07	124.68
18	aJ	204	BCR	C15-C16-C17	-3.42	116.47	123.47
15	b4	414	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
15	a6	403	CLA	CMB-C2B-C3B	3.42	131.07	124.68
18	aA	848	BCR	C15-C16-C17	-3.41	116.48	123.47
16	aA	846	PQN	C11-C12-C13	-3.41	121.11	126.79
15	c2	405	CLA	CMB-C2B-C3B	3.41	131.06	124.68
15	bA	814	CLA	CMB-C2B-C3B	3.41	131.06	124.68
18	a1	418	BCR	C34-C9-C10	-3.41	118.15	122.92
15	cA	809	CLA	CMB-C2B-C3B	3.41	131.06	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cJ	103	BCR	C15-C16-C17	-3.41	116.49	123.47
15	c1	402	CLA	CMB-C2B-C3B	3.41	131.05	124.68
15	aA	810	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
18	c4	418	BCR	C2-C1-C6	3.41	115.73	110.48
18	cA	847	BCR	C15-C16-C17	-3.40	116.50	123.47
15	a2	415	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
15	b1	404	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
15	cA	843	CLA	CHB-C4A-NA	3.40	129.22	124.51
15	cA	814	CLA	CMB-C2B-C3B	3.40	131.05	124.68
18	a2	419	BCR	C30-C25-C26	-3.40	117.82	122.61
15	b5	420	CLA	C3A-C2A-C1A	3.40	106.43	101.34
18	c5	418	BCR	C30-C25-C26	-3.39	117.83	122.61
16	cA	845	PQN	C11-C12-C13	-3.39	121.14	126.79
15	bL	202	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
15	a2	413	CLA	CMC-C2C-C1C	-3.39	119.87	125.04
18	b4	418	BCR	C2-C1-C6	3.39	115.71	110.48
18	a5	401	BCR	C11-C10-C9	-3.39	122.47	127.31
15	a4	421	CLA	C1-C2-C3	-3.39	120.18	126.04
15	aA	818	CLA	CHB-C4A-NA	3.39	129.20	124.51
15	cL	201	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
15	b5	412	CLA	CMC-C2C-C1C	-3.39	119.88	125.04
15	c2	415	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
15	cA	842	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
15	a1	401	CLA	CMB-C2B-C3B	3.39	131.01	124.68
18	b1	419	BCR	C34-C9-C10	-3.39	118.18	122.92
15	aA	843	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
18	a5	418	BCR	C30-C25-C26	-3.38	117.85	122.61
15	aB	832	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
15	b1	405	CLA	CAC-C3C-C2C	-3.38	121.75	127.53
15	a4	406	CLA	CMB-C2B-C3B	3.38	131.00	124.68
14	aA	801	CL0	CHD-C1D-ND	-3.38	121.35	124.45
18	a4	418	BCR	C2-C1-C6	3.38	115.68	110.48
15	b2	413	CLA	CMC-C2C-C1C	-3.37	119.90	125.04
18	bA	851	BCR	C24-C23-C22	-3.37	121.14	126.23
18	b2	401	BCR	C7-C8-C9	-3.37	121.14	126.23
15	a5	412	CLA	CMC-C2C-C1C	-3.37	119.90	125.04
15	b6	422	CLA	C6-C5-C3	-3.37	104.61	113.45
15	bB	814	CLA	C1-C2-C3	-3.37	120.21	126.04
18	cA	849	BCR	C24-C23-C22	-3.37	121.14	126.23
15	c1	405	CLA	CAC-C3C-C2C	-3.37	121.77	127.53
15	aA	809	CLA	CMB-C2B-C3B	3.37	130.98	124.68
15	bA	818	CLA	CHB-C4A-NA	3.37	129.17	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	809	CLA	CMB-C2B-C3B	3.36	130.97	124.68
14	bA	801	CL0	CHD-C1D-ND	-3.36	121.36	124.45
18	b2	420	BCR	C2-C1-C6	3.36	115.66	110.48
15	b5	402	CLA	CMB-C2B-C3B	3.36	130.97	124.68
15	c5	412	CLA	CMC-C2C-C1C	-3.36	119.92	125.04
14	cA	801	CL0	CHD-C1D-ND	-3.36	121.37	124.45
15	bA	843	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
15	cB	832	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
18	aA	850	BCR	C24-C23-C22	-3.35	121.17	126.23
15	b1	402	CLA	CMB-C2B-C3B	3.35	130.95	124.68
15	cA	818	CLA	CHB-C4A-NA	3.35	129.15	124.51
15	a5	402	CLA	CMB-C2B-C3B	3.35	130.94	124.68
18	bB	847	BCR	C40-C30-C25	3.35	115.73	110.30
15	cB	814	CLA	C1-C2-C3	-3.35	120.25	126.04
18	bF	202	BCR	C16-C15-C14	-3.35	116.62	123.47
18	c2	401	BCR	C7-C8-C9	-3.35	121.18	126.23
15	cA	837	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
18	c2	420	BCR	C2-C1-C6	3.35	115.63	110.48
15	b2	406	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
15	c4	406	CLA	CMB-C2B-C3B	3.34	130.94	124.68
18	a2	420	BCR	C2-C1-C6	3.34	115.63	110.48
15	c5	402	CLA	CMB-C2B-C3B	3.34	130.93	124.68
15	aA	815	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
15	b2	415	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
18	b5	401	BCR	C11-C10-C9	-3.34	122.54	127.31
15	bB	832	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
18	cF	204	BCR	C16-C15-C14	-3.34	116.63	123.47
18	c3	418	BCR	C2-C1-C6	3.34	115.62	110.48
15	bA	837	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
15	aB	814	CLA	C1-C2-C3	-3.34	120.28	126.04
15	aA	837	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
14	cA	801	CL0	CBC-CAC-C3C	-3.33	103.24	112.43
14	bA	801	CL0	CBC-CAC-C3C	-3.33	103.25	112.43
15	bB	816	CLA	CHB-C4A-NA	3.33	129.12	124.51
15	b2	403	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
15	bA	815	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
15	aA	827	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
18	aB	847	BCR	C40-C30-C25	3.33	115.69	110.30
15	bB	835	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
15	c2	422	CLA	CGD-CBD-CAD	-3.33	99.96	110.73
15	cA	827	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
15	cA	802	CLA	C1B-CHB-C4A	-3.33	123.53	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aF	202	BCR	C16-C15-C14	-3.33	116.66	123.47
15	cA	815	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
18	b6	419	BCR	C2-C1-C6	3.32	115.60	110.48
14	aA	801	CL0	CBC-CAC-C3C	-3.32	103.27	112.43
18	c6	419	BCR	C2-C1-C6	3.32	115.59	110.48
15	bA	827	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
18	c2	419	BCR	C30-C25-C26	-3.32	117.94	122.61
15	b4	406	CLA	CMB-C2B-C3B	3.32	130.89	124.68
15	aB	816	CLA	CHB-C4A-NA	3.32	129.10	124.51
18	cB	847	BCR	C40-C30-C25	3.31	115.67	110.30
18	bB	848	BCR	C11-C10-C9	-3.31	122.58	127.31
15	a2	406	CLA	C6-C5-C3	-3.31	104.77	113.45
15	aB	835	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
15	a2	422	CLA	CGD-CBD-CAD	-3.31	100.01	110.73
15	a6	422	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
15	c2	406	CLA	C6-C5-C3	-3.31	104.78	113.45
15	aA	802	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
15	aA	804	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
15	a1	422	CLA	C6-C5-C3	-3.31	104.78	113.45
18	c1	401	BCR	C11-C10-C9	-3.31	122.59	127.31
15	cB	835	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
18	a6	419	BCR	C2-C1-C6	3.31	115.57	110.48
15	bA	828	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
15	bA	802	CLA	C1B-CHB-C4A	-3.30	123.57	130.12
18	cB	846	BCR	C15-C16-C17	-3.30	116.71	123.47
15	bA	804	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
15	cB	816	CLA	CHB-C4A-NA	3.30	129.07	124.51
18	a2	401	BCR	C7-C8-C9	-3.30	121.25	126.23
15	a1	404	CLA	CAC-C3C-C2C	-3.30	121.89	127.53
15	cA	804	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
15	b2	406	CLA	C6-C5-C3	-3.30	104.81	113.45
18	a1	420	BCR	C2-C1-C6	3.30	115.56	110.48
19	bA	855	LHG	O8-C23-C24	3.30	120.02	111.38
19	cA	853	LHG	O8-C23-C24	3.30	120.02	111.38
18	bL	205	BCR	C11-C10-C9	-3.29	122.61	127.31
18	bB	846	BCR	C15-C16-C17	-3.29	116.73	123.47
15	bJ	101	CLA	CHB-C4A-NA	3.29	129.07	124.51
18	cB	848	BCR	C11-C10-C9	-3.29	122.61	127.31
15	cA	809	CLA	CHB-C4A-NA	3.29	129.06	124.51
15	cB	810	CLA	CMB-C2B-C3B	3.29	130.83	124.68
18	cJ	103	BCR	C15-C14-C13	-3.29	122.62	127.31
15	c5	410	CLA	C2D-C1D-ND	-3.29	107.68	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	809	CLA	CHB-C4A-NA	3.29	129.06	124.51
15	a6	413	CLA	CMC-C2C-C1C	-3.29	120.04	125.04
15	aA	828	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
15	b2	422	CLA	CGD-CBD-CAD	-3.28	100.10	110.73
18	aB	846	BCR	C15-C16-C17	-3.28	116.75	123.47
18	aB	848	BCR	C11-C10-C9	-3.28	122.62	127.31
15	bB	810	CLA	CMB-C2B-C3B	3.28	130.82	124.68
15	bA	810	CLA	CHB-C4A-NA	3.28	129.05	124.51
15	cA	816	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
15	aA	834	CLA	CHB-C4A-NA	3.28	129.05	124.51
18	a3	418	BCR	C2-C1-C6	3.28	115.53	110.48
19	aA	854	LHG	O8-C23-C24	3.28	119.98	111.38
15	cA	828	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
15	cA	810	CLA	CHB-C4A-NA	3.28	129.04	124.51
15	c1	405	CLA	CHD-C1D-ND	-3.27	121.44	124.45
18	cB	848	BCR	C2-C1-C6	3.27	115.52	110.48
15	aA	809	CLA	CHB-C4A-NA	3.27	129.04	124.51
15	aJ	202	CLA	CHB-C4A-NA	3.27	129.03	124.51
15	cB	821	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
15	aA	808	CLA	CMB-C2B-C3B	3.27	130.79	124.68
15	bA	808	CLA	CMB-C2B-C3B	3.27	130.79	124.68
18	aF	203	BCR	C2-C1-C6	3.27	115.51	110.48
18	bJ	105	BCR	C2-C1-C6	3.27	115.51	110.48
15	c2	413	CLA	CMC-C2C-C1C	-3.27	120.06	125.04
18	c3	420	BCR	C28-C27-C26	-3.27	108.25	114.08
15	bB	825	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
15	aA	810	CLA	CHB-C4A-NA	3.26	129.02	124.51
15	aB	825	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
18	aB	848	BCR	C2-C1-C6	3.26	115.50	110.48
15	aB	810	CLA	CBA-CAA-C2A	-3.26	104.24	113.86
15	cJ	101	CLA	CHB-C4A-NA	3.26	129.02	124.51
15	aB	821	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
18	bJ	103	BCR	C15-C14-C13	-3.26	122.66	127.31
15	cB	810	CLA	CBA-CAA-C2A	-3.26	104.25	113.86
15	cA	808	CLA	CMB-C2B-C3B	3.26	130.77	124.68
15	aA	816	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
15	aA	845	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
15	aA	832	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
15	bB	821	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
18	aJ	204	BCR	C15-C14-C13	-3.25	122.67	127.31
15	c2	403	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
15	bB	833	CLA	O2D-CGD-O1D	-3.25	117.48	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	422	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
15	bA	830	CLA	CHB-C4A-NA	3.25	129.00	124.51
18	b3	418	BCR	C2-C1-C6	3.25	115.48	110.48
15	bB	810	CLA	CBA-CAA-C2A	-3.25	104.28	113.86
15	cB	833	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	cB	825	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	b5	410	CLA	C2D-C1D-ND	-3.25	107.71	110.10
15	b2	406	CLA	C16-C15-C13	-3.25	105.42	115.92
18	b2	401	BCR	C15-C14-C13	-3.25	122.68	127.31
18	c2	401	BCR	C15-C14-C13	-3.25	122.68	127.31
15	aB	833	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	bA	832	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
15	a1	415	CLA	CHB-C4A-NA	3.24	129.00	124.51
15	b1	405	CLA	CHD-C1D-ND	-3.24	121.47	124.45
15	bB	836	CLA	O2D-CGD-CBD	3.24	117.03	111.27
15	aB	810	CLA	CMB-C2B-C3B	3.24	130.75	124.68
15	aB	836	CLA	O2D-CGD-CBD	3.24	117.03	111.27
15	b2	422	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
15	cL	203	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
15	cA	830	CLA	CHB-C4A-NA	3.24	128.99	124.51
15	cB	836	CLA	O2D-CGD-CBD	3.24	117.02	111.27
15	aL	203	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
18	cL	204	BCR	C11-C10-C9	-3.24	122.69	127.31
15	bA	834	CLA	CHB-C4A-NA	3.23	128.99	124.51
18	cA	848	BCR	C2-C1-C6	3.23	115.46	110.48
15	cA	839	CLA	CMB-C2B-C3B	3.23	130.73	124.68
15	bA	809	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	a1	419	BCR	C28-C27-C26	-3.23	108.31	114.08
15	bA	816	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	c2	404	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	a2	404	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	c2	422	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
15	cB	823	CLA	CHB-C4A-NA	3.23	128.98	124.51
15	c6	413	CLA	CMC-C2C-C1C	-3.23	120.12	125.04
15	cB	838	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	aA	830	CLA	CHB-C4A-NA	3.23	128.98	124.51
15	bA	839	CLA	CMB-C2B-C3B	3.23	130.72	124.68
18	a1	421	BCR	C2-C1-C6	3.23	115.45	110.48
15	bL	204	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
18	aI	103	BCR	C11-C10-C9	-3.23	122.70	127.31
15	cK	102	CLA	CMB-C2B-C3B	3.23	130.72	124.68
15	cB	819	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	416	CLA	CHB-C4A-NA	3.23	128.97	124.51
18	a3	420	BCR	C28-C27-C26	-3.22	108.32	114.08
15	aA	839	CLA	CMB-C2B-C3B	3.22	130.71	124.68
15	cA	832	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
15	cA	834	CLA	CHB-C4A-NA	3.22	128.97	124.51
15	c4	410	CLA	C2D-C1D-ND	-3.22	107.73	110.10
18	cF	205	BCR	C2-C1-C6	3.22	115.44	110.48
15	cA	844	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
18	b1	418	BCR	C30-C25-C26	-3.22	118.08	122.61
15	a5	410	CLA	C2D-C1D-ND	-3.22	107.73	110.10
15	b4	410	CLA	C2D-C1D-ND	-3.22	107.73	110.10
15	bB	823	CLA	CHB-C4A-NA	3.22	128.96	124.51
15	aK	102	CLA	CMB-C2B-C3B	3.22	130.70	124.68
15	cA	809	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
15	aA	809	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
15	bB	838	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
18	aA	849	BCR	C2-C1-C6	3.22	115.43	110.48
18	bB	848	BCR	C2-C1-C6	3.22	115.43	110.48
15	cB	836	CLA	CMB-C2B-C3B	3.21	130.69	124.68
15	b3	408	CLA	C2D-C1D-ND	-3.21	107.73	110.10
16	cB	843	PQN	C11-C12-C13	-3.21	121.44	126.79
15	aA	831	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
15	bL	203	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
15	a2	417	CLA	CHB-C4A-NA	3.21	128.96	124.51
18	c1	401	BCR	C2-C1-C6	3.21	115.43	110.48
15	a6	422	CLA	O2D-CGD-CBD	3.21	116.98	111.27
15	bA	808	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	bA	850	BCR	C2-C1-C6	3.21	115.42	110.48
15	bK	101	CLA	CMB-C2B-C3B	3.21	130.68	124.68
18	b1	401	BCR	C34-C9-C8	-3.21	113.03	118.08
15	aL	202	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
15	bB	825	CLA	CHB-C4A-NA	3.21	128.94	124.51
15	cA	808	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
15	a1	404	CLA	CHD-C1D-ND	-3.20	121.51	124.45
15	b4	415	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
15	a4	410	CLA	C2D-C1D-ND	-3.20	107.74	110.10
15	aA	804	CLA	CMD-C2D-C1D	-3.20	119.07	124.71
18	bB	847	BCR	C27-C26-C25	3.20	127.38	122.73
15	bB	819	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
14	aA	801	CL0	C4C-C3C-C2C	-3.20	102.23	106.90
18	b3	420	BCR	C28-C27-C26	-3.20	108.36	114.08
15	bB	835	CLA	CHB-C4A-NA	3.20	128.94	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	845	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
15	b5	420	CLA	CHB-C4A-NA	3.20	128.94	124.51
15	cA	804	CLA	CMD-C2D-C1D	-3.20	119.07	124.71
18	b4	420	BCR	C28-C27-C26	-3.20	108.36	114.08
15	aB	823	CLA	CHB-C4A-NA	3.20	128.94	124.51
15	aB	812	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
15	bA	831	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
15	b1	405	CLA	CMD-C2D-C1D	3.20	130.35	124.71
15	b1	414	CLA	CMB-C2B-C3B	3.20	130.66	124.68
18	c2	421	BCR	C28-C27-C26	-3.20	108.37	114.08
18	c6	401	BCR	C11-C10-C9	-3.20	122.75	127.31
18	a1	417	BCR	C30-C25-C26	-3.20	118.11	122.61
18	a4	420	BCR	C28-C27-C26	-3.20	108.37	114.08
15	bA	804	CLA	CMD-C2D-C1D	-3.19	119.08	124.71
15	c5	420	CLA	CHB-C4A-NA	3.19	128.93	124.51
15	a4	405	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
16	bB	843	PQN	C11-C12-C13	-3.19	121.48	126.79
18	a2	421	BCR	C28-C27-C26	-3.19	108.38	114.08
18	b3	418	BCR	C3-C4-C5	-3.19	108.38	114.08
15	aB	825	CLA	CHB-C4A-NA	3.19	128.93	124.51
15	bA	822	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
15	cB	835	CLA	CHB-C4A-NA	3.19	128.92	124.51
15	bB	837	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
18	c4	420	BCR	C28-C27-C26	-3.19	108.39	114.08
15	bB	812	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
15	b1	416	CLA	CHB-C4A-NA	3.19	128.92	124.51
15	a1	422	CLA	CED-O2D-CGD	3.19	123.14	115.94
15	cB	808	CLA	CMB-C2B-C3B	3.19	130.64	124.68
15	bA	845	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
15	cA	831	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
14	bA	801	CL0	C4C-C3C-C2C	-3.18	102.26	106.90
14	cA	801	CL0	C4C-C3C-C2C	-3.18	102.26	106.90
15	aA	845	CLA	O2A-CGA-O1A	-3.18	115.56	123.59
15	cA	844	CLA	O2A-CGA-O1A	-3.18	115.56	123.59
18	c1	418	BCR	C30-C25-C26	-3.18	118.13	122.61
15	aB	836	CLA	CMB-C2B-C3B	3.18	130.63	124.68
15	bB	836	CLA	CMB-C2B-C3B	3.18	130.63	124.68
15	aB	838	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
15	b6	406	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
15	cB	812	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	aB	819	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	cL	202	CLA	O2D-CGD-O1D	-3.18	117.62	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	835	CLA	CHB-C4A-NA	3.18	128.91	124.51
15	aB	809	CLA	CBA-CAA-C2A	3.18	123.25	113.86
18	a2	401	BCR	C15-C14-C13	-3.18	122.77	127.31
15	cB	825	CLA	CHB-C4A-NA	3.18	128.91	124.51
15	a3	412	CLA	CMC-C2C-C1C	-3.18	120.20	125.04
15	aA	819	CLA	CMB-C2B-C3B	3.18	130.62	124.68
14	cA	801	CL0	CHC-C1C-C2C	-3.18	117.93	126.72
15	a3	421	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	aA	808	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
15	aA	822	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
15	bB	811	CLA	CHB-C4A-NA	3.18	128.90	124.51
15	b2	417	CLA	CHB-C4A-NA	3.18	128.90	124.51
15	bB	829	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
15	a3	421	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
18	a6	401	BCR	C11-C10-C9	-3.17	122.78	127.31
16	aB	843	PQN	C11-C12-C13	-3.17	121.51	126.79
15	a3	410	CLA	C2D-C1D-ND	-3.17	107.77	110.10
18	aB	847	BCR	C27-C26-C25	3.17	127.34	122.73
15	c1	405	CLA	CMD-C2D-C1D	3.17	130.31	124.71
14	bA	801	CL0	CHC-C1C-C2C	-3.17	117.94	126.72
15	c2	406	CLA	C16-C15-C13	-3.17	105.67	115.92
15	cB	811	CLA	CHB-C4A-NA	3.17	128.90	124.51
15	aB	811	CLA	CHB-C4A-NA	3.17	128.90	124.51
15	cB	837	CLA	CHB-C4A-NA	3.17	128.90	124.51
15	cB	809	CLA	CBA-CAA-C2A	3.17	123.22	113.86
18	cB	847	BCR	C27-C26-C25	3.17	127.33	122.73
15	b3	412	CLA	CMC-C2C-C1C	-3.17	120.21	125.04
15	aB	837	CLA	CHB-C4A-NA	3.17	128.89	124.51
18	b6	421	BCR	C2-C1-C6	3.17	115.36	110.48
15	cA	822	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
15	b4	405	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
14	aA	801	CL0	CHC-C1C-C2C	-3.17	117.96	126.72
15	b3	421	CLA	CHA-C1A-NA	-3.17	119.15	126.40
15	bB	809	CLA	CBA-CAA-C2A	3.17	123.21	113.86
15	bA	820	CLA	O2D-CGD-CBD	3.16	116.89	111.27
20	aB	850	LMG	O6-C1-O1	-3.16	102.48	109.97
20	bB	851	LMG	O6-C1-O1	-3.16	102.48	109.97
15	bB	808	CLA	CMB-C2B-C3B	3.16	130.60	124.68
15	bA	832	CLA	O2D-CGD-CBD	3.16	116.89	111.27
15	c4	405	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
15	bB	837	CLA	CHB-C4A-NA	3.16	128.89	124.51
15	b3	421	CLA	O2D-CGD-O1D	-3.16	117.66	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	837	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	aB	837	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	b3	410	CLA	C2D-C1D-ND	-3.16	107.78	110.10
15	c6	414	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	aB	829	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
15	a1	403	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
15	bA	819	CLA	CMB-C2B-C3B	3.16	130.58	124.68
18	b1	420	BCR	C28-C27-C26	-3.16	108.44	114.08
15	a2	422	CLA	C16-C15-C13	-3.16	105.72	115.92
20	cB	850	LMG	O6-C1-O1	-3.16	102.50	109.97
15	a1	411	CLA	C1B-CHB-C4A	-3.16	123.87	130.12
15	a6	406	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
15	a5	420	CLA	CHB-C4A-NA	3.16	128.88	124.51
15	c2	422	CLA	C16-C15-C13	-3.15	105.72	115.92
15	b3	404	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
15	a3	421	CLA	CHA-C1A-NA	-3.15	119.17	126.40
15	c6	406	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
15	b6	411	CLA	C2D-C1D-ND	-3.15	107.78	110.10
15	aA	820	CLA	O2D-CGD-CBD	3.15	116.87	111.27
18	c1	420	BCR	C28-C27-C26	-3.15	108.45	114.08
15	a2	422	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
15	cA	820	CLA	O2D-CGD-CBD	3.15	116.87	111.27
15	b2	404	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
18	a4	401	BCR	C11-C10-C9	-3.15	122.81	127.31
15	cA	819	CLA	CMB-C2B-C3B	3.15	130.57	124.68
15	a3	408	CLA	C2D-C1D-ND	-3.15	107.78	110.10
15	cB	826	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
15	c3	421	CLA	CHA-C1A-NA	-3.15	119.19	126.40
15	b6	407	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
15	b2	422	CLA	C16-C15-C13	-3.15	105.75	115.92
15	aB	808	CLA	CMB-C2B-C3B	3.15	130.56	124.68
15	c3	421	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
18	b4	401	BCR	C11-C10-C9	-3.14	122.82	127.31
15	a2	406	CLA	C16-C15-C13	-3.14	105.76	115.92
15	cB	840	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
15	a1	411	CLA	CMC-C2C-C1C	-3.14	120.25	125.04
15	cA	832	CLA	O2D-CGD-CBD	3.14	116.85	111.27
15	aA	844	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
15	aA	817	CLA	CMB-C2B-C3B	3.14	130.55	124.68
15	cA	817	CLA	CMB-C2B-C3B	3.14	130.55	124.68
15	cB	829	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
15	cB	813	CLA	CMB-C2B-C3B	3.14	130.55	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b6	401	BCR	C11-C10-C9	-3.14	122.83	127.31
15	c5	408	CLA	C2D-C1D-ND	-3.14	107.79	110.10
15	c2	417	CLA	CHB-C4A-NA	3.14	128.85	124.51
15	a6	414	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
15	b6	413	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
15	a1	407	CLA	C2D-C1D-ND	-3.13	107.79	110.10
15	cA	803	CLA	CHB-C4A-NA	3.13	128.85	124.51
15	bB	828	CLA	CHB-C4A-NA	3.13	128.84	124.51
15	c4	415	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
15	a2	403	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
15	aA	832	CLA	O2D-CGD-CBD	3.13	116.83	111.27
15	aA	817	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
15	c3	412	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
15	bA	807	CLA	CHB-C4A-NA	3.13	128.84	124.51
15	bA	817	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
18	a3	418	BCR	C3-C4-C5	-3.13	108.49	114.08
15	a6	414	CLA	C2D-C1D-ND	-3.13	107.80	110.10
15	bA	817	CLA	CMB-C2B-C3B	3.13	130.53	124.68
15	aB	840	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
15	aA	835	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
15	cA	817	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
15	bB	840	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
15	cA	835	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
15	c3	410	CLA	C2D-C1D-ND	-3.13	107.80	110.10
15	cB	834	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
18	b2	421	BCR	C28-C27-C26	-3.12	108.50	114.08
15	bB	826	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
15	aA	836	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
15	aB	834	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
15	bA	803	CLA	CHB-C4A-NA	3.12	128.83	124.51
15	cA	836	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
15	cB	829	CLA	CHB-C4A-NA	3.12	128.83	124.51
15	aB	826	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	cA	829	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	aA	803	CLA	CHB-C4A-NA	3.12	128.83	124.51
15	a1	404	CLA	CMD-C2D-C1D	3.12	130.21	124.71
15	c6	406	CLA	CHD-C1D-ND	-3.12	121.59	124.45
15	bB	834	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
15	bB	817	CLA	O2D-CGD-CBD	3.12	116.81	111.27
15	aA	829	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	b4	417	CLA	C2C-C1C-NC	-3.12	107.05	109.97
15	aB	817	CLA	O2D-CGD-CBD	3.12	116.81	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	828	CLA	CHB-C4A-NA	3.12	128.82	124.51
15	c4	417	CLA	C2C-C1C-NC	-3.12	107.05	109.97
15	bA	844	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
15	a3	416	CLA	CHB-C4A-NA	3.11	128.82	124.51
15	c1	408	CLA	C2D-C1D-ND	-3.11	107.81	110.10
15	c1	416	CLA	C1-C2-C3	-3.11	121.72	126.75
15	bA	821	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
15	a2	405	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	b4	405	CLA	CMD-C2D-C1D	3.11	130.19	124.71
15	cA	837	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	a3	404	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	b3	416	CLA	CHB-C4A-NA	3.11	128.81	124.51
18	cI	102	BCR	C15-C14-C13	-3.11	122.87	127.31
15	aA	807	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	a6	407	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	a6	417	CLA	CHB-C4A-NA	3.11	128.81	124.51
18	a6	421	BCR	C2-C1-C6	3.11	115.26	110.48
18	c4	401	BCR	C11-C10-C9	-3.11	122.88	127.31
15	cB	828	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	c3	405	CLA	CMD-C2D-C1D	3.11	130.19	124.71
15	aB	809	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
15	cA	807	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	aA	821	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
15	bB	809	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
15	b3	421	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
15	bA	835	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
15	aB	829	CLA	CHB-C4A-NA	3.10	128.80	124.51
15	a4	415	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
15	c6	417	CLA	CHB-C4A-NA	3.10	128.80	124.51
15	aB	834	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
15	bA	845	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
15	bX	102	CLA	CMB-C2B-C3B	3.10	130.48	124.68
15	cA	843	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
18	cA	851	BCR	C39-C30-C25	-3.10	105.27	110.30
18	c4	419	BCR	C24-C23-C22	-3.10	121.55	126.23
15	a3	405	CLA	CMD-C2D-C1D	3.10	130.18	124.71
15	bB	813	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	bI	102	BCR	C15-C14-C13	-3.10	122.89	127.31
15	bA	836	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
15	b2	418	CLA	CHB-C4A-NA	3.10	128.80	124.51
15	cA	821	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
15	b6	422	CLA	CGD-CBD-CAD	-3.10	100.70	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	402	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
15	c2	416	CLA	C2D-C1D-ND	-3.10	107.82	110.10
15	aB	813	CLA	CMB-C2B-C3B	3.10	130.47	124.68
15	b6	422	CLA	C3A-C2A-C1A	3.10	105.97	101.34
15	aB	811	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
18	aI	102	BCR	C15-C14-C13	-3.09	122.89	127.31
15	c6	407	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
18	c1	419	BCR	C3-C4-C5	-3.09	108.55	114.08
15	a4	417	CLA	C2C-C1C-NC	-3.09	107.07	109.97
15	b2	405	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
15	aX	102	CLA	CMB-C2B-C3B	3.09	130.46	124.68
15	cA	835	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	bA	829	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
15	aA	837	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	a5	402	CLA	C1-C2-C3	-3.09	120.70	126.04
15	cB	834	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	a1	418	BCR	C3-C4-C5	-3.09	108.56	114.08
15	c3	416	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	bB	829	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	aA	811	CLA	CMB-C2B-C3B	3.09	130.45	124.68
15	aA	835	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	b5	408	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	c5	402	CLA	C1-C2-C3	-3.09	120.70	126.04
15	bB	834	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
15	cA	811	CLA	CMB-C2B-C3B	3.09	130.45	124.68
15	cB	817	CLA	O2D-CGD-CBD	3.09	116.75	111.27
15	c3	408	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	a2	418	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	bA	842	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
15	a5	415	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
15	aB	827	CLA	CHB-C4A-NA	3.08	128.78	124.51
15	b4	421	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
15	c5	413	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
15	cB	838	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
15	c4	405	CLA	CMD-C2D-C1D	3.08	130.14	124.71
15	aA	829	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
15	b1	412	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
15	aB	813	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
15	b1	404	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
15	c2	411	CLA	C2D-C1D-ND	-3.08	107.83	110.10
15	bA	829	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
15	a5	405	CLA	CMD-C2D-C1D	3.08	130.14	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	413	CLA	CMB-C2B-C3B	3.08	130.44	124.68
15	c2	405	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
18	bA	853	BCR	C39-C30-C25	-3.08	105.31	110.30
15	c1	404	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
15	c4	402	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
15	b6	417	CLA	CHB-C4A-NA	3.08	128.77	124.51
15	bB	811	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
15	c1	417	CLA	CHB-C4A-NA	3.08	128.77	124.51
15	cX	102	CLA	CMB-C2B-C3B	3.08	130.44	124.68
15	b5	405	CLA	CMD-C2D-C1D	3.08	130.13	124.71
15	aB	818	CLA	CHB-C4A-NA	3.08	128.77	124.51
15	aA	845	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
15	c3	421	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
15	c5	417	CLA	C2C-C1C-NC	-3.08	107.09	109.97
15	a5	413	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
15	a6	411	CLA	C2D-C1D-ND	-3.07	107.84	110.10
15	c5	415	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
15	cA	829	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
15	c2	417	CLA	C1C-C2C-C3C	-3.07	103.72	106.96
15	bB	838	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
15	a5	408	CLA	C2D-C1D-ND	-3.07	107.84	110.10
18	b6	420	BCR	C28-C27-C26	-3.07	108.59	114.08
15	a5	406	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
15	c2	418	CLA	CHB-C4A-NA	3.07	128.76	124.51
15	c3	408	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
15	bJ	102	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
15	cA	844	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
15	a1	416	CLA	CHB-C4A-NA	3.07	128.75	124.51
15	c6	411	CLA	C2D-C1D-ND	-3.07	107.84	110.10
15	a6	406	CLA	CHD-C1D-ND	-3.07	121.64	124.45
15	a2	417	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
15	bB	813	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
15	b3	408	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
15	cB	809	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
15	c5	405	CLA	CMD-C2D-C1D	3.07	130.12	124.71
18	aA	852	BCR	C39-C30-C25	-3.06	105.33	110.30
15	aB	838	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
15	b4	402	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
15	c1	408	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
15	c1	412	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
15	a3	404	CLA	C1-C2-C3	-3.06	120.74	126.04
15	aA	807	CLA	CAA-C2A-C3A	-3.06	104.39	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	811	CLA	CMB-C2B-C3B	3.06	130.41	124.68
15	a1	422	CLA	CHB-C4A-NA	3.06	128.75	124.51
15	b5	413	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
15	bB	827	CLA	CHB-C4A-NA	3.06	128.75	124.51
15	cF	201	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
15	aJ	203	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
18	c5	419	BCR	C28-C27-C26	-3.06	108.61	114.08
15	b6	406	CLA	CHD-C1D-ND	-3.06	121.64	124.45
15	cB	820	CLA	CMB-C2B-C3B	3.06	130.40	124.68
15	b4	411	CLA	CHB-C4A-NA	3.06	128.74	124.51
15	cB	818	CLA	CHB-C4A-NA	3.06	128.74	124.51
15	b6	414	CLA	CHD-C1D-ND	-3.06	121.64	124.45
15	b3	405	CLA	CMD-C2D-C1D	3.06	130.10	124.71
15	b5	417	CLA	C2C-C1C-NC	-3.06	107.11	109.97
15	a4	421	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
15	c1	414	CLA	CMB-C2B-C3B	3.06	130.40	124.68
18	c3	418	BCR	C3-C4-C5	-3.06	108.62	114.08
15	b1	417	CLA	C2C-C1C-NC	-3.06	107.11	109.97
15	a6	404	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	bA	807	CLA	CAA-C2A-C3A	-3.05	104.41	112.78
15	cA	807	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
15	c5	403	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	b5	402	CLA	C1-C2-C3	-3.05	120.76	126.04
15	c3	404	CLA	C1-C2-C3	-3.05	120.76	126.04
15	c6	409	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
15	a6	406	CLA	CMD-C2D-C1D	3.05	130.09	124.71
15	bA	837	CLA	CHB-C4A-NA	3.05	128.73	124.51
15	cB	811	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
15	a4	405	CLA	CMD-C2D-C1D	3.05	130.09	124.71
15	cJ	102	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
15	cB	813	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	bB	818	CLA	CHB-C4A-NA	3.05	128.73	124.51
15	b6	404	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
15	cB	827	CLA	CHB-C4A-NA	3.05	128.73	124.51
15	bB	809	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
15	bA	835	CLA	C2D-C1D-ND	-3.05	107.86	110.10
15	a3	408	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	cA	848	BCR	C15-C16-C17	-3.04	117.24	123.47
18	c6	419	BCR	C3-C4-C5	-3.04	108.64	114.08
18	b4	419	BCR	C24-C23-C22	-3.04	121.64	126.23
18	aA	849	BCR	C15-C16-C17	-3.04	117.24	123.47
15	cA	828	CLA	O2D-CGD-O1D	-3.04	117.89	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	830	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	cB	847	BCR	C15-C16-C17	-3.04	117.24	123.47
15	cA	840	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
15	aB	826	CLA	CAA-C2A-C1A	-3.04	102.01	111.97
15	cA	830	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	aB	847	BCR	C15-C16-C17	-3.04	117.25	123.47
15	aB	820	CLA	CMB-C2B-C3B	3.04	130.37	124.68
15	bA	840	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
15	aA	842	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
15	aA	827	CLA	CAA-CBA-CGA	-3.04	104.37	113.25
18	b5	419	BCR	C28-C27-C26	-3.04	108.65	114.08
15	b6	414	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
15	aA	830	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
18	c6	420	BCR	C28-C27-C26	-3.04	108.66	114.08
15	a6	409	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
18	bA	850	BCR	C15-C16-C17	-3.04	117.25	123.47
15	bB	820	CLA	CMB-C2B-C3B	3.04	130.36	124.68
15	b5	403	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
15	cB	826	CLA	CAA-C2A-C1A	-3.03	102.03	111.97
15	bA	828	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
15	bA	826	CLA	CHB-C4A-NA	3.03	128.71	124.51
18	a4	419	BCR	C24-C23-C22	-3.03	121.65	126.23
15	aB	809	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
15	cA	827	CLA	CAA-CBA-CGA	-3.03	104.39	113.25
15	a2	418	CLA	C2C-C1C-NC	-3.03	107.13	109.97
15	b5	406	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
18	b1	419	BCR	C3-C4-C5	-3.03	108.67	114.08
18	b6	419	BCR	C3-C4-C5	-3.03	108.67	114.08
18	a5	419	BCR	C28-C27-C26	-3.03	108.67	114.08
15	b6	409	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
15	c5	406	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
15	bB	841	CLA	CMB-C2B-C3B	3.03	130.34	124.68
15	bA	827	CLA	CAA-CBA-CGA	-3.03	104.40	113.25
18	a6	420	BCR	C28-C27-C26	-3.03	108.67	114.08
15	b1	403	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
15	b1	417	CLA	CHB-C4A-NA	3.03	128.70	124.51
15	b5	416	CLA	CHB-C4A-NA	3.03	128.70	124.51
15	cB	841	CLA	CMB-C2B-C3B	3.03	130.34	124.68
15	a1	409	CLA	C2D-C1D-ND	-3.03	107.87	110.10
15	bB	826	CLA	CAA-C2A-C1A	-3.03	102.06	111.97
18	b4	418	BCR	C27-C26-C25	3.03	127.12	122.73
15	cB	803	CLA	C1B-CHB-C4A	-3.03	124.13	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	405	CLA	CMD-C2D-C1D	3.02	130.04	124.71
15	a5	403	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
15	aB	839	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
15	b2	411	CLA	C2D-C1D-ND	-3.02	107.88	110.10
15	b2	405	CLA	CMD-C2D-C1D	3.02	130.04	124.71
15	aA	831	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
15	cA	823	CLA	CMB-C2B-C3B	3.02	130.34	124.68
18	c4	418	BCR	C27-C26-C25	3.02	127.12	122.73
15	aB	803	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
15	bB	839	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
18	bB	844	BCR	C11-C10-C9	-3.02	123.00	127.31
15	c1	417	CLA	C2C-C1C-NC	-3.02	107.14	109.97
15	aB	841	CLA	CMB-C2B-C3B	3.02	130.33	124.68
18	a6	419	BCR	C3-C4-C5	-3.02	108.68	114.08
15	aA	828	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	a1	402	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	bA	831	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
15	c1	403	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	aA	826	CLA	CHB-C4A-NA	3.02	128.69	124.51
15	b5	415	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
15	aA	840	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
18	bB	847	BCR	C15-C16-C17	-3.02	117.30	123.47
15	cB	839	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
15	c1	412	CLA	CMC-C2C-C1C	-3.01	120.45	125.04
15	cA	831	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
18	aI	102	BCR	C2-C1-C6	3.01	115.12	110.48
15	cB	809	CLA	O2A-CGA-O1A	-3.01	115.99	123.59
15	c3	408	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
15	bB	803	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
15	bB	819	CLA	CHB-C4A-NA	3.01	128.68	124.51
15	bA	823	CLA	CMB-C2B-C3B	3.01	130.31	124.68
15	a1	407	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
15	c4	416	CLA	CHB-C4A-NA	3.01	128.67	124.51
15	b6	422	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
15	b1	408	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
15	c6	406	CLA	CMD-C2D-C1D	3.01	130.01	124.71
15	c4	421	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
15	a2	407	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	b2	415	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	a2	416	CLA	C2D-C1D-ND	-3.00	107.89	110.10
15	aL	202	CLA	O2D-CGD-CBD	3.00	116.60	111.27
15	a2	405	CLA	CMD-C2D-C1D	3.00	130.00	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	826	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	bA	810	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	c6	404	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	a1	409	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	aB	844	BCR	C15-C16-C17	-3.00	117.33	123.47
15	cJ	102	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	c5	416	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	aA	823	CLA	CMB-C2B-C3B	3.00	130.29	124.68
18	cB	844	BCR	C15-C16-C17	-3.00	117.33	123.47
18	c1	419	BCR	C2-C1-C6	3.00	115.10	110.48
18	cI	102	BCR	C2-C1-C6	3.00	115.10	110.48
18	bI	101	BCR	C2-C1-C6	3.00	115.09	110.48
18	c4	420	BCR	C15-C14-C13	-3.00	123.03	127.31
15	a5	416	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	b2	418	CLA	C2C-C1C-NC	-3.00	107.17	109.97
15	c3	415	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
15	b1	408	CLA	C2D-C1D-ND	-3.00	107.90	110.10
15	a6	422	CLA	C16-C15-C13	-3.00	106.23	115.92
15	bB	842	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
18	aI	101	BCR	C2-C1-C6	3.00	115.09	110.48
15	b6	406	CLA	CMD-C2D-C1D	2.99	129.99	124.71
18	a1	418	BCR	C2-C1-C6	2.99	115.09	110.48
15	aB	839	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	c5	417	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	cB	839	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	b6	414	CLA	C3C-C4C-NC	-2.99	107.22	110.57
15	cF	201	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
15	bA	818	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
15	bB	805	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	cX	102	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
15	cB	842	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
18	bB	844	BCR	C15-C16-C17	-2.99	117.35	123.47
15	aB	833	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	a4	411	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	bB	839	CLA	CHB-C4A-NA	2.99	128.64	124.51
15	b3	411	CLA	CHB-C4A-NA	2.99	128.64	124.51
15	aA	810	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	b3	408	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	b5	405	CLA	CHD-C1D-ND	-2.99	121.71	124.45
15	c2	407	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	cA	810	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	b3	404	CLA	C1-C2-C3	-2.99	120.88	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b4	405	CLA	C3C-C4C-NC	-2.99	107.22	110.57
15	a5	405	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	cA	849	BCR	C11-C10-C9	-2.98	123.05	127.31
18	a4	418	BCR	C27-C26-C25	2.98	127.06	122.73
15	bL	203	CLA	O2D-CGD-CBD	2.98	116.57	111.27
15	c5	405	CLA	CHD-C1D-ND	-2.98	121.71	124.45
15	cL	202	CLA	O2D-CGD-CBD	2.98	116.57	111.27
15	b4	404	CLA	C1-C2-C3	-2.98	120.88	126.04
15	aA	818	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
15	bX	102	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
18	cB	844	BCR	C11-C10-C9	-2.98	123.05	127.31
15	cB	817	CLA	CHB-C4A-NA	2.98	128.64	124.51
15	aA	802	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
15	aA	842	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
15	cB	819	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	aB	806	CLA	O2A-C1-C2	-2.98	100.80	108.64
15	aB	819	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	a3	408	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
18	cI	101	BCR	C2-C1-C6	2.98	115.06	110.48
15	cB	837	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
15	aB	842	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
15	b5	414	CLA	CAA-C2A-C3A	-2.98	109.15	116.10
15	cB	833	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	a1	406	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	b6	418	CLA	C2C-C1C-NC	-2.97	107.19	109.97
15	b4	402	CLA	C1-C2-C3	-2.97	120.90	126.04
15	aX	102	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
18	bI	102	BCR	C2-C1-C6	2.97	115.06	110.48
18	aB	844	BCR	C11-C10-C9	-2.97	123.06	127.31
15	a1	422	CLA	C6-C7-C8	-2.97	106.31	115.92
15	b1	406	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
15	c5	404	CLA	CMB-C2B-C3B	2.97	130.24	124.68
15	b3	415	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
18	b2	419	BCR	C27-C26-C25	2.97	127.05	122.73
15	bB	833	CLA	CHB-C4A-NA	2.97	128.62	124.51
15	c4	410	CLA	CMC-C2C-C3C	2.97	134.18	126.12
15	bB	806	CLA	O2A-C1-C2	-2.97	100.83	108.64
15	b2	416	CLA	C2D-C1D-ND	-2.97	107.92	110.10
15	aB	837	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
15	a5	408	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
18	bJ	103	BCR	C24-C23-C22	-2.97	121.75	126.23
15	b1	407	CLA	CHB-C4A-NA	2.97	128.62	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aJ	205	BCR	C15-C16-C17	-2.97	117.39	123.47
15	a1	416	CLA	C2C-C1C-NC	-2.97	107.19	109.97
18	cJ	104	BCR	C15-C16-C17	-2.97	117.40	123.47
15	b6	422	CLA	C6-C7-C8	-2.97	106.33	115.92
15	bB	837	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
15	cB	806	CLA	O2A-C1-C2	-2.97	100.84	108.64
15	a4	414	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	bB	817	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	b6	422	CLA	CHB-C4A-NA	2.96	128.61	124.51
15	b5	404	CLA	CMB-C2B-C3B	2.96	130.22	124.68
18	bA	851	BCR	C11-C10-C9	-2.96	123.08	127.31
15	cA	818	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
15	c2	418	CLA	C2C-C1C-NC	-2.96	107.19	109.97
15	b1	410	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	bJ	104	BCR	C15-C16-C17	-2.96	117.40	123.47
15	c2	415	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	b6	420	BCR	C15-C14-C13	-2.96	123.08	127.31
15	c3	404	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
15	b1	412	CLA	CMC-C2C-C1C	-2.96	120.53	125.04
15	cA	802	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
15	b1	416	CLA	C1-C2-C3	-2.96	121.96	126.75
18	c2	420	BCR	C24-C23-C22	-2.96	121.76	126.23
15	a2	415	CLA	CHB-C4A-NA	2.96	128.60	124.51
15	c6	414	CLA	CHD-C1D-ND	-2.96	121.73	124.45
14	bA	801	CL0	CAC-C3C-C4C	2.96	128.65	124.81
15	a6	422	CLA	C6-C5-C3	-2.96	105.69	113.45
15	a2	417	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
15	cB	805	CLA	CHB-C4A-NA	2.96	128.60	124.51
15	b4	405	CLA	CHD-C1D-ND	-2.96	121.74	124.45
18	aA	850	BCR	C11-C10-C9	-2.96	123.09	127.31
18	b1	419	BCR	C2-C1-C6	2.96	115.03	110.48
15	a4	402	CLA	C1-C2-C3	-2.96	120.93	126.04
15	bB	834	CLA	C2D-C1D-ND	-2.96	107.92	110.10
15	bB	814	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
15	b2	417	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
18	cI	102	BCR	C15-C16-C17	-2.96	117.42	123.47
15	c2	411	CLA	CMC-C2C-C3C	2.96	134.14	126.12
15	b1	412	CLA	CMB-C2B-C3B	2.96	130.21	124.68
18	a6	420	BCR	C15-C14-C13	-2.96	123.09	127.31
15	c2	410	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
15	aB	814	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
15	bA	842	CLA	CMB-C2B-C1B	-2.96	123.92	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c6	401	BCR	C24-C23-C22	-2.95	121.77	126.23
15	c4	421	CLA	CAA-CBA-CGA	-2.95	104.62	113.25
15	a5	404	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	a5	417	CLA	C2C-C1C-NC	-2.95	107.20	109.97
14	aA	801	CL0	CAC-C3C-C4C	2.95	128.64	124.81
15	a2	410	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
15	a1	405	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	cA	833	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	c6	405	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	c4	408	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
15	a4	421	CLA	C6-C7-C8	-2.95	106.38	115.92
15	bJ	102	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	aJ	203	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	b4	410	CLA	CMC-C2C-C3C	2.95	134.13	126.12
15	b4	416	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	b2	402	CLA	C1-C2-C3	-2.95	120.94	126.04
15	cA	812	CLA	CMB-C2B-C3B	2.95	130.20	124.68
15	b5	408	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
15	cB	829	CLA	C2D-C1D-ND	-2.95	107.93	110.10
15	a6	422	CLA	C6-C7-C8	-2.95	106.38	115.92
15	c4	411	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	aA	818	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
15	b4	412	CLA	CMC-C2C-C1C	-2.95	120.55	125.04
15	a5	404	CLA	CMB-C2B-C3B	2.95	130.19	124.68
16	bB	843	PQN	C14-C13-C15	2.95	120.23	115.27
15	a4	404	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
15	bA	833	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	bB	848	BCR	C3-C4-C5	-2.95	108.81	114.08
15	c4	421	CLA	C6-C7-C8	-2.95	106.39	115.92
15	aA	833	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	a6	403	CLA	C1-C2-C3	-2.95	120.95	126.04
15	cA	809	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
15	cA	818	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
15	b2	410	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
15	a3	414	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	bA	802	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	c6	403	CLA	C1-C2-C3	-2.95	120.95	126.04
18	aJ	204	BCR	C24-C23-C22	-2.95	121.78	126.23
18	c6	420	BCR	C15-C14-C13	-2.94	123.11	127.31
15	a5	404	CLA	CHB-C4A-NA	2.94	128.58	124.51
15	b5	405	CLA	C3C-C4C-NC	-2.94	107.27	110.57
15	b5	412	CLA	C1B-CHB-C4A	-2.94	124.29	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	409	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
18	a6	401	BCR	C24-C23-C22	-2.94	121.79	126.23
15	b4	421	CLA	C6-C7-C8	-2.94	106.41	115.92
18	cB	848	BCR	C3-C4-C5	-2.94	108.82	114.08
15	b2	407	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
15	a5	405	CLA	C3C-C4C-NC	-2.94	107.27	110.57
15	c5	414	CLA	CAA-C2A-C3A	-2.94	109.23	116.10
15	cB	817	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
15	b5	412	CLA	CMB-C2B-C3B	2.94	130.18	124.68
15	aA	812	CLA	CMB-C2B-C3B	2.94	130.18	124.68
15	a4	404	CLA	CMB-C2B-C3B	2.94	130.18	124.68
15	aA	826	CLA	C2A-C1A-CHA	2.94	129.00	123.86
18	a6	401	BCR	C15-C16-C17	-2.94	117.45	123.47
15	c1	410	CLA	CMC-C2C-C3C	2.94	134.09	126.12
15	aA	804	CLA	O2D-CGD-CBD	2.94	116.49	111.27
15	a5	412	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
15	a1	409	CLA	CMC-C2C-C3C	2.94	134.09	126.12
15	bA	818	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
15	cA	815	CLA	CMB-C2B-C3B	2.94	130.17	124.68
15	a6	422	CLA	CHB-C4A-NA	2.94	128.57	124.51
15	b1	410	CLA	CMC-C2C-C3C	2.94	134.09	126.12
15	aA	815	CLA	CMB-C2B-C3B	2.94	130.17	124.68
18	aI	102	BCR	C15-C16-C17	-2.94	117.46	123.47
15	cA	826	CLA	C2A-C1A-CHA	2.94	128.99	123.86
15	b5	417	CLA	CHB-C4A-NA	2.94	128.57	124.51
15	b2	411	CLA	CMC-C2C-C3C	2.94	134.09	126.12
18	b4	420	BCR	C15-C14-C13	-2.94	123.12	127.31
15	c4	402	CLA	C1-C2-C3	-2.93	120.97	126.04
15	bA	809	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
15	a4	416	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	a5	417	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	a2	411	CLA	CMC-C2C-C3C	2.93	134.08	126.12
15	a6	405	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	bA	812	CLA	CMB-C2B-C3B	2.93	130.17	124.68
16	aB	843	PQN	C14-C13-C15	2.93	120.21	115.27
14	cA	801	CL0	CAC-C3C-C4C	2.93	128.62	124.81
15	a2	412	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	a6	416	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	a1	415	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
15	cB	814	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	a3	414	CLA	CMB-C2B-C3B	2.93	130.16	124.68
15	b2	412	CLA	CHB-C4A-NA	2.93	128.57	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	827	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
15	c5	408	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
15	aA	824	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	c1	407	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	c2	412	CLA	CHB-C4A-NA	2.93	128.56	124.51
18	bJ	105	BCR	C15-C14-C13	-2.93	123.13	127.31
15	aA	809	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
15	a6	413	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
15	b4	414	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	a1	412	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
15	aB	817	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	aA	806	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
15	b6	403	CLA	C1-C2-C3	-2.93	120.98	126.04
15	a3	412	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
15	a3	417	CLA	C2C-C1C-NC	-2.93	107.23	109.97
15	bA	815	CLA	CMB-C2B-C3B	2.93	130.16	124.68
15	b6	405	CLA	CMB-C2B-C3B	2.93	130.16	124.68
15	cA	827	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
15	bA	806	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
15	c4	404	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	a4	410	CLA	CMC-C2C-C3C	2.93	134.06	126.12
15	c6	408	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	aB	805	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	a6	418	CLA	C2C-C1C-NC	-2.93	107.23	109.97
18	cJ	104	BCR	C11-C10-C9	-2.93	123.14	127.31
15	b4	421	CLA	CAA-CBA-CGA	-2.93	104.70	113.25
18	b1	419	BCR	C15-C16-C17	-2.93	117.48	123.47
15	a4	421	CLA	CAA-CBA-CGA	-2.92	104.71	113.25
15	a2	411	CLA	C2D-C1D-ND	-2.92	107.95	110.10
15	c2	422	CLA	CED-O2D-CGD	2.92	122.55	115.94
18	bI	102	BCR	C15-C16-C17	-2.92	117.48	123.47
15	a4	421	CLA	CHA-C1A-NA	-2.92	119.70	126.40
15	c4	404	CLA	C1-C2-C3	-2.92	120.99	126.04
15	a3	411	CLA	CHB-C4A-NA	2.92	128.56	124.51
15	a3	406	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
15	bA	826	CLA	C2A-C1A-CHA	2.92	128.97	123.86
15	b4	421	CLA	CHA-C1A-NA	-2.92	119.70	126.40
15	c6	416	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
18	a1	420	BCR	C24-C23-C22	-2.92	121.82	126.23
15	c1	410	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	c5	414	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	a5	414	CLA	CMB-C2B-C3B	2.92	130.15	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aF	203	BCR	C15-C14-C13	-2.92	123.14	127.31
15	c2	402	CLA	C1-C2-C3	-2.92	120.99	126.04
15	a6	405	CLA	CMB-C2B-C3B	2.92	130.14	124.68
18	aJ	205	BCR	C11-C10-C9	-2.92	123.14	127.31
15	bB	819	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
15	cA	806	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
15	a5	410	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	cA	819	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	b4	408	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
15	c4	414	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	b2	404	CLA	CMB-C2B-C3B	2.92	130.14	124.68
18	b4	418	BCR	C40-C30-C29	-2.92	97.23	108.91
15	b2	416	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
15	b3	416	CLA	C1-C2-C3	-2.92	122.03	126.75
15	b6	416	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
15	c3	404	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	c5	404	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
15	cA	824	CLA	CHB-C4A-NA	2.92	128.54	124.51
15	c6	409	CLA	C2D-C1D-ND	-2.92	107.95	110.10
15	a6	408	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
15	bB	817	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
15	cB	819	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
15	a4	405	CLA	C3C-C4C-NC	-2.91	107.30	110.57
15	a4	406	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
15	b1	415	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	bA	824	CLA	CHB-C4A-NA	2.91	128.54	124.51
15	b2	417	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
15	c6	413	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
15	bB	829	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	b6	409	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	c3	412	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
18	aB	848	BCR	C3-C4-C5	-2.91	108.88	114.08
18	cF	205	BCR	C15-C14-C13	-2.91	123.15	127.31
18	c1	419	BCR	C24-C23-C22	-2.91	121.83	126.23
15	c1	413	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
15	c4	407	CLA	CHB-C4A-NA	2.91	128.54	124.51
15	a2	409	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
18	a2	420	BCR	C24-C23-C22	-2.91	121.84	126.23
16	cB	843	PQN	C14-C13-C15	2.91	120.17	115.27
15	b5	414	CLA	CHB-C4A-NA	2.91	128.54	124.51
15	b3	412	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
15	b2	409	CLA	C1B-CHB-C4A	-2.91	124.35	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b4	404	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
15	c3	410	CLA	CMC-C2C-C3C	2.91	134.01	126.12
15	c2	417	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
18	a4	420	BCR	C15-C14-C13	-2.91	123.16	127.31
15	a5	414	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	b2	401	BCR	C1-C6-C5	-2.91	118.52	122.61
18	a4	418	BCR	C40-C30-C29	-2.91	97.28	108.91
15	b5	404	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
15	c4	412	CLA	CMC-C2C-C1C	-2.91	120.61	125.04
15	aB	819	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
15	b6	413	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
15	c4	421	CLA	CHA-C1A-NA	-2.91	119.74	126.40
15	b4	406	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
15	c2	404	CLA	C1-C2-C3	-2.91	121.02	126.04
15	aA	827	CLA	CAA-C2A-C1A	-2.91	102.45	111.97
15	a4	408	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
18	cJ	103	BCR	C24-C23-C22	-2.91	121.84	126.23
15	c1	410	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	a3	415	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
15	bA	819	CLA	CHB-C4A-NA	2.90	128.53	124.51
15	c5	412	CLA	CMB-C2B-C3B	2.90	130.11	124.68
15	cA	804	CLA	O2D-CGD-CBD	2.90	116.43	111.27
15	c6	405	CLA	CMB-C2B-C3B	2.90	130.11	124.68
15	b4	417	CLA	CHB-C4A-NA	2.90	128.53	124.51
15	c3	411	CLA	CHB-C4A-NA	2.90	128.53	124.51
15	b3	414	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
15	b4	404	CLA	CMB-C2B-C3B	2.90	130.11	124.68
15	a4	404	CLA	C1-C2-C3	-2.90	121.02	126.04
15	b6	408	CLA	CHB-C4A-NA	2.90	128.53	124.51
18	bJ	104	BCR	C11-C10-C9	-2.90	123.17	127.31
15	aA	813	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
15	a5	412	CLA	CMB-C2B-C3B	2.90	130.11	124.68
15	b2	405	CLA	CHD-C1D-ND	-2.90	121.79	124.45
15	c2	404	CLA	CMB-C2B-C3B	2.90	130.11	124.68
15	a2	406	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	a6	409	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	c5	412	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
15	aA	830	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	a2	404	CLA	CMB-C2B-C3B	2.90	130.10	124.68
15	b4	407	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c4	417	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c6	417	CLA	O2D-CGD-O1D	-2.90	118.17	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a6	414	CLA	CAC-C3C-C2C	-2.90	122.57	127.53
18	a1	418	BCR	C24-C23-C22	-2.90	121.86	126.23
15	cA	830	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	aL	202	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
15	c3	417	CLA	C2C-C1C-NC	-2.90	107.26	109.97
15	c3	416	CLA	C1-C2-C3	-2.90	122.06	126.75
15	a4	405	CLA	CHD-C1D-ND	-2.90	121.79	124.45
15	bA	804	CLA	O2D-CGD-CBD	2.90	116.42	111.27
15	b1	402	CLA	C1-C2-C3	-2.90	121.03	126.04
15	aB	829	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	c4	414	CLA	CAA-C2A-C3A	-2.90	109.34	116.10
15	bA	809	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
15	a1	414	CLA	C2D-C1D-ND	-2.90	107.97	110.10
18	c4	418	BCR	C40-C30-C29	-2.90	97.32	108.91
15	c1	408	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c3	408	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c5	404	CLA	CHB-C4A-NA	2.89	128.51	124.51
15	c2	416	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	a1	411	CLA	CMB-C2B-C3B	2.89	130.09	124.68
15	a2	405	CLA	C3C-C4C-NC	-2.89	107.33	110.57
15	c2	405	CLA	CHD-C1D-ND	-2.89	121.80	124.45
15	b6	417	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	bA	836	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
15	a4	412	CLA	CMB-C2B-C3B	2.89	130.09	124.68
18	c6	401	BCR	C15-C16-C17	-2.89	117.55	123.47
15	cA	813	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	a2	402	CLA	C1-C2-C3	-2.89	121.04	126.04
15	b1	404	CLA	C1-C2-C3	-2.89	121.04	126.04
15	a5	414	CLA	CAA-C2A-C3A	-2.89	109.35	116.10
15	c5	410	CLA	CMC-C2C-C3C	2.89	133.97	126.12
15	aB	817	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
15	bA	822	CLA	CHB-C4A-NA	2.89	128.51	124.51
15	b1	410	CLA	C2D-C1D-ND	-2.89	107.97	110.10
15	b1	413	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	a6	402	BCR	C7-C8-C9	-2.89	121.87	126.23
18	c2	401	BCR	C1-C6-C5	-2.89	118.54	122.61
18	b1	419	BCR	C24-C23-C22	-2.89	121.87	126.23
18	b2	420	BCR	C24-C23-C22	-2.89	121.87	126.23
15	aA	844	CLA	CMB-C2B-C3B	2.89	130.08	124.68
18	b6	401	BCR	C24-C23-C22	-2.89	121.87	126.23
15	b4	414	CLA	CAA-C2A-C3A	-2.89	109.36	116.10
15	c6	418	CLA	C2C-C1C-NC	-2.89	107.27	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	801	CL0	CMB-C2B-C3B	2.89	130.08	124.68
15	bA	838	CLA	CHB-C4A-NA	2.89	128.50	124.51
15	cA	822	CLA	CHB-C4A-NA	2.89	128.50	124.51
18	bI	102	BCR	C24-C23-C22	-2.89	121.87	126.23
15	bA	813	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
15	bB	830	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
15	a4	413	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
15	a5	405	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	b1	401	BCR	C15-C16-C17	-2.88	117.57	123.47
14	aA	801	CL0	CMB-C2B-C3B	2.88	130.07	124.68
18	a2	401	BCR	C1-C6-C5	-2.88	118.55	122.61
15	c4	405	CLA	C3C-C4C-NC	-2.88	107.34	110.57
15	b2	414	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
15	a3	416	CLA	C1-C2-C3	-2.88	122.09	126.75
15	b5	404	CLA	CHB-C4A-NA	2.88	128.50	124.51
15	c3	412	CLA	CMB-C2B-C3B	2.88	130.07	124.68
18	aA	849	BCR	C3-C4-C5	-2.88	108.93	114.08
15	cB	816	CLA	O2D-CGD-CBD	2.88	116.39	111.27
18	b6	401	BCR	C15-C16-C17	-2.88	117.57	123.47
15	a1	406	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
15	b6	422	CLA	CAA-CBA-CGA	-2.88	104.83	113.25
15	b3	408	CLA	CHB-C4A-NA	2.88	128.50	124.51
15	cA	838	CLA	CHB-C4A-NA	2.88	128.50	124.51
15	aA	816	CLA	CHB-C4A-NA	2.88	128.49	124.51
15	b6	409	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
15	a2	416	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
15	aB	834	CLA	C2D-C1D-ND	-2.88	107.98	110.10
18	cJ	104	BCR	C27-C26-C25	2.88	126.91	122.73
18	aI	102	BCR	C24-C23-C22	-2.88	121.89	126.23
15	a4	412	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
15	cA	836	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
18	a1	420	BCR	C15-C16-C17	-2.88	117.58	123.47
15	aA	843	CLA	CHB-C4A-NA	2.88	128.49	124.51
15	c6	405	CLA	C1-C2-C3	-2.88	121.07	126.04
15	bL	203	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
15	bK	101	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	a4	412	CLA	CMC-C2C-C1C	-2.87	120.66	125.04
15	b6	405	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	cB	801	CLA	CMB-C2B-C3B	2.87	130.06	124.68
15	b4	421	CLA	CHB-C4A-NA	2.87	128.49	124.51
15	cA	809	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
15	b4	413	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b6	415	CLA	CMB-C2B-C3B	2.87	130.05	124.68
15	a1	415	CLA	C1-C2-C3	-2.87	122.10	126.75
15	a4	414	CLA	CAA-C2A-C3A	-2.87	109.39	116.10
15	b3	414	CLA	CMB-C2B-C3B	2.87	130.05	124.68
15	cB	830	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
15	b3	406	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	aB	816	CLA	O2D-CGD-CBD	2.87	116.37	111.27
15	a2	404	CLA	C1-C2-C3	-2.87	121.08	126.04
15	b2	405	CLA	C3C-C4C-NC	-2.87	107.35	110.57
15	cB	804	CLA	CBC-CAC-C3C	2.87	120.35	112.43
15	aA	804	CLA	CHB-C4A-NA	2.87	128.48	124.51
15	a6	415	CLA	CMB-C2B-C3B	2.87	130.05	124.68
15	c3	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	b3	417	CLA	C2C-C1C-NC	-2.87	107.28	109.97
15	aB	801	CLA	CMB-C2B-C3B	2.87	130.05	124.68
18	a2	419	BCR	C40-C30-C29	-2.87	97.43	108.91
18	b3	418	BCR	C27-C26-C25	2.87	126.90	122.73
15	c2	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	c2	417	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
15	a3	402	CLA	C1-C2-C3	-2.87	121.08	126.04
15	a1	403	CLA	C1-C2-C3	-2.87	121.08	126.04
15	c5	410	CLA	CHB-C4A-NA	2.87	128.48	124.51
15	aA	836	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
15	aA	841	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	c4	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	b3	410	CLA	CMC-C2C-C3C	2.87	133.90	126.12
16	cB	843	PQN	C16-C17-C18	-2.87	106.65	115.92
15	cA	842	CLA	CHB-C4A-NA	2.87	128.48	124.51
15	b4	412	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
18	b2	401	BCR	C15-C16-C17	-2.87	117.60	123.47
15	bB	804	CLA	CBC-CAC-C3C	2.87	120.33	112.43
15	bA	830	CLA	C2D-C1D-ND	-2.87	107.99	110.10
15	cA	843	CLA	CMB-C2B-C3B	2.87	130.04	124.68
16	bB	843	PQN	C16-C17-C18	-2.87	106.66	115.92
15	cB	832	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
15	a1	407	CLA	CHB-C4A-NA	2.87	128.47	124.51
15	c3	414	CLA	CHB-C4A-NA	2.87	128.47	124.51
18	b6	402	BCR	C7-C8-C9	-2.86	121.91	126.23
18	bB	845	BCR	C28-C27-C26	-2.86	108.96	114.08
15	bA	820	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	cL	202	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
15	a6	417	CLA	O2D-CGD-O1D	-2.86	118.24	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a3	418	BCR	C27-C26-C25	2.86	126.89	122.73
15	aB	804	CLA	CBC-CAC-C3C	2.86	120.33	112.43
18	aJ	205	BCR	C27-C26-C25	2.86	126.89	122.73
15	c2	405	CLA	C3C-C4C-NC	-2.86	107.36	110.57
15	b6	408	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	cB	820	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	bJ	104	BCR	C27-C26-C25	2.86	126.89	122.73
15	bB	811	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
15	c3	403	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	b3	403	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	c6	402	BCR	C7-C8-C9	-2.86	121.91	126.23
15	aB	811	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
15	aK	102	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	c1	406	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	b6	419	BCR	C27-C26-C25	2.86	126.89	122.73
15	b3	417	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	aA	809	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
15	c3	414	CLA	CAA-C2A-C3A	-2.86	109.42	116.10
16	aB	843	PQN	C16-C17-C18	-2.86	106.67	115.92
15	bB	801	CLA	CMB-C2B-C3B	2.86	130.03	124.68
18	b4	420	BCR	C35-C13-C14	-2.86	118.92	122.92
15	c5	414	CLA	CMB-C2B-C3B	2.86	130.03	124.68
15	b5	414	CLA	CMB-C2B-C3B	2.86	130.03	124.68
15	a4	417	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	a6	408	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	cK	102	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	cA	801	CL0	CMB-C2B-C3B	2.86	130.03	124.68
15	c4	411	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
15	aB	815	CLA	CHB-C4A-NA	2.86	128.46	124.51
18	cB	845	BCR	C28-C27-C26	-2.86	108.97	114.08
18	a1	418	BCR	C15-C16-C17	-2.86	117.62	123.47
15	b1	408	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	b3	407	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	cA	816	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	a1	415	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
15	b2	413	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
15	b5	410	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	cB	811	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
15	c4	412	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
15	bA	844	CLA	CMB-C2B-C3B	2.86	130.02	124.68
15	a6	409	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
15	cB	818	CLA	O2D-CGD-O1D	-2.86	118.25	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c2	419	BCR	C40-C30-C29	-2.86	97.48	108.91
15	c3	410	CLA	CAC-C3C-C2C	2.86	132.41	127.53
18	a1	421	BCR	C15-C16-C17	-2.86	117.62	123.47
18	a6	421	BCR	C15-C16-C17	-2.86	117.62	123.47
15	a3	412	CLA	CMB-C2B-C3B	2.86	130.02	124.68
18	bA	850	BCR	C3-C4-C5	-2.86	108.98	114.08
15	cB	822	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	c1	407	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	c2	406	CLA	C6-C7-C8	-2.85	106.69	115.92
15	c6	415	CLA	CMB-C2B-C3B	2.85	130.02	124.68
15	a2	417	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
18	c1	401	BCR	C15-C16-C17	-2.85	117.63	123.47
18	b3	419	BCR	C24-C23-C22	-2.85	121.92	126.23
18	aB	845	BCR	C28-C27-C26	-2.85	108.98	114.08
15	a2	405	CLA	CHD-C1D-ND	-2.85	121.83	124.45
15	c3	405	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	a3	419	BCR	C24-C23-C22	-2.85	121.92	126.23
18	a6	419	BCR	C27-C26-C25	2.85	126.87	122.73
18	c1	419	BCR	C15-C16-C17	-2.85	117.63	123.47
18	b1	401	BCR	C24-C23-C22	-2.85	121.92	126.23
15	c3	417	CLA	CHB-C4A-NA	2.85	128.46	124.51
15	bB	816	CLA	O2D-CGD-CBD	2.85	116.34	111.27
15	c4	404	CLA	CMB-C2B-C3B	2.85	130.01	124.68
15	bA	816	CLA	CHB-C4A-NA	2.85	128.46	124.51
15	cA	804	CLA	CHB-C4A-NA	2.85	128.46	124.51
15	c3	409	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
15	c4	408	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	bB	822	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	cA	848	BCR	C3-C4-C5	-2.85	108.99	114.08
15	c5	405	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	bB	832	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
15	b2	413	CLA	C2D-C1D-ND	-2.85	108.00	110.10
15	aA	822	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c1	402	CLA	C1-C2-C3	-2.85	121.12	126.04
18	c6	419	BCR	C27-C26-C25	2.85	126.87	122.73
18	cB	845	BCR	C30-C25-C26	-2.85	118.60	122.61
18	cF	204	BCR	C30-C25-C26	-2.85	118.60	122.61
15	cA	826	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
15	c5	405	CLA	C3C-C4C-NC	-2.85	107.38	110.57
15	cA	841	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	bL	206	BCR	C3-C4-C5	-2.85	108.99	114.08
15	bA	843	CLA	CHB-C4A-NA	2.85	128.45	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	405	CLA	CHD-C1D-ND	-2.85	121.84	124.45
15	a3	417	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c1	404	CLA	C1-C2-C3	-2.85	121.12	126.04
18	b4	419	BCR	C15-C14-C13	-2.85	123.25	127.31
15	a5	410	CLA	CMC-C2C-C3C	2.85	133.84	126.12
15	b3	404	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c6	417	CLA	C1-C2-C3	-2.85	122.15	126.75
15	a1	411	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	b2	417	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
15	b1	411	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	c4	419	BCR	C15-C14-C13	-2.85	123.25	127.31
15	aL	201	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
15	c2	413	CLA	C1B-CHB-C4A	-2.84	124.48	130.12
15	aB	832	CLA	C1B-CHB-C4A	-2.84	124.48	130.12
15	aB	822	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a2	406	CLA	C6-C7-C8	-2.84	106.73	115.92
18	c3	419	BCR	C24-C23-C22	-2.84	121.94	126.23
15	b2	406	CLA	C6-C7-C8	-2.84	106.73	115.92
15	a4	407	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	b2	419	BCR	C40-C30-C29	-2.84	97.53	108.91
18	a2	419	BCR	C27-C26-C25	2.84	126.86	122.73
15	c2	409	CLA	C2D-C1D-ND	-2.84	108.01	110.10
15	b2	409	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a2	413	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
15	bL	202	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
18	a5	418	BCR	C3-C4-C5	-2.84	109.00	114.08
15	aB	818	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	c2	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	aB	848	BCR	C15-C14-C13	-2.84	123.25	127.31
15	bA	804	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	c4	421	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	c6	418	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a1	401	CLA	C1-C2-C3	-2.84	121.13	126.04
15	b3	402	CLA	C1-C2-C3	-2.84	121.13	126.04
15	a2	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	c3	414	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	cB	811	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
15	aB	830	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
15	aA	819	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a3	410	CLA	CMC-C2C-C3C	2.84	133.83	126.12
15	c6	408	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	b2	422	CLA	CED-O2D-CGD	2.84	122.36	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	405	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	bB	820	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	c2	414	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	cB	826	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
15	c1	410	CLA	CAC-C3C-C2C	2.84	132.38	127.53
15	cB	834	CLA	C2D-C1D-ND	-2.84	108.01	110.10
15	aA	826	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
15	bA	841	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	a1	411	CLA	C2D-C1D-ND	-2.84	108.01	110.10
15	b4	412	CLA	CMB-C2B-C3B	2.84	129.99	124.68
15	b1	407	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	aA	838	CLA	CHB-C4A-NA	2.84	128.43	124.51
15	a3	409	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
15	b5	410	CLA	CMC-C2C-C3C	2.83	133.81	126.12
18	cI	102	BCR	C24-C23-C22	-2.83	121.95	126.23
15	b1	416	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
15	bA	824	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	c1	416	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
15	cB	815	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	c2	409	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	c5	411	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	aA	824	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	b3	405	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	c4	412	CLA	CMB-C2B-C3B	2.83	129.98	124.68
15	c4	413	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	b4	403	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	bA	826	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
15	c6	411	CLA	CMC-C2C-C3C	2.83	133.80	126.12
15	aB	820	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	c1	415	CLA	C2D-C1D-ND	-2.83	108.02	110.10
15	b6	405	CLA	C1-C2-C3	-2.83	121.15	126.04
15	bA	825	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	c1	411	CLA	CHB-C4A-NA	2.83	128.42	124.51
18	c5	418	BCR	C40-C30-C29	-2.83	97.59	108.91
15	c3	402	CLA	C1-C2-C3	-2.83	121.15	126.04
15	b2	406	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	c5	402	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	c5	420	CLA	C16-C15-C13	-2.83	106.78	115.92
18	c2	401	BCR	C35-C13-C14	-2.83	118.96	122.92
15	a5	411	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	c1	412	CLA	CMB-C2B-C3B	2.83	129.97	124.68
15	b3	409	CLA	C1B-CHB-C4A	-2.83	124.52	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	408	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	c3	407	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	b2	404	CLA	C1-C2-C3	-2.83	121.15	126.04
15	aB	811	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
15	aA	820	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	b3	414	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	c2	413	CLA	CMB-C2B-C3B	2.83	129.97	124.68
15	aA	809	CLA	O2D-CGD-CBD	2.83	116.29	111.27
15	bB	815	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	a6	405	CLA	C1-C2-C3	-2.83	121.16	126.04
15	cL	201	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
15	a5	402	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
18	bL	201	BCR	C3-C4-C5	-2.82	109.03	114.08
15	a3	407	CLA	CHB-C4A-NA	2.82	128.42	124.51
15	b2	406	CLA	CHB-C4A-NA	2.82	128.42	124.51
15	aB	826	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
15	cA	824	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	c5	418	BCR	C3-C4-C5	-2.82	109.04	114.08
15	aA	824	CLA	CMB-C2B-C3B	2.82	129.96	124.68
15	aA	825	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	a4	419	BCR	C15-C14-C13	-2.82	123.28	127.31
15	c6	409	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	c2	419	BCR	C27-C26-C25	2.82	126.83	122.73
15	a5	420	CLA	C16-C15-C13	-2.82	106.80	115.92
18	c1	401	BCR	C24-C23-C22	-2.82	121.97	126.23
15	bB	834	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	cA	825	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	c1	412	CLA	C2D-C1D-ND	-2.82	108.03	110.10
15	aA	806	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
18	bB	846	BCR	C15-C14-C13	-2.82	123.29	127.31
15	bB	809	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	bB	811	CLA	O2A-CGA-O1A	-2.82	116.48	123.59
15	b2	402	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
15	a4	421	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	b6	409	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	b3	405	CLA	CHD-C1D-ND	-2.82	121.86	124.45
15	c3	416	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
15	cA	821	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	cJ	103	BCR	C35-C13-C14	-2.82	118.98	122.92
18	bF	202	BCR	C30-C25-C26	-2.82	118.65	122.61
15	bB	818	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
15	b3	412	CLA	CMB-C2B-C3B	2.82	129.94	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c3	401	BCR	C15-C16-C17	-2.81	117.71	123.47
18	bB	848	BCR	C15-C14-C13	-2.81	123.29	127.31
15	b5	404	CLA	C1-C2-C3	-2.81	121.17	126.04
18	aF	202	BCR	C30-C25-C26	-2.81	118.65	122.61
15	c6	405	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	aJ	204	BCR	C35-C13-C14	-2.81	118.98	122.92
15	a6	411	CLA	CMC-C2C-C3C	2.81	133.76	126.12
15	b6	411	CLA	CMC-C2C-C3C	2.81	133.76	126.12
15	bL	203	CLA	CHD-C1D-ND	-2.81	121.87	124.45
15	b4	408	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	aA	837	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
15	a1	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	a6	409	CLA	CHB-C4A-NA	2.81	128.40	124.51
15	c3	414	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	bL	205	BCR	C15-C14-C13	-2.81	123.30	127.31
18	cB	846	BCR	C15-C14-C13	-2.81	123.30	127.31
15	c2	413	CLA	C2D-C1D-ND	-2.81	108.03	110.10
15	a2	406	CLA	CHB-C4A-NA	2.81	128.40	124.51
15	cA	820	CLA	CHB-C4A-NA	2.81	128.40	124.51
15	cA	837	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
18	a2	401	BCR	C35-C13-C14	-2.81	118.99	122.92
15	cA	809	CLA	O2D-CGD-CBD	2.81	116.26	111.27
15	a4	408	CLA	C2D-C1D-ND	-2.81	108.03	110.10
15	a3	416	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
15	c3	405	CLA	C3C-C4C-NC	-2.81	107.42	110.57
15	a4	403	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	a3	404	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	a5	418	BCR	C40-C30-C29	-2.81	97.67	108.91
18	aL	205	BCR	C3-C4-C5	-2.81	109.06	114.08
18	c3	418	BCR	C40-C30-C29	-2.81	97.67	108.91
15	aL	201	CLA	CMB-C2B-C3B	2.81	129.93	124.68
15	a2	413	CLA	CMB-C2B-C3B	2.81	129.93	124.68
15	cL	201	CLA	CMB-C2B-C3B	2.81	129.93	124.68
15	a2	414	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
15	a2	409	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	bJ	103	BCR	C35-C13-C14	-2.81	118.99	122.92
18	cL	204	BCR	C15-C14-C13	-2.81	123.30	127.31
15	a6	417	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
15	c6	417	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
15	a6	422	CLA	CHA-C1A-NA	-2.81	119.97	126.40
15	a6	412	CLA	CHB-C4A-NA	2.81	128.39	124.51
15	b3	416	CLA	CHC-C1C-C2C	-2.81	118.96	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	409	CLA	C2D-C1D-ND	-2.81	108.04	110.10
18	c2	401	BCR	C15-C16-C17	-2.81	117.73	123.47
15	b6	417	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
15	cB	814	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
18	b2	401	BCR	C35-C13-C14	-2.81	118.99	122.92
15	bB	824	CLA	CHD-C1D-ND	-2.81	121.88	124.45
18	a1	417	BCR	C40-C30-C29	-2.81	97.69	108.91
15	a1	405	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
15	a3	405	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	a3	405	CLA	C3C-C4C-NC	-2.80	107.43	110.57
15	bA	824	CLA	CMB-C2B-C3B	2.80	129.92	124.68
18	b3	418	BCR	C40-C30-C29	-2.80	97.69	108.91
18	cB	849	BCR	C27-C26-C25	2.80	126.80	122.73
15	cL	202	CLA	CHD-C1D-ND	-2.80	121.88	124.45
15	a4	416	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
15	b3	406	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
15	b1	404	CLA	CHB-C4A-NA	2.80	128.39	124.51
15	b6	417	CLA	C1-C2-C3	-2.80	122.22	126.75
18	aJ	204	BCR	C7-C8-C9	-2.80	122.00	126.23
15	bB	826	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
15	a1	413	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	a2	406	CLA	CMB-C2B-C3B	2.80	129.91	124.68
15	a3	403	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
15	a3	414	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	cB	809	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	bA	820	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
15	cA	806	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
18	a4	418	BCR	C3-C4-C5	-2.80	109.08	114.08
15	bA	845	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	b5	402	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
15	a6	417	CLA	C1-C2-C3	-2.80	122.23	126.75
18	cA	848	BCR	C40-C30-C25	2.80	114.84	110.30
18	b5	418	BCR	C40-C30-C29	-2.80	97.72	108.91
18	bB	850	BCR	C27-C26-C25	2.80	126.79	122.73
18	b6	419	BCR	C40-C30-C29	-2.80	97.72	108.91
15	c6	415	CLA	CHB-C4A-NA	2.80	128.38	124.51
18	a2	401	BCR	C15-C16-C17	-2.80	117.75	123.47
15	a5	408	CLA	CHB-C4A-NA	2.79	128.38	124.51
15	c6	412	CLA	CHB-C4A-NA	2.79	128.38	124.51
18	cF	204	BCR	C35-C13-C14	-2.79	119.01	122.92
15	b1	412	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
15	aA	821	CLA	CHB-C4A-NA	2.79	128.38	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	824	CLA	CMB-C2B-C3B	2.79	129.91	124.68
18	a3	418	BCR	C40-C30-C29	-2.79	97.73	108.91
18	a1	420	BCR	C34-C9-C8	-2.79	113.67	118.08
15	b2	413	CLA	CMB-C2B-C3B	2.79	129.91	124.68
15	c1	414	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	aA	849	BCR	C27-C26-C25	2.79	126.79	122.73
15	b6	405	CLA	CHB-C4A-NA	2.79	128.38	124.51
15	aB	840	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
15	c3	411	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	a3	420	BCR	C15-C14-C13	-2.79	123.32	127.31
15	bB	834	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
18	aB	845	BCR	C30-C25-C26	-2.79	118.68	122.61
15	a4	407	CLA	C2A-C1A-CHA	2.79	128.74	123.86
15	c4	416	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
15	bA	809	CLA	O2D-CGD-CBD	2.79	116.23	111.27
15	bA	806	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
15	b5	420	CLA	C16-C15-C13	-2.79	106.89	115.92
18	aB	849	BCR	C27-C26-C25	2.79	126.78	122.73
15	aA	820	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
18	c3	419	BCR	C15-C16-C17	-2.79	117.76	123.47
18	c4	418	BCR	C3-C4-C5	-2.79	109.09	114.08
15	cB	840	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
15	c2	406	CLA	CMB-C2B-C3B	2.79	129.90	124.68
18	bB	848	BCR	C27-C26-C25	2.79	126.78	122.73
15	b6	407	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
15	b4	416	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
15	aB	809	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	c2	406	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	c1	412	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	cJ	103	BCR	C7-C8-C9	-2.79	122.02	126.23
18	bB	845	BCR	C30-C25-C26	-2.79	118.69	122.61
19	bA	854	LHG	O8-C23-C24	2.79	120.66	111.91
15	bB	814	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
18	c4	420	BCR	C35-C13-C14	-2.79	119.02	122.92
18	bA	850	BCR	C27-C26-C25	2.79	126.78	122.73
15	bA	837	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
15	b3	414	CLA	CAA-C2A-C3A	-2.79	109.59	116.10
19	cA	852	LHG	O8-C23-C24	2.79	120.65	111.91
15	c6	417	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
15	aA	845	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	b6	418	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	b2	406	CLA	CGD-CBD-CAD	-2.79	101.71	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	814	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
18	aA	849	BCR	C40-C30-C25	2.79	114.82	110.30
15	aB	834	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
18	a6	419	BCR	C40-C30-C29	-2.79	97.77	108.91
15	c4	403	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
15	bL	202	CLA	CMB-C2B-C3B	2.78	129.89	124.68
15	b1	406	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
18	a4	420	BCR	C35-C13-C14	-2.78	119.02	122.92
15	bA	825	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
18	bA	850	BCR	C40-C30-C25	2.78	114.81	110.30
15	aB	834	CLA	CHB-C4A-NA	2.78	128.36	124.51
15	cB	834	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
19	aA	853	LHG	O8-C23-C24	2.78	120.64	111.91
20	cB	850	LMG	C40-C39-C38	-2.78	100.30	114.42
15	b1	402	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
15	a3	404	CLA	CMB-C2B-C3B	2.78	129.88	124.68
15	b3	404	CLA	CMB-C2B-C3B	2.78	129.88	124.68
18	b6	421	BCR	C15-C16-C17	-2.78	117.78	123.47
15	a6	407	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
18	bJ	103	BCR	C7-C8-C9	-2.78	122.03	126.23
15	c1	406	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
15	a3	414	CLA	CAA-C2A-C3A	-2.78	109.61	116.10
18	c3	418	BCR	C27-C26-C25	2.78	126.77	122.73
15	bA	821	CLA	CHB-C4A-NA	2.78	128.36	124.51
15	cB	834	CLA	CHB-C4A-NA	2.78	128.36	124.51
18	c6	419	BCR	C40-C30-C29	-2.78	97.79	108.91
15	aB	820	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
15	a3	416	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
15	a2	413	CLA	C2D-C1D-ND	-2.78	108.06	110.10
14	bA	801	CL0	CHB-C4A-NA	2.78	128.35	124.51
15	a1	410	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	a3	406	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
15	aA	811	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
15	bA	831	CLA	C2D-C1D-ND	-2.78	108.06	110.10
15	c6	409	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	bB	840	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
18	b4	419	BCR	C11-C10-C9	-2.78	123.35	127.31
18	cA	848	BCR	C27-C26-C25	2.78	126.76	122.73
15	c5	416	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
15	aB	841	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	bB	808	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	c1	404	CLA	CHB-C4A-NA	2.78	128.35	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	825	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
15	b1	405	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
15	b5	416	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
15	a3	421	CLA	C6-C7-C8	-2.78	106.95	115.92
18	c4	419	BCR	C15-C16-C17	-2.78	117.79	123.47
15	aA	803	CLA	CAA-CBA-CGA	-2.77	105.14	113.25
15	b5	411	CLA	CHB-C4A-NA	2.77	128.35	124.51
15	bB	820	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
15	c4	406	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
15	b5	408	CLA	CHB-C4A-NA	2.77	128.35	124.51
15	bB	836	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
18	c5	418	BCR	C27-C26-C25	2.77	126.76	122.73
15	c2	406	CLA	CGD-CBD-CAD	-2.77	101.75	110.73
15	a5	404	CLA	C1-C2-C3	-2.77	121.25	126.04
15	a4	406	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
15	cA	820	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
15	a2	422	CLA	CED-O2D-CGD	2.77	122.21	115.94
15	b2	407	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
18	aB	846	BCR	C15-C14-C13	-2.77	123.35	127.31
15	b3	421	CLA	C6-C7-C8	-2.77	106.96	115.92
15	a2	406	CLA	CGD-CBD-CAD	-2.77	101.75	110.73
15	a5	416	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
15	b4	411	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	bB	816	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
15	bA	817	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	a1	422	CLA	CGD-CBD-CAD	-2.77	101.76	110.73
15	aB	836	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
14	cA	801	CL0	CHB-C4A-NA	2.77	128.34	124.51
15	a3	409	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	cA	803	CLA	CAA-CBA-CGA	-2.77	105.16	113.25
18	b3	420	BCR	C15-C14-C13	-2.77	123.36	127.31
15	a5	407	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	a5	414	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	c1	405	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	b1	418	BCR	C40-C30-C29	-2.77	97.83	108.91
20	aB	850	LMG	C40-C39-C38	-2.77	100.37	114.42
20	bB	851	LMG	C40-C39-C38	-2.77	100.37	114.42
18	cB	848	BCR	C15-C14-C13	-2.77	123.36	127.31
15	c1	402	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
15	c6	407	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
15	b2	406	CLA	CMB-C2B-C3B	2.77	129.85	124.68
18	b4	418	BCR	C3-C4-C5	-2.77	109.14	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b5	418	BCR	C27-C26-C25	2.77	126.75	122.73
18	cB	846	BCR	C27-C26-C25	2.77	126.75	122.73
15	a6	415	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	bA	803	CLA	CAA-CBA-CGA	-2.77	105.17	113.25
15	a3	410	CLA	CAC-C3C-C2C	2.76	132.26	127.53
15	cB	841	CLA	CHB-C4A-NA	2.76	128.34	124.51
15	cB	816	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
18	aI	103	BCR	C15-C14-C13	-2.76	123.36	127.31
18	a4	419	BCR	C11-C10-C9	-2.76	123.36	127.31
18	bF	202	BCR	C35-C13-C14	-2.76	119.05	122.92
15	aB	824	CLA	CHD-C1D-ND	-2.76	121.91	124.45
18	aB	846	BCR	C40-C30-C25	2.76	114.78	110.30
18	c1	418	BCR	C40-C30-C29	-2.76	97.85	108.91
18	a3	401	BCR	C15-C16-C17	-2.76	117.81	123.47
18	b2	421	BCR	C15-C14-C13	-2.76	123.37	127.31
15	b6	412	CLA	CHB-C4A-NA	2.76	128.33	124.51
15	cB	808	CLA	CHB-C4A-NA	2.76	128.33	124.51
15	c2	422	CLA	C6-C7-C8	-2.76	106.99	115.92
15	b3	405	CLA	C3C-C4C-NC	-2.76	107.47	110.57
15	cB	820	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
15	c3	416	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
15	aA	817	CLA	CHB-C4A-NA	2.76	128.33	124.51
15	cA	811	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	a6	418	CLA	C3A-C2A-C1A	2.76	105.47	101.34
18	aB	848	BCR	C27-C26-C25	2.76	126.74	122.73
18	aF	203	BCR	C7-C8-C9	-2.76	122.06	126.23
15	a6	418	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	cB	846	BCR	C40-C30-C25	2.76	114.78	110.30
18	c6	402	BCR	C15-C14-C13	-2.76	123.37	127.31
18	b3	401	BCR	C15-C16-C17	-2.76	117.82	123.47
15	aA	804	CLA	CMB-C2B-C3B	2.76	129.84	124.68
15	aB	811	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	a4	408	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	b3	416	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
15	cB	836	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
15	b3	421	CLA	C6-C5-C3	-2.76	106.22	113.45
15	aA	840	CLA	O2D-CGD-CBD	2.76	116.17	111.27
15	a5	416	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	b5	414	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	cA	829	CLA	O2D-CGD-CBD	2.76	116.17	111.27
15	c4	409	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
19	cA	852	LHG	C20-C19-C18	-2.76	100.43	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	411	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
15	cB	824	CLA	CHD-C1D-ND	-2.76	121.92	124.45
15	aB	808	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	b4	408	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	b6	415	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	cA	844	CLA	CHB-C4A-NA	2.76	128.32	124.51
18	bJ	105	BCR	C7-C8-C9	-2.76	122.07	126.23
19	aA	853	LHG	C20-C19-C18	-2.76	100.44	114.42
15	cA	817	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	aA	829	CLA	O2D-CGD-CBD	2.75	116.16	111.27
15	c4	412	CLA	C2D-C1D-ND	-2.75	108.07	110.10
15	bB	841	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	b3	401	BCR	C15-C14-C13	-2.75	123.38	127.31
15	aB	816	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
15	b4	412	CLA	C2D-C1D-ND	-2.75	108.08	110.10
15	aJ	202	CLA	CMB-C2B-C3B	2.75	129.83	124.68
15	cA	825	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
18	aF	202	BCR	C35-C13-C14	-2.75	119.07	122.92
15	a5	407	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	b2	409	CLA	C2D-C1D-ND	-2.75	108.08	110.10
15	bA	829	CLA	O2D-CGD-CBD	2.75	116.16	111.27
18	a2	421	BCR	C15-C14-C13	-2.75	123.38	127.31
18	c3	420	BCR	C15-C14-C13	-2.75	123.38	127.31
15	a6	405	CLA	CHB-C4A-NA	2.75	128.32	124.51
15	a1	415	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	b5	408	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	b1	420	BCR	C35-C13-C14	-2.75	119.07	122.92
15	cA	832	CLA	CHB-C4A-NA	2.75	128.31	124.51
15	cA	841	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	b3	401	BCR	C7-C8-C9	-2.75	122.08	126.23
15	c1	416	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
15	c2	407	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
15	bB	811	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	b5	416	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	c4	419	BCR	C11-C10-C9	-2.75	123.39	127.31
15	aA	832	CLA	CHB-C4A-NA	2.75	128.31	124.51
15	aA	841	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	bB	846	BCR	C27-C26-C25	2.75	126.72	122.73
15	aA	837	CLA	CMB-C2B-C3B	2.75	129.82	124.68
15	a4	405	CLA	CHD-C1D-C2D	2.75	131.24	125.48
15	cB	811	CLA	C2A-C1A-CHA	2.75	128.66	123.86
18	cF	204	BCR	C27-C26-C25	2.75	126.72	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a4	419	BCR	C15-C16-C17	-2.75	117.85	123.47
15	a2	404	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	aA	801	CL0	CHB-C4A-NA	2.75	128.31	124.51
15	c5	409	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
15	bA	837	CLA	CMB-C2B-C3B	2.74	129.81	124.68
15	a1	401	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
15	b2	417	CLA	C1-C2-C3	-2.74	122.31	126.75
18	bF	202	BCR	C27-C26-C25	2.74	126.71	122.73
18	a3	401	BCR	C15-C14-C13	-2.74	123.39	127.31
15	a6	417	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
18	a5	418	BCR	C27-C26-C25	2.74	126.71	122.73
15	b1	410	CLA	CAC-C3C-C2C	2.74	132.22	127.53
15	a3	411	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	bA	852	BCR	C15-C16-C17	-2.74	117.86	123.47
15	a2	418	CLA	C3A-C2A-C1A	2.74	105.45	101.34
19	bA	854	LHG	C20-C19-C18	-2.74	100.51	114.42
15	a5	409	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
15	bA	811	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	c2	420	BCR	C15-C14-C13	-2.74	123.40	127.31
18	cA	850	BCR	C15-C16-C17	-2.74	117.86	123.47
15	cJ	101	CLA	CMB-C2B-C3B	2.74	129.81	124.68
15	b4	406	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
15	c5	405	CLA	CHD-C1D-C2D	2.74	131.23	125.48
15	b3	410	CLA	CAC-C3C-C2C	2.74	132.22	127.53
15	a2	407	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
15	a5	405	CLA	CHD-C1D-C2D	2.74	131.23	125.48
15	a3	405	CLA	CHD-C1D-ND	-2.74	121.94	124.45
15	a4	414	CLA	CMB-C2B-C3B	2.74	129.80	124.68
15	b1	405	CLA	CHD-C1D-C2D	2.74	131.23	125.48
15	b1	403	CLA	CHB-C4A-NA	2.74	128.30	124.51
18	b3	419	BCR	C15-C16-C17	-2.74	117.86	123.47
15	c3	421	CLA	C6-C5-C3	-2.74	106.27	113.45
15	b4	409	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
15	a5	408	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
15	aB	811	CLA	C2A-C1A-CHA	2.74	128.65	123.86
18	b5	418	BCR	C3-C4-C5	-2.74	109.19	114.08
15	bJ	101	CLA	CMB-C2B-C3B	2.74	129.80	124.68
15	a3	421	CLA	C6-C5-C3	-2.74	106.28	113.45
15	c3	406	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
15	bA	841	CLA	CMB-C2B-C3B	2.74	129.80	124.68
15	b6	418	CLA	C3A-C2A-C1A	2.74	105.44	101.34
15	a1	409	CLA	CAC-C3C-C2C	2.74	132.21	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	837	CLA	CMB-C2B-C3B	2.74	129.80	124.68
18	cF	205	BCR	C7-C8-C9	-2.74	122.10	126.23
15	cF	203	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
15	c1	404	CLA	CMB-C2B-C3B	2.73	129.79	124.68
15	bB	842	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
15	c5	408	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
15	a4	408	CLA	CHB-C4A-NA	2.73	128.29	124.51
15	a2	411	CLA	CAC-C3C-C2C	2.73	132.21	127.53
15	bB	811	CLA	C2A-C1A-CHA	2.73	128.64	123.86
15	bF	201	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
15	b1	414	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
15	bA	804	CLA	CMB-C2B-C3B	2.73	129.79	124.68
15	cB	842	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	b6	414	CLA	CAC-C3C-C4C	2.73	128.35	124.81
15	a2	406	CLA	O2D-CGD-CBD	2.73	116.12	111.27
15	aJ	201	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
15	cB	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	cA	831	CLA	C2D-C1D-ND	-2.73	108.09	110.10
15	a3	416	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	b5	407	CLA	CHB-C4A-NA	2.73	128.29	124.51
15	c4	408	CLA	CHB-C4A-NA	2.73	128.29	124.51
15	b4	405	CLA	CHD-C1D-C2D	2.73	131.21	125.48
15	cA	804	CLA	CMB-C2B-C3B	2.73	129.79	124.68
15	bA	840	CLA	O2D-CGD-CBD	2.73	116.12	111.27
18	aA	851	BCR	C15-C16-C17	-2.73	117.88	123.47
15	b5	420	CLA	CMB-C2B-C3B	2.73	129.78	124.68
15	c3	404	CLA	CMB-C2B-C3B	2.73	129.78	124.68
15	aL	202	CLA	CHD-C1D-ND	-2.73	121.95	124.45
15	a4	412	CLA	C2D-C1D-ND	-2.73	108.09	110.10
15	c4	407	CLA	C2A-C1A-CHA	2.73	128.63	123.86
15	b2	422	CLA	C6-C7-C8	-2.73	107.10	115.92
15	c3	421	CLA	C6-C7-C8	-2.73	107.10	115.92
15	a3	410	CLA	CHB-C4A-NA	2.73	128.28	124.51
15	a6	410	CLA	CHB-C4A-NA	2.73	128.28	124.51
15	c3	413	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
15	bB	824	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
15	c5	404	CLA	C1-C2-C3	-2.73	121.33	126.04
15	c5	408	CLA	CHB-C4A-NA	2.73	128.28	124.51
15	c2	417	CLA	C1-C2-C3	-2.73	122.34	126.75
18	aB	846	BCR	C27-C26-C25	2.73	126.69	122.73
18	aI	103	BCR	C27-C26-C25	2.73	126.69	122.73
15	a2	415	CLA	CMB-C2B-C3B	2.73	129.78	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b1	419	BCR	C8-C9-C10	2.73	123.12	118.94
18	bB	847	BCR	C15-C14-C13	-2.73	123.39	127.30
18	bL	206	BCR	C7-C8-C9	-2.72	122.12	126.23
15	cB	811	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
19	bA	854	LHG	C11-C10-C9	-2.72	100.60	114.42
15	b5	407	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c5	407	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c5	416	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	cA	830	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
15	a3	412	CLA	C2D-C1D-ND	-2.72	108.10	110.10
15	b4	408	CLA	C2D-C1D-ND	-2.72	108.10	110.10
15	aA	805	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c3	416	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	b3	411	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	b6	402	BCR	C15-C14-C13	-2.72	123.42	127.31
15	b1	412	CLA	C2D-C1D-ND	-2.72	108.10	110.10
15	b4	407	CLA	C2A-C1A-CHA	2.72	128.62	123.86
15	b3	413	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	cB	824	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
15	a4	404	CLA	CHB-C4A-NA	2.72	128.28	124.51
15	a2	422	CLA	C6-C7-C8	-2.72	107.12	115.92
15	c4	408	CLA	C2D-C1D-ND	-2.72	108.10	110.10
19	aA	853	LHG	C11-C10-C9	-2.72	100.61	114.42
15	c2	404	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	cB	848	BCR	C27-C26-C25	2.72	126.68	122.73
15	bB	817	CLA	CAC-C3C-C4C	2.72	128.34	124.81
15	bB	826	CLA	CAA-CBA-CGA	-2.72	105.31	113.25
15	a6	411	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	c5	409	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	aF	201	BCR	C27-C26-C25	2.72	126.68	122.73
15	a2	417	CLA	C1-C2-C3	-2.72	122.35	126.75
15	bB	807	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	c2	415	CLA	CMB-C2B-C3B	2.72	129.76	124.68
15	a1	403	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	b5	405	CLA	CHD-C1D-C2D	2.72	131.18	125.48
15	b6	417	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
15	cA	840	CLA	O2D-CGD-CBD	2.72	116.10	111.27
18	bL	201	BCR	C7-C8-C9	-2.72	122.13	126.23
15	aB	826	CLA	CAA-CBA-CGA	-2.72	105.31	113.25
15	b6	410	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
18	bB	846	BCR	C40-C30-C25	2.72	114.70	110.30
18	a3	419	BCR	C15-C16-C17	-2.72	117.91	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b4	416	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
15	cA	805	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
15	a4	410	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	aB	818	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
15	c6	418	CLA	C3A-C2A-C1A	2.72	105.41	101.34
19	cA	852	LHG	C11-C10-C9	-2.71	100.64	114.42
15	bA	830	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
15	a5	409	CLA	CHB-C4A-NA	2.71	128.27	124.51
15	b2	418	CLA	C3A-C2A-C1A	2.71	105.40	101.34
15	aB	837	CLA	CBA-CAA-C2A	2.71	121.87	113.86
18	a6	402	BCR	C15-C14-C13	-2.71	123.44	127.31
15	b3	416	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
15	c5	414	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
15	b6	422	CLA	C16-C15-C13	-2.71	107.15	115.92
15	aB	825	CLA	C2A-C1A-CHA	2.71	128.60	123.86
15	aB	824	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
15	aB	842	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
18	b4	419	BCR	C15-C16-C17	-2.71	117.92	123.47
18	cF	202	BCR	C27-C26-C25	2.71	126.67	122.73
15	c4	405	CLA	CHD-C1D-C2D	2.71	131.17	125.48
15	b5	409	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
15	b4	410	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	b4	414	CLA	CMB-C2B-C3B	2.71	129.75	124.68
15	a4	416	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	c6	406	CLA	C3C-C4C-NC	-2.71	107.53	110.57
18	a3	401	BCR	C7-C8-C9	-2.71	122.14	126.23
15	a6	410	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
15	a3	402	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	bB	837	CLA	CBA-CAA-C2A	2.71	121.86	113.86
18	b5	419	BCR	C35-C13-C14	-2.71	119.13	122.92
15	c4	404	CLA	CHB-C4A-NA	2.71	128.26	124.51
18	aA	852	BCR	C27-C26-C25	2.71	126.66	122.73
15	bB	835	CLA	CMB-C2B-C3B	2.71	129.75	124.68
18	cB	847	BCR	C30-C25-C26	-2.71	118.80	122.61
18	aF	202	BCR	C27-C26-C25	2.71	126.66	122.73
15	aA	808	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	bA	832	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	bA	805	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
15	b5	406	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
15	cB	836	CLA	CHB-C4A-NA	2.71	128.25	124.51
15	a6	416	CLA	C2D-C1D-ND	-2.71	108.11	110.10
15	c1	405	CLA	CHD-C1D-C2D	2.71	131.16	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	808	CLA	CHB-C4A-NA	2.71	128.25	124.51
15	b3	410	CLA	CHB-C4A-NA	2.71	128.25	124.51
15	a1	422	CLA	CMB-C2B-C3B	2.70	129.74	124.68
15	a6	422	CLA	C11-C10-C8	-2.70	107.18	115.92
18	bL	205	BCR	C27-C26-C25	2.70	126.66	122.73
15	c1	414	CLA	CAA-C2A-C3A	-2.70	109.79	116.10
15	b3	407	CLA	C2A-C1A-CHA	2.70	128.59	123.86
15	cA	805	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
15	a1	413	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	a2	403	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	c4	421	CLA	C6-C5-C3	-2.70	106.36	113.45
15	a1	404	CLA	CHD-C1D-C2D	2.70	131.15	125.48
15	b2	411	CLA	CAC-C3C-C2C	2.70	132.15	127.53
15	aA	805	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
18	bA	853	BCR	C27-C26-C25	2.70	126.66	122.73
15	c2	418	CLA	C3A-C2A-C1A	2.70	105.39	101.34
18	cA	847	BCR	C15-C14-C13	-2.70	123.45	127.31
15	cA	833	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	cB	826	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
15	b1	409	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
15	c6	410	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
15	c3	412	CLA	C2D-C1D-ND	-2.70	108.11	110.10
15	c4	416	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
18	b2	420	BCR	C15-C16-C17	-2.70	117.94	123.47
15	cB	817	CLA	CAC-C3C-C4C	2.70	128.31	124.81
14	bA	801	CL0	CHD-C4C-NC	2.70	128.46	124.20
15	a4	409	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
15	a5	406	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
18	a1	418	BCR	C8-C9-C10	2.70	123.09	118.94
15	a1	415	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
15	c5	407	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	cA	811	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
15	c5	420	CLA	CMB-C2B-C3B	2.70	129.73	124.68
15	bA	805	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
15	aB	807	CLA	C7-C6-C5	-2.70	106.03	113.36
18	cA	851	BCR	C30-C25-C26	-2.70	118.81	122.61
15	b6	410	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	cB	807	CLA	C7-C6-C5	-2.70	106.03	113.36
15	a5	402	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	c3	409	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	cB	837	CLA	CBA-CAA-C2A	2.70	121.83	113.86
15	bB	807	CLA	C7-C6-C5	-2.70	106.03	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c1	419	BCR	C8-C9-C10	2.70	123.08	118.94
15	bA	811	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
15	c1	409	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
15	aB	821	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	a1	403	CLA	CMB-C2B-C3B	2.70	129.72	124.68
15	cB	835	CLA	CMB-C2B-C3B	2.70	129.72	124.68
15	a2	415	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
15	b3	409	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	c5	419	BCR	C35-C13-C14	-2.70	119.15	122.92
15	aA	820	CLA	C1-C2-C3	-2.70	121.38	126.04
15	c4	414	CLA	CMB-C2B-C3B	2.70	129.72	124.68
18	cA	851	BCR	C27-C26-C25	2.70	126.64	122.73
18	aB	847	BCR	C15-C14-C13	-2.69	123.44	127.30
18	cB	847	BCR	C15-C14-C13	-2.69	123.44	127.30
18	cL	204	BCR	C27-C26-C25	2.69	126.64	122.73
15	c2	422	CLA	CHA-C1A-NA	-2.69	120.23	126.40
18	bA	849	BCR	C15-C14-C13	-2.69	123.47	127.31
15	c1	414	CLA	CHB-C4A-NA	2.69	128.24	124.51
15	c6	410	CLA	CHB-C4A-NA	2.69	128.24	124.51
18	aB	847	BCR	C30-C25-C26	-2.69	118.82	122.61
18	bB	847	BCR	C30-C25-C26	-2.69	118.82	122.61
15	bB	836	CLA	CHB-C4A-NA	2.69	128.24	124.51
15	c2	411	CLA	CAC-C3C-C2C	2.69	132.13	127.53
15	c5	410	CLA	CAC-C3C-C2C	2.69	132.13	127.53
15	b6	403	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
15	cB	835	CLA	O1D-CGD-CBD	2.69	129.99	124.48
15	aB	807	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
18	bB	849	BCR	C27-C26-C25	2.69	126.64	122.73
18	c2	419	BCR	C3-C4-C5	-2.69	109.27	114.08
18	aA	848	BCR	C15-C14-C13	-2.69	123.47	127.31
15	c3	403	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	cA	836	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	aA	817	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	b2	422	CLA	C6-C5-C3	-2.69	106.40	113.45
18	a5	401	BCR	C15-C14-C13	-2.69	123.47	127.31
18	c2	421	BCR	C15-C14-C13	-2.69	123.47	127.31
15	a2	410	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	b3	409	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	a6	413	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	aA	830	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
15	bA	819	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
15	b2	404	CLA	CHB-C4A-NA	2.69	128.23	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bA	853	BCR	C32-C1-C6	2.69	114.66	110.30
18	a2	420	BCR	C15-C14-C13	-2.69	123.47	127.31
15	bB	818	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
15	b5	410	CLA	CAC-C3C-C2C	2.69	132.12	127.53
15	bB	803	CLA	C1-C2-C3	-2.69	121.40	126.04
15	cB	818	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
15	b6	412	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
15	c3	402	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
15	b2	415	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
15	aA	804	CLA	CMD-C2D-C3D	2.69	133.79	127.61
15	cA	819	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
15	b2	403	CLA	CHB-C4A-NA	2.69	128.22	124.51
18	c3	401	BCR	C7-C8-C9	-2.68	122.18	126.23
15	aB	803	CLA	C1-C2-C3	-2.68	121.40	126.04
18	a2	419	BCR	C3-C4-C5	-2.68	109.28	114.08
15	b2	405	CLA	CHD-C1D-C2D	2.68	131.11	125.48
15	b5	402	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	aA	852	BCR	C32-C1-C6	2.68	114.65	110.30
15	aA	811	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
18	aF	203	BCR	C27-C26-C25	2.68	126.63	122.73
15	a6	412	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
15	a2	422	CLA	CHA-C1A-NA	-2.68	120.25	126.40
15	bA	833	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	bB	835	CLA	O1D-CGD-CBD	2.68	129.97	124.48
18	c1	420	BCR	C35-C13-C14	-2.68	119.17	122.92
18	b2	419	BCR	C3-C4-C5	-2.68	109.29	114.08
15	a5	420	CLA	C6-C5-C3	-2.68	106.42	113.45
15	b5	420	CLA	C6-C7-C8	-2.68	107.25	115.92
18	cA	851	BCR	C32-C1-C6	2.68	114.65	110.30
15	a5	410	CLA	CAC-C3C-C2C	2.68	132.12	127.53
14	cA	801	CL0	CHD-C4C-NC	2.68	128.43	124.20
18	bJ	105	BCR	C27-C26-C25	2.68	126.62	122.73
18	b1	418	BCR	C27-C26-C25	2.68	126.62	122.73
15	b3	402	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	aB	817	CLA	CAC-C3C-C4C	2.68	128.29	124.81
15	c5	406	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
18	aL	205	BCR	C7-C8-C9	-2.68	122.19	126.23
15	c2	403	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	aB	849	BCR	C35-C13-C14	-2.68	119.17	122.92
18	a2	420	BCR	C15-C16-C17	-2.68	117.99	123.47
15	aB	835	CLA	CMB-C2B-C3B	2.68	129.69	124.68
15	c2	415	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	836	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	bB	825	CLA	C2A-C1A-CHA	2.68	128.54	123.86
15	cB	840	CLA	CAA-CBA-CGA	-2.68	105.43	113.25
15	b6	416	CLA	C2D-C1D-ND	-2.68	108.13	110.10
15	aA	833	CLA	CHB-C4A-NA	2.68	128.21	124.51
18	a5	419	BCR	C35-C13-C14	-2.68	119.17	122.92
15	cB	825	CLA	C2A-C1A-CHA	2.68	128.54	123.86
15	c1	405	CLA	C3C-C4C-NC	-2.68	107.57	110.57
18	cF	205	BCR	C27-C26-C25	2.68	126.62	122.73
14	aA	801	CL0	CHD-C4C-NC	2.68	128.42	124.20
15	b5	409	CLA	CHB-C4A-NA	2.68	128.21	124.51
15	a2	405	CLA	CHD-C1D-C2D	2.68	131.09	125.48
15	a5	420	CLA	C6-C7-C8	-2.68	107.27	115.92
15	cA	808	CLA	CHB-C4A-NA	2.68	128.21	124.51
15	a5	407	CLA	C2A-C1A-CHA	2.68	128.54	123.86
15	c2	405	CLA	CHD-C1D-C2D	2.67	131.09	125.48
15	aA	831	CLA	C2D-C1D-ND	-2.67	108.13	110.10
18	c1	418	BCR	C27-C26-C25	2.67	126.61	122.73
15	a6	422	CLA	CMB-C2B-C1B	-2.67	124.35	128.46
15	cA	834	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
15	a4	421	CLA	CED-O2D-CGD	2.67	121.98	115.94
15	bB	840	CLA	CAA-CBA-CGA	-2.67	105.44	113.25
15	c5	420	CLA	C6-C5-C3	-2.67	106.45	113.45
15	a5	420	CLA	CMB-C2B-C3B	2.67	129.68	124.68
15	b5	416	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
15	bA	836	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	b4	404	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	b5	407	CLA	C2A-C1A-CHA	2.67	128.53	123.86
15	b5	420	CLA	C6-C5-C3	-2.67	106.45	113.45
15	b6	411	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	b1	416	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
18	cJ	103	BCR	C11-C10-C9	-2.67	123.50	127.31
15	aA	836	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	a2	408	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	cA	841	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	aA	803	CLA	C1-O2A-CGA	2.67	123.45	116.44
18	cA	847	BCR	C24-C23-C22	-2.67	122.20	126.23
15	a6	415	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	bB	807	CLA	C11-C12-C13	-2.67	107.29	115.92
15	b1	404	CLA	CMB-C2B-C3B	2.67	129.67	124.68
18	cB	849	BCR	C35-C13-C14	-2.67	119.19	122.92
18	aA	852	BCR	C30-C25-C26	-2.67	118.86	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bJ	103	BCR	C11-C10-C9	-2.67	123.50	127.31
15	aB	829	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
15	c5	420	CLA	C6-C7-C8	-2.67	107.30	115.92
15	aA	829	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	b2	415	CLA	CMB-C2B-C3B	2.67	129.67	124.68
15	b3	405	CLA	CHD-C1D-C2D	2.67	131.07	125.48
15	cB	840	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
15	c5	416	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
15	cB	811	CLA	O2A-C1-C2	-2.67	101.63	108.64
15	b6	415	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	b2	410	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	a3	407	CLA	C2A-C1A-CHA	2.67	128.52	123.86
15	c3	405	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
15	c6	412	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
15	c5	407	CLA	C2A-C1A-CHA	2.67	128.52	123.86
15	b2	406	CLA	O2D-CGD-CBD	2.67	116.00	111.27
15	cB	829	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
15	a3	413	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	a6	403	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	cA	804	CLA	CMD-C2D-C3D	2.66	133.74	127.61
15	c6	415	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	b1	414	CLA	CAA-C2A-C3A	-2.66	109.89	116.10
15	b3	412	CLA	C2D-C1D-ND	-2.66	108.14	110.10
15	aB	811	CLA	O2A-C1-C2	-2.66	101.64	108.64
15	c6	411	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	cB	801	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
15	aB	840	CLA	CAA-CBA-CGA	-2.66	105.48	113.25
15	bA	817	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
15	bA	841	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	c3	410	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	cK	101	BCR	C24-C23-C22	-2.66	122.22	126.23
15	c6	411	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
15	cB	803	CLA	C1-C2-C3	-2.66	121.44	126.04
18	b1	401	BCR	C15-C14-C13	-2.66	123.52	127.31
15	cB	807	CLA	C11-C12-C13	-2.66	107.33	115.92
15	cA	815	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	aA	839	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	bB	829	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
15	bB	834	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
18	b2	420	BCR	C15-C14-C13	-2.66	123.52	127.31
15	cA	803	CLA	C1-O2A-CGA	2.66	123.41	116.44
15	a1	404	CLA	C3C-C4C-NC	-2.66	107.59	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	422	CLA	C6-C5-C3	-2.66	106.49	113.45
15	a1	408	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
15	b2	422	CLA	CHA-C1A-NA	-2.65	120.32	126.40
15	aB	815	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
15	a4	421	CLA	C6-C5-C3	-2.65	106.50	113.45
15	bA	803	CLA	C1-O2A-CGA	2.65	123.41	116.44
15	bA	804	CLA	CMD-C2D-C3D	2.65	133.72	127.61
15	aB	807	CLA	C11-C12-C13	-2.65	107.34	115.92
15	aB	831	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
18	a1	419	BCR	C24-C23-C22	-2.65	122.23	126.23
15	b2	406	CLA	CAA-C2A-C1A	2.65	120.67	111.97
15	a6	411	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
15	bB	802	CLA	CBA-CAA-C2A	-2.65	106.03	113.86
18	c2	420	BCR	C15-C16-C17	-2.65	118.04	123.47
18	c3	401	BCR	C15-C14-C13	-2.65	123.53	127.31
15	cA	820	CLA	C1-C2-C3	-2.65	121.46	126.04
15	a3	415	CLA	C2D-C1D-ND	-2.65	108.15	110.10
18	bA	853	BCR	C30-C25-C26	-2.65	118.88	122.61
15	aB	808	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
18	cA	847	BCR	C28-C27-C26	-2.65	109.34	114.08
15	b6	406	CLA	C3C-C4C-NC	-2.65	107.60	110.57
15	cB	834	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
15	bB	821	CLA	CHB-C4A-NA	2.65	128.18	124.51
15	aA	802	CLA	CAA-CBA-CGA	-2.65	105.51	113.25
15	c3	405	CLA	CHD-C1D-C2D	2.65	131.04	125.48
15	aA	814	CLA	CHB-C4A-NA	2.65	128.18	124.51
15	b3	403	CLA	CHB-C4A-NA	2.65	128.18	124.51
15	aB	835	CLA	O1D-CGD-CBD	2.65	129.90	124.48
15	bA	810	CLA	CMB-C2B-C3B	2.65	129.63	124.68
15	c6	413	CLA	C2D-C1D-ND	-2.65	108.15	110.10
15	aA	819	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
15	aB	802	CLA	CBA-CAA-C2A	-2.65	106.05	113.86
15	bB	811	CLA	O2A-C1-C2	-2.65	101.68	108.64
15	c4	410	CLA	CHB-C4A-NA	2.65	128.17	124.51
15	c4	421	CLA	CED-O2D-CGD	2.65	121.92	115.94
15	c6	413	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
15	bB	840	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
15	b6	408	CLA	C2A-C1A-CHA	2.65	128.49	123.86
15	bA	839	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	bA	849	BCR	C28-C27-C26	-2.65	109.35	114.08
18	a1	417	BCR	C27-C26-C25	2.65	126.57	122.73
15	bA	829	CLA	CHB-C4A-NA	2.65	128.17	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	408	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	c1	420	BCR	C15-C14-C13	-2.65	123.53	127.31
15	bA	820	CLA	C1-C2-C3	-2.64	121.47	126.04
20	aB	850	LMG	O3-C3-C2	-2.64	104.23	110.35
15	a1	402	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	aA	834	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	cA	815	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
18	bB	850	BCR	C35-C13-C14	-2.64	119.22	122.92
15	bB	808	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
15	b1	416	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	c6	403	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	c2	408	CLA	C2A-C1A-CHA	2.64	128.48	123.86
15	aB	834	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
15	cA	814	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	cA	829	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	a2	406	CLA	CAA-C2A-C1A	2.64	120.63	111.97
20	bB	851	LMG	O3-C3-C2	-2.64	104.24	110.35
15	cA	802	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
15	aA	810	CLA	CMB-C2B-C3B	2.64	129.62	124.68
15	bA	834	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	aB	801	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
15	cB	802	CLA	CBA-CAA-C2A	-2.64	106.07	113.86
15	bB	815	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
15	c1	415	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
15	a5	416	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
15	c2	410	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	a6	413	CLA	C2D-C1D-ND	-2.64	108.16	110.10
15	b4	412	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
15	bA	814	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	cB	821	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	a1	413	CLA	CAA-C2A-C3A	-2.64	109.94	116.10
15	c1	403	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	b4	421	CLA	CED-O2D-CGD	2.64	121.90	115.94
15	aB	840	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
15	c6	404	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	c4	415	CLA	C2D-C1D-ND	-2.64	108.16	110.10
18	b3	419	BCR	C15-C14-C13	-2.64	123.55	127.31
15	a6	414	CLA	C3C-C4C-NC	-2.64	107.61	110.57
15	c5	402	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	aK	101	BCR	C24-C23-C22	-2.63	122.25	126.23
18	bA	848	BCR	C24-C23-C22	-2.63	122.25	126.23
15	b2	413	CLA	CMC-C2C-C3C	2.63	133.27	126.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c5	401	BCR	C15-C14-C13	-2.63	123.55	127.31
15	c3	407	CLA	C2A-C1A-CHA	2.63	128.47	123.86
15	cF	201	CLA	C2D-C1D-ND	-2.63	108.16	110.10
15	bB	801	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
15	b6	422	CLA	C11-C10-C8	-2.63	107.41	115.92
20	cB	850	LMG	O3-C3-C2	-2.63	104.26	110.35
15	b6	406	CLA	CHD-C1D-C2D	2.63	131.00	125.48
18	b5	419	BCR	C15-C14-C13	-2.63	123.55	127.31
15	aB	811	CLA	CMB-C2B-C3B	2.63	129.60	124.68
15	c6	416	CLA	C2D-C1D-ND	-2.63	108.16	110.10
15	cA	810	CLA	CMB-C2B-C3B	2.63	129.60	124.68
15	b1	415	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
15	bA	802	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
15	cB	808	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
18	aJ	204	BCR	C11-C10-C9	-2.63	123.56	127.31
15	b2	422	CLA	C3A-C2A-C1A	2.63	105.28	101.34
15	cA	817	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
15	c6	406	CLA	CHD-C1D-C2D	2.63	131.00	125.48
15	c3	407	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
18	b1	420	BCR	C15-C14-C13	-2.63	123.56	127.31
15	a6	406	CLA	C3C-C4C-NC	-2.63	107.62	110.57
15	c4	410	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
15	b2	406	CLA	CHA-C1A-NA	-2.63	120.38	126.40
15	bB	831	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
18	c5	419	BCR	C15-C14-C13	-2.63	123.56	127.31
15	b6	411	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
15	b3	415	CLA	C2D-C1D-ND	-2.63	108.17	110.10
15	a2	413	CLA	CMC-C2C-C3C	2.63	133.25	126.12
15	b4	410	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
18	aI	103	BCR	C31-C1-C6	2.63	114.56	110.30
15	aA	839	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
15	a1	414	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
15	bB	826	CLA	C2D-C1D-ND	-2.62	108.17	110.10
18	aK	101	BCR	C28-C27-C26	-2.62	109.39	114.08
15	cA	839	CLA	CHB-C4A-NA	2.62	128.14	124.51
15	b6	406	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
18	a1	421	BCR	C7-C8-C9	-2.62	122.27	126.23
18	aA	848	BCR	C28-C27-C26	-2.62	109.39	114.08
18	c1	401	BCR	C15-C14-C13	-2.62	123.57	127.31
15	c2	415	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
15	a2	422	CLA	C3A-C2A-C1A	2.62	105.27	101.34
15	bA	812	CLA	O2D-CGD-O1D	-2.62	118.71	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	412	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
15	b4	410	CLA	CAC-C3C-C2C	2.62	132.01	127.53
15	aA	815	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
15	cA	812	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
15	a2	408	CLA	C2A-C1A-CHA	2.62	128.44	123.86
14	cA	801	CL0	C1-C2-C3	-2.62	121.51	126.04
15	c1	413	CLA	CMB-C2B-C3B	2.62	129.58	124.68
15	a1	406	CLA	C2A-C1A-CHA	2.62	128.44	123.86
15	a6	408	CLA	C2A-C1A-CHA	2.62	128.44	123.86
15	c2	422	CLA	C6-C5-C3	-2.62	106.59	113.45
15	aA	834	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
15	aA	841	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	bA	848	BCR	C28-C27-C26	-2.62	109.40	114.08
18	a5	419	BCR	C15-C14-C13	-2.62	123.58	127.31
15	b6	413	CLA	CMB-C2B-C3B	2.62	129.57	124.68
18	aA	848	BCR	C24-C23-C22	-2.62	122.28	126.23
18	cK	101	BCR	C28-C27-C26	-2.62	109.41	114.08
15	aA	815	CLA	CHB-C4A-NA	2.62	128.13	124.51
15	bA	815	CLA	CHB-C4A-NA	2.62	128.13	124.51
15	b5	414	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
15	cB	815	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
18	bA	849	BCR	C24-C23-C22	-2.61	122.28	126.23
14	bA	801	CL0	C4-C3-C5	2.61	119.67	115.27
15	c3	409	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
15	b4	421	CLA	C6-C5-C3	-2.61	106.60	113.45
18	bL	205	BCR	C31-C1-C6	2.61	114.54	110.30
14	cA	801	CL0	CGD-CBD-CAD	-2.61	102.27	110.73
15	aA	844	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
15	a6	406	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
15	b2	408	CLA	C2A-C1A-CHA	2.61	128.43	123.86
15	c4	410	CLA	CAC-C3C-C2C	2.61	132.00	127.53
15	a3	403	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	b6	413	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
15	a3	405	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
15	a6	406	CLA	CHD-C1D-C2D	2.61	130.96	125.48
18	aB	846	BCR	C39-C30-C25	-2.61	106.06	110.30
15	c2	412	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
15	bA	834	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	bA	839	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	b4	403	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	b3	417	CLA	C3A-C2A-C1A	2.61	105.25	101.34
15	c2	422	CLA	C3A-C2A-C1A	2.61	105.25	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	804	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	cA	834	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	c5	414	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	b3	405	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
14	aA	801	CL0	C4-C3-C5	2.61	119.66	115.27
15	c2	406	CLA	O2D-CGD-CBD	2.61	115.91	111.27
15	b6	411	CLA	CAC-C3C-C2C	2.61	131.99	127.53
15	cB	831	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
15	a1	406	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	c2	406	CLA	CAA-C2A-C1A	2.61	120.53	111.97
15	b2	411	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	aA	804	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
18	c3	419	BCR	C15-C14-C13	-2.61	123.59	127.31
15	c6	414	CLA	C3C-C4C-NC	-2.61	107.65	110.57
14	aA	801	CL0	C1-C2-C3	-2.61	121.53	126.04
15	bA	844	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
15	aA	842	CLA	C2D-C1D-ND	-2.61	108.18	110.10
15	b6	413	CLA	C2D-C1D-ND	-2.61	108.18	110.10
15	aA	838	CLA	O2D-CGD-CBD	2.61	115.90	111.27
15	a3	407	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	bA	801	CL0	CGD-CBD-CAD	-2.61	102.29	110.73
15	a3	402	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	c4	401	BCR	C24-C23-C22	-2.61	122.30	126.23
18	cB	845	BCR	C29-C30-C25	2.61	114.49	110.48
15	bA	838	CLA	O2D-CGD-CBD	2.61	115.90	111.27
15	c2	402	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	bB	811	CLA	CMB-C2B-C3B	2.61	129.55	124.68
15	c4	413	CLA	CMB-C2B-C3B	2.61	129.55	124.68
18	cM	101	BCR	C33-C5-C6	-2.60	121.60	124.53
14	aA	801	CL0	CGD-CBD-CAD	-2.60	102.30	110.73
15	cA	838	CLA	O2D-CGD-CBD	2.60	115.90	111.27
18	bB	846	BCR	C39-C30-C25	-2.60	106.08	110.30
15	c5	413	CLA	CMB-C2B-C3B	2.60	129.55	124.68
15	bA	815	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
18	c6	420	BCR	C29-C30-C25	2.60	114.49	110.48
15	aA	822	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
15	cA	839	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
15	b4	416	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
15	c3	413	CLA	CMB-C2B-C3B	2.60	129.55	124.68
15	c6	408	CLA	C2A-C1A-CHA	2.60	128.41	123.86
15	cB	826	CLA	C2D-C1D-ND	-2.60	108.19	110.10
15	b1	407	CLA	C1B-CHB-C4A	-2.60	124.97	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	820	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	aA	848	BCR	C11-C10-C9	-2.60	123.60	127.31
15	a5	414	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
15	a2	411	CLA	CHB-C4A-NA	2.60	128.11	124.51
15	c3	405	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
15	b2	410	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	cB	827	CLA	O2A-C1-C2	-2.60	101.80	108.64
15	bB	837	CLA	CHD-C1D-ND	-2.60	122.07	124.45
15	b6	404	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	a1	404	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
15	cA	843	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
18	bL	201	BCR	C24-C23-C22	-2.60	122.31	126.23
15	aB	827	CLA	O2A-C1-C2	-2.60	101.81	108.64
14	bA	801	CL0	C1-C2-C3	-2.60	121.55	126.04
15	c2	408	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	c1	416	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	c4	403	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	b3	413	CLA	CMB-C2B-C3B	2.60	129.53	124.68
15	c4	412	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
18	cL	204	BCR	C31-C1-C6	2.59	114.51	110.30
15	cB	833	CLA	O2D-CGD-CBD	2.59	115.88	111.27
15	c5	403	CLA	CHB-C4A-NA	2.59	128.10	124.51
15	b1	407	CLA	C2A-C1A-CHA	2.59	128.40	123.86
15	c6	411	CLA	CAC-C3C-C2C	2.59	131.97	127.53
18	a6	420	BCR	C29-C30-C25	2.59	114.47	110.48
15	a4	407	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	bL	206	BCR	C24-C23-C22	-2.59	122.32	126.23
15	c2	413	CLA	CMC-C2C-C3C	2.59	133.15	126.12
18	c6	420	BCR	C3-C4-C5	-2.59	109.45	114.08
18	a1	419	BCR	C15-C14-C13	-2.59	123.61	127.31
15	b6	422	CLA	O2D-CGD-CBD	2.59	115.87	111.27
15	a4	417	CLA	CHD-C1D-ND	-2.59	122.07	124.45
15	bB	833	CLA	O2D-CGD-CBD	2.59	115.87	111.27
15	b1	414	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	c2	411	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
15	a3	405	CLA	CHD-C1D-C2D	2.59	130.91	125.48
18	aM	101	BCR	C33-C5-C6	-2.59	121.62	124.53
18	bM	101	BCR	C33-C5-C6	-2.59	121.62	124.53
15	c6	406	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
15	c2	410	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
15	aL	203	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
15	a6	404	CLA	CHB-C4A-NA	2.59	128.09	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	416	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
18	cB	846	BCR	C39-C30-C25	-2.59	106.10	110.30
15	bB	834	CLA	CMB-C2B-C3B	2.59	129.52	124.68
15	bA	804	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
15	bA	822	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
15	cB	831	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	aA	812	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
20	aB	850	LMG	O2-C2-C1	-2.59	103.76	110.05
18	a1	420	BCR	C15-C14-C13	-2.59	123.62	127.31
19	aA	854	LHG	C11-C10-C9	-2.59	101.30	114.42
15	aB	825	CLA	CHA-C1A-NA	-2.59	120.48	126.40
15	aA	834	CLA	CAA-CBA-CGA	-2.59	105.70	113.25
18	c6	420	BCR	C35-C13-C14	-2.59	119.30	122.92
15	aA	824	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
15	c5	410	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
15	cA	809	CLA	CAA-C2A-C1A	-2.58	103.50	111.97
15	b1	413	CLA	CMB-C2B-C3B	2.58	129.51	124.68
15	aA	819	CLA	CBC-CAC-C3C	2.58	119.56	112.43
15	c3	402	CLA	CHB-C4A-NA	2.58	128.09	124.51
15	bA	819	CLA	CBC-CAC-C3C	2.58	119.55	112.43
15	aB	837	CLA	CHD-C1D-ND	-2.58	122.08	124.45
15	bA	824	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
15	cA	827	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
15	cB	825	CLA	CHA-C1A-NA	-2.58	120.48	126.40
15	c2	411	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	aL	205	BCR	C24-C23-C22	-2.58	122.33	126.23
18	bB	845	BCR	C29-C30-C25	2.58	114.46	110.48
15	aA	827	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
15	a3	417	CLA	C3A-C2A-C1A	2.58	105.20	101.34
15	cB	811	CLA	CMB-C2B-C3B	2.58	129.51	124.68
15	a5	403	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	b5	403	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	aB	845	BCR	C29-C30-C25	2.58	114.45	110.48
18	b6	420	BCR	C3-C4-C5	-2.58	109.47	114.08
15	bB	802	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
15	cA	822	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
15	aA	809	CLA	CAA-C2A-C1A	-2.58	103.52	111.97
15	cA	824	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
18	a3	419	BCR	C15-C14-C13	-2.58	123.63	127.31
18	c3	419	BCR	C11-C10-C9	-2.58	123.63	127.31
15	bB	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	bB	815	CLA	O2D-CGD-CBD	2.58	115.85	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	818	CLA	O2D-CGD-CBD	2.58	115.85	111.27
15	bA	827	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
19	bA	855	LHG	C11-C10-C9	-2.58	101.33	114.42
15	aA	835	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	b6	403	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	c3	410	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
19	cA	853	LHG	C11-C10-C9	-2.58	101.34	114.42
15	bB	815	CLA	C2D-C1D-ND	-2.58	108.20	110.10
15	cA	819	CLA	CBC-CAC-C3C	2.58	119.53	112.43
15	bB	827	CLA	O2A-C1-C2	-2.58	101.86	108.64
15	bA	834	CLA	CAA-CBA-CGA	-2.58	105.72	113.25
15	cA	834	CLA	CAA-CBA-CGA	-2.58	105.73	113.25
15	b5	415	CLA	C2D-C1D-ND	-2.58	108.21	110.10
15	bA	835	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
15	b3	402	CLA	CHB-C4A-NA	2.58	128.07	124.51
15	cB	833	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
15	b6	422	CLA	CHA-C1A-NA	-2.57	120.50	126.40
15	bA	805	CLA	O2D-CGD-CBD	2.57	115.84	111.27
15	bA	809	CLA	CAA-C2A-C1A	-2.57	103.54	111.97
15	cA	835	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
14	cA	801	CL0	C4-C3-C5	2.57	119.60	115.27
18	b6	420	BCR	C29-C30-C25	2.57	114.44	110.48
15	bA	835	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	cB	815	CLA	O2D-CGD-CBD	2.57	115.84	111.27
15	aB	826	CLA	C2D-C1D-ND	-2.57	108.21	110.10
15	c1	410	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	aL	201	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	cA	848	BCR	C15-C14-C13	-2.57	123.64	127.31
15	aB	834	CLA	CMB-C2B-C3B	2.57	129.49	124.68
15	c1	407	CLA	C2A-C1A-CHA	2.57	128.35	123.86
15	a4	405	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
15	a4	410	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	bL	204	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
15	bB	831	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	b1	405	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
15	bB	807	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	cA	804	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
15	b2	412	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
15	a5	412	CLA	CMC-C2C-C3C	2.57	133.09	126.12
15	b4	417	CLA	CHD-C1D-ND	-2.57	122.09	124.45
15	c4	409	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
20	cB	850	LMG	O2-C2-C1	-2.57	103.81	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	409	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
15	cL	203	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
15	bB	818	CLA	O2D-CGD-CBD	2.57	115.83	111.27
15	c6	413	CLA	CMB-C2B-C3B	2.57	129.48	124.68
15	c5	412	CLA	C2D-C1D-ND	-2.57	108.21	110.10
15	cB	820	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	bB	825	CLA	CHA-C1A-NA	-2.57	120.52	126.40
15	cB	837	CLA	CHD-C1D-ND	-2.57	122.09	124.45
18	b5	401	BCR	C15-C14-C13	-2.57	123.65	127.31
15	c6	403	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	a6	411	CLA	CAC-C3C-C2C	2.57	131.92	127.53
15	b4	415	CLA	C2D-C1D-ND	-2.57	108.21	110.10
15	c4	405	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
15	a4	403	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	aB	807	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	aB	833	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
15	c1	407	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
15	b2	415	CLA	CAA-C2A-C3A	-2.56	110.11	116.10
15	a5	412	CLA	C2D-C1D-ND	-2.56	108.21	110.10
15	bA	838	CLA	C2D-C1D-ND	-2.56	108.21	110.10
18	aJ	205	BCR	C15-C14-C13	-2.56	123.65	127.31
15	bB	809	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
15	bL	202	CLA	CHB-C4A-NA	2.56	128.06	124.51
15	bA	804	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
15	aB	815	CLA	O2D-CGD-CBD	2.56	115.82	111.27
18	bA	849	BCR	C11-C10-C9	-2.56	123.65	127.31
18	cJ	104	BCR	C15-C14-C13	-2.56	123.65	127.31
15	aA	835	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
15	bA	842	CLA	C2D-C1D-ND	-2.56	108.22	110.10
18	a2	421	BCR	C15-C16-C17	-2.56	118.23	123.47
15	aA	804	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
18	a6	420	BCR	C3-C4-C5	-2.56	109.50	114.08
18	cB	849	BCR	C10-C11-C12	-2.56	115.22	123.22
18	cA	847	BCR	C11-C10-C9	-2.56	123.66	127.31
15	c4	407	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
15	cB	831	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
15	a4	405	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
15	bB	833	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
15	a2	402	CLA	CHB-C4A-NA	2.56	128.05	124.51
15	aA	805	CLA	O2D-CGD-CBD	2.56	115.82	111.27
15	aB	831	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
20	bB	851	LMG	O2-C2-C1	-2.56	103.83	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	839	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
15	b4	405	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
15	a2	411	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	bB	812	CLA	CHD-C1D-ND	-2.56	122.10	124.45
15	cB	801	CLA	C2D-C1D-ND	-2.56	108.22	110.10
15	b5	412	CLA	CMC-C2C-C3C	2.56	133.06	126.12
15	bB	833	CLA	CMB-C2B-C3B	2.56	129.46	124.68
18	a1	419	BCR	C35-C13-C14	-2.56	119.34	122.92
15	b3	407	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	bB	801	CLA	C2D-C1D-ND	-2.56	108.22	110.10
15	c3	415	CLA	C2D-C1D-ND	-2.56	108.22	110.10
15	cB	834	CLA	CMB-C2B-C3B	2.56	129.46	124.68
15	aB	809	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
18	bB	850	BCR	C10-C11-C12	-2.56	115.24	123.22
15	bB	809	CLA	O2D-CGD-CBD	2.56	115.81	111.27
15	b1	408	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	b4	407	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	a4	415	CLA	CBA-CAA-C2A	2.56	121.41	113.86
15	b2	413	CLA	C1D-ND-C4D	2.55	108.15	106.33
15	aB	818	CLA	O2D-CGD-CBD	2.55	115.81	111.27
15	cA	831	CLA	O2D-CGD-CBD	2.55	115.81	111.27
15	a6	413	CLA	CMB-C2B-C3B	2.55	129.46	124.68
15	bB	831	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
15	a1	422	CLA	C11-C10-C8	-2.55	107.66	115.92
15	a4	416	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
15	aB	833	CLA	CMB-C2B-C3B	2.55	129.46	124.68
15	aB	802	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
15	cL	201	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	aB	809	CLA	O2D-CGD-CBD	2.55	115.80	111.27
15	c3	417	CLA	C3A-C2A-C1A	2.55	105.16	101.34
15	a5	413	CLA	CMB-C2B-C3B	2.55	129.45	124.68
18	bA	850	BCR	C15-C14-C13	-2.55	123.67	127.31
15	cB	802	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
18	b2	421	BCR	C29-C30-C25	2.55	114.41	110.48
15	c2	406	CLA	CHA-C1A-NA	-2.55	120.56	126.40
18	aB	849	BCR	C10-C11-C12	-2.55	115.25	123.22
15	cA	835	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	bJ	104	BCR	C15-C14-C13	-2.55	123.67	127.31
15	cB	833	CLA	CMB-C2B-C3B	2.55	129.45	124.68
15	cB	809	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
15	aB	831	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	b1	402	CLA	CHB-C4A-NA	2.55	128.04	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	406	CLA	CHA-C1A-NA	-2.55	120.56	126.40
15	cF	201	CLA	CMB-C2B-C3B	2.55	129.45	124.68
15	a4	414	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
15	a3	413	CLA	CMB-C2B-C3B	2.55	129.45	124.68
15	aB	833	CLA	O2D-CGD-CBD	2.55	115.80	111.27
15	cB	809	CLA	O2D-CGD-CBD	2.55	115.80	111.27
15	bB	839	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
18	c1	418	BCR	C3-C4-C5	-2.55	109.53	114.08
15	cA	809	CLA	C1-C2-C3	-2.55	121.64	126.04
15	bB	823	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	bB	804	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	cF	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	bB	814	CLA	CAC-C3C-C2C	2.55	131.89	127.53
15	a6	403	CLA	CHB-C4A-NA	2.55	128.03	124.51
15	a2	415	CLA	CAA-C2A-C3A	-2.55	110.15	116.10
15	cB	823	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	b6	417	CLA	C3C-C4C-NC	-2.55	107.72	110.57
15	bB	804	CLA	CMD-C2D-C3D	2.55	133.47	127.61
15	bA	831	CLA	O2D-CGD-CBD	2.55	115.79	111.27
18	bJ	103	BCR	C27-C26-C25	2.55	126.43	122.73
15	aA	831	CLA	O2D-CGD-CBD	2.55	115.79	111.27
15	a5	410	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	a2	412	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
15	cB	807	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	a4	410	CLA	CAC-C3C-C2C	2.54	131.88	127.53
15	cA	805	CLA	O2D-CGD-CBD	2.54	115.79	111.27
15	c1	412	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	c1	405	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
18	b3	419	BCR	C11-C10-C9	-2.54	123.68	127.31
15	bB	802	CLA	C6-C5-C3	-2.54	106.79	113.45
15	c5	412	CLA	CMC-C2C-C3C	2.54	133.02	126.12
15	bA	819	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	aB	812	CLA	CHD-C1D-ND	-2.54	122.12	124.45
15	a1	411	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	b5	412	CLA	C2D-C1D-ND	-2.54	108.23	110.10
15	aA	825	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	bF	201	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	a3	419	BCR	C11-C10-C9	-2.54	123.69	127.31
15	b4	411	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
15	b4	414	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
15	c4	405	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
15	bA	815	CLA	O2D-CGD-O1D	-2.54	118.87	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	819	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
18	cB	849	BCR	C23-C22-C21	-2.54	115.05	118.94
15	c4	407	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
15	cB	802	CLA	C6-C5-C3	-2.54	106.80	113.45
15	aJ	201	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	bA	805	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	b1	412	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	b2	402	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	c1	402	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	aB	804	CLA	CMD-C2D-C3D	2.54	133.45	127.61
15	cB	839	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
15	aB	814	CLA	CAC-C3C-C2C	2.54	131.87	127.53
18	b1	418	BCR	C3-C4-C5	-2.54	109.55	114.08
15	aB	823	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
15	cB	804	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	cB	814	CLA	CAC-C3C-C2C	2.54	131.87	127.53
15	c1	416	CLA	C3C-C4C-NC	-2.54	107.73	110.57
15	a5	415	CLA	C2D-C1D-ND	-2.54	108.23	110.10
15	b2	407	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	aA	815	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
15	b5	405	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
15	cB	824	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
18	a6	421	BCR	C15-C14-C13	-2.54	123.69	127.31
15	aA	842	CLA	CMB-C2B-C3B	2.54	129.42	124.68
15	a2	417	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
15	cA	825	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
15	aX	102	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
15	b4	405	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
15	bX	102	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
18	b1	401	BCR	C34-C9-C10	-2.53	119.37	122.92
15	c5	415	CLA	C2D-C1D-ND	-2.53	108.24	110.10
15	c4	417	CLA	CHD-C1D-ND	-2.53	122.13	124.45
15	c2	417	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
15	aB	811	CLA	C1-O2A-CGA	2.53	123.08	116.44
15	bB	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	c6	416	CLA	CBA-CAA-C2A	2.53	121.33	113.86
15	a1	411	CLA	C1D-ND-C4D	2.53	108.13	106.33
15	cA	838	CLA	C2D-C1D-ND	-2.53	108.24	110.10
15	aA	805	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	aB	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	a1	401	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	cB	844	BCR	C15-C14-C13	-2.53	123.70	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	802	CLA	C6-C5-C3	-2.53	106.83	113.45
15	bA	812	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
15	b1	411	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
15	b3	412	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
18	a6	420	BCR	C35-C13-C14	-2.53	119.38	122.92
15	bB	828	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
18	cJ	103	BCR	C27-C26-C25	2.53	126.40	122.73
18	c2	421	BCR	C29-C30-C25	2.53	114.37	110.48
15	c2	407	CLA	CHB-C4A-NA	2.53	128.00	124.51
18	aA	849	BCR	C15-C14-C13	-2.53	123.71	127.31
15	aB	824	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
20	cB	850	LMG	C38-C37-C36	-2.53	101.61	114.42
15	aA	808	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
15	a5	405	CLA	CAA-C2A-C3A	-2.52	105.86	112.78
15	b2	411	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
18	aB	849	BCR	C23-C22-C21	-2.52	115.07	118.94
15	b4	407	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
15	a2	417	CLA	C2A-C1A-CHA	2.52	128.27	123.86
15	cB	804	CLA	CMD-C2D-C3D	2.52	133.42	127.61
15	a3	410	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
15	b4	414	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
15	aB	801	CLA	C2D-C1D-ND	-2.52	108.24	110.10
18	cA	850	BCR	C15-C14-C13	-2.52	123.71	127.31
18	aJ	204	BCR	C27-C26-C25	2.52	126.39	122.73
18	bB	844	BCR	C15-C14-C13	-2.52	123.71	127.31
15	bB	811	CLA	C1-O2A-CGA	2.52	123.06	116.44
18	b6	420	BCR	C35-C13-C14	-2.52	119.39	122.92
15	a2	410	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	a6	417	CLA	C3C-C4C-NC	-2.52	107.74	110.57
15	c6	415	CLA	CAA-C2A-C3A	-2.52	110.21	116.10
15	cB	811	CLA	C1-O2A-CGA	2.52	123.06	116.44
15	b3	416	CLA	C3C-C4C-NC	-2.52	107.74	110.57
18	aB	847	BCR	C38-C26-C27	-2.52	108.77	113.62
18	aL	205	BCR	C15-C16-C17	-2.52	118.31	123.47
15	c4	411	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
15	b4	413	CLA	CMB-C2B-C3B	2.52	129.39	124.68
15	bA	825	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	cA	815	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	b1	405	CLA	C3C-C4C-NC	-2.52	107.75	110.57
15	a4	414	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
18	b3	420	BCR	C29-C30-C25	2.52	114.36	110.48
15	aB	804	CLA	CHB-C4A-NA	2.52	127.99	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bB	847	BCR	C38-C26-C27	-2.52	108.78	113.62
15	bB	805	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
20	aB	850	LMG	C38-C37-C36	-2.52	101.64	114.42
18	aB	844	BCR	C15-C14-C13	-2.52	123.72	127.31
15	cB	815	CLA	C2D-C1D-ND	-2.52	108.25	110.10
15	cA	826	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	a2	413	CLA	C1D-ND-C4D	2.52	108.12	106.33
15	b6	414	CLA	CAC-C3C-C2C	-2.52	123.22	127.53
18	bA	852	BCR	C15-C14-C13	-2.52	123.72	127.31
15	bB	824	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	bA	825	CLA	C2D-C1D-ND	-2.52	108.25	110.10
18	c3	420	BCR	C35-C13-C14	-2.52	119.40	122.92
20	bB	851	LMG	C38-C37-C36	-2.52	101.65	114.42
15	c6	417	CLA	C3C-C4C-NC	-2.52	107.75	110.57
18	c6	402	BCR	C1-C6-C5	-2.52	119.07	122.61
15	b2	406	CLA	C3A-C2A-C1A	2.51	105.11	101.34
18	aA	851	BCR	C15-C14-C13	-2.51	123.72	127.31
18	bB	850	BCR	C23-C22-C21	-2.51	115.08	118.94
15	c2	413	CLA	C1D-ND-C4D	2.51	108.12	106.33
15	bA	827	CLA	CMD-C2D-C1D	-2.51	120.28	124.71
15	cX	102	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
15	aA	832	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
15	aA	825	CLA	C2D-C1D-ND	-2.51	108.25	110.10
15	c6	414	CLA	C2D-C1D-ND	-2.51	108.25	110.10
15	cB	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	a2	422	CLA	C11-C10-C8	-2.51	107.80	115.92
15	b6	410	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
15	b6	407	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	b5	413	CLA	CMB-C2B-C3B	2.51	129.38	124.68
15	c5	405	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
15	aB	810	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
15	b2	417	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
18	bL	201	BCR	C15-C16-C17	-2.51	118.33	123.47
18	b4	401	BCR	C15-C16-C17	-2.51	118.33	123.47
15	cA	807	CLA	O1D-CGD-CBD	2.51	129.62	124.48
15	aA	809	CLA	C1-C2-C3	-2.51	121.70	126.04
18	c5	419	BCR	C29-C30-C25	2.51	114.34	110.48
18	bL	205	BCR	C15-C16-C17	-2.51	118.34	123.47
18	b6	402	BCR	C1-C6-C5	-2.51	119.08	122.61
15	bA	809	CLA	C1-C2-C3	-2.51	121.71	126.04
15	a2	407	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	a3	405	CLA	C1B-CHB-C4A	-2.51	125.15	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c6	402	BCR	C15-C16-C17	-2.51	118.34	123.47
15	b4	402	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	aM	101	BCR	C7-C8-C9	-2.51	122.45	126.23
15	cB	835	CLA	C1B-CHB-C4A	-2.51	125.16	130.12
15	aA	819	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
18	a6	402	BCR	C1-C6-C5	-2.51	119.08	122.61
15	b2	414	CLA	C2D-C1D-ND	-2.50	108.26	110.10
18	a6	402	BCR	C15-C16-C17	-2.50	118.34	123.47
15	cB	828	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	bA	807	CLA	O1D-CGD-CBD	2.50	129.61	124.48
15	c2	417	CLA	C2A-C1A-CHA	2.50	128.24	123.86
15	a2	422	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	cM	101	BCR	C7-C8-C9	-2.50	122.45	126.23
15	b1	416	CLA	C3C-C4C-NC	-2.50	107.76	110.57
15	a5	407	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	a2	406	CLA	C3A-C2A-C1A	2.50	105.09	101.34
18	a4	401	BCR	C24-C23-C22	-2.50	122.45	126.23
15	b6	415	CLA	CAA-C2A-C3A	-2.50	110.26	116.10
15	b6	422	CLA	CHA-C4D-ND	2.50	137.74	132.50
18	cB	847	BCR	C38-C26-C27	-2.50	108.81	113.62
15	c5	416	CLA	C3C-C4C-NC	-2.50	107.76	110.57
18	c4	420	BCR	C29-C30-C25	2.50	114.33	110.48
15	bA	808	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
18	c2	421	BCR	C15-C16-C17	-2.50	118.35	123.47
15	bA	803	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	cB	812	CLA	CHD-C1D-ND	-2.50	122.16	124.45
15	cB	836	CLA	C2A-C1A-CHA	2.50	128.23	123.86
15	cA	812	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	aA	826	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
15	bB	810	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
15	bA	826	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
15	cA	827	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	a3	420	BCR	C35-C13-C14	-2.50	119.42	122.92
15	cA	808	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
18	aI	101	BCR	C15-C16-C17	-2.50	118.36	123.47
15	a1	412	CLA	CMB-C2B-C3B	2.50	129.35	124.68
15	bA	842	CLA	CMB-C2B-C3B	2.50	129.35	124.68
18	bI	101	BCR	C15-C16-C17	-2.50	118.36	123.47
15	aB	823	CLA	C2A-C1A-CHA	2.50	128.22	123.86
15	aB	815	CLA	C2D-C1D-ND	-2.50	108.26	110.10
15	c4	414	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
15	c3	416	CLA	C3C-C4C-NC	-2.50	107.77	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	402	CLA	CHB-C4A-NA	2.50	127.96	124.51
15	a6	415	CLA	CAA-C2A-C3A	-2.50	110.27	116.10
15	c3	414	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
20	aB	850	LMG	C42-C41-C40	-2.50	101.75	114.42
20	cB	850	LMG	C42-C41-C40	-2.50	101.75	114.42
15	aA	827	CLA	CHB-C4A-NA	2.50	127.96	124.51
15	cA	803	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
15	c1	411	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
15	a5	416	CLA	C3C-C4C-NC	-2.49	107.77	110.57
18	cI	101	BCR	C15-C16-C17	-2.49	118.36	123.47
15	aA	836	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
15	b5	410	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
15	a4	407	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
15	b3	406	CLA	CHB-C4A-NA	2.49	127.96	124.51
15	bB	836	CLA	C2A-C1A-CHA	2.49	128.22	123.86
15	a4	413	CLA	CMB-C2B-C3B	2.49	129.34	124.68
18	a3	420	BCR	C29-C30-C25	2.49	114.32	110.48
15	bB	835	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
15	a1	422	CLA	CHA-C1A-NA	-2.49	120.69	126.40
15	cA	827	CLA	CMD-C2D-C1D	-2.49	120.32	124.71
15	aB	835	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
15	b6	416	CLA	CBA-CAA-C2A	2.49	121.22	113.86
15	b2	417	CLA	C2A-C1A-CHA	2.49	128.22	123.86
15	bA	827	CLA	CHB-C4A-NA	2.49	127.96	124.51
15	cB	801	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	aF	203	BCR	C11-C10-C9	-2.49	123.75	127.31
18	b5	419	BCR	C24-C23-C22	-2.49	122.47	126.23
18	aI	103	BCR	C15-C16-C17	-2.49	118.37	123.47
15	cA	805	CLA	CHB-C4A-NA	2.49	127.96	124.51
15	aB	804	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
18	b3	420	BCR	C35-C13-C14	-2.49	119.43	122.92
15	bB	823	CLA	C2A-C1A-CHA	2.49	128.22	123.86
15	aB	828	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
15	bB	822	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
15	cB	804	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
20	bB	851	LMG	C42-C41-C40	-2.49	101.78	114.42
18	b4	401	BCR	C24-C23-C22	-2.49	122.47	126.23
15	bB	832	CLA	CHB-C4A-NA	2.49	127.95	124.51
15	c6	407	CLA	CHB-C4A-NA	2.49	127.95	124.51
15	cA	832	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
15	aB	836	CLA	C2A-C1A-CHA	2.49	128.21	123.86
15	c2	409	CLA	O2D-CGD-O1D	-2.49	118.97	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	826	CLA	C3C-C4C-NC	-2.49	107.78	110.57
15	aB	814	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
15	cB	814	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
15	bB	814	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
15	b5	417	CLA	CHD-C1D-ND	-2.49	122.17	124.45
15	b5	405	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
18	bA	852	BCR	C10-C11-C12	-2.49	115.46	123.22
18	bL	206	BCR	C15-C16-C17	-2.49	118.38	123.47
15	aA	812	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
15	cB	841	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
15	c2	406	CLA	C3A-C2A-C1A	2.49	105.06	101.34
15	b2	412	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	cL	203	CLA	O2D-CGD-CBD	2.49	115.69	111.27
15	bB	804	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
15	c5	405	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
18	b6	421	BCR	C15-C14-C13	-2.49	123.76	127.31
15	a6	416	CLA	CBA-CAA-C2A	2.49	121.20	113.86
15	a1	410	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	a1	415	CLA	C3C-C4C-NC	-2.49	107.78	110.57
18	b2	421	BCR	C15-C16-C17	-2.48	118.38	123.47
15	aB	832	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	cB	804	CLA	C1C-C2C-C3C	2.48	109.57	106.96
15	a4	411	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
15	cB	810	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
15	cB	822	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
15	cB	842	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
15	b5	412	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	bL	204	CLA	O2D-CGD-CBD	2.48	115.68	111.27
18	a1	417	BCR	C3-C4-C5	-2.48	109.64	114.08
18	b4	420	BCR	C29-C30-C25	2.48	114.30	110.48
15	a1	405	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	bA	832	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
15	aA	803	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	c3	420	BCR	C29-C30-C25	2.48	114.30	110.48
15	c4	414	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
18	c1	420	BCR	C24-C23-C22	-2.48	122.49	126.23
15	a3	414	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
15	cB	805	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
15	b3	414	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
15	cB	832	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	a6	421	BCR	C24-C23-C22	-2.48	122.49	126.23
15	bB	801	CLA	O2D-CGD-O1D	-2.48	118.99	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	826	CLA	C3C-C4C-NC	-2.48	107.79	110.57
15	a3	412	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
15	aB	842	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
15	cB	833	CLA	C6-C7-C8	-2.48	107.91	115.92
15	bA	811	CLA	CHB-C4A-NA	2.48	127.94	124.51
15	aA	807	CLA	O1D-CGD-CBD	2.48	129.56	124.48
18	a1	421	BCR	C15-C14-C13	-2.48	123.77	127.31
18	cL	204	BCR	C15-C16-C17	-2.48	118.40	123.47
15	bA	836	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
15	cB	823	CLA	C2A-C1A-CHA	2.48	128.19	123.86
15	a3	421	CLA	CMB-C2B-C3B	2.48	129.31	124.68
15	a1	422	CLA	CHA-C4D-ND	2.48	137.68	132.50
15	cB	801	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
15	b1	409	CLA	CHB-C4A-NA	2.48	127.94	124.51
15	aA	826	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
18	a2	421	BCR	C29-C30-C25	2.47	114.29	110.48
15	aA	827	CLA	CMD-C2D-C1D	-2.47	120.35	124.71
18	bJ	105	BCR	C11-C10-C9	-2.47	123.78	127.31
15	c3	417	CLA	CHD-C1D-ND	-2.47	122.18	124.45
15	aB	805	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
15	a5	405	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
15	aA	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
15	a4	415	CLA	C2D-C1D-ND	-2.47	108.28	110.10
15	c4	415	CLA	CBA-CAA-C2A	2.47	121.16	113.86
15	a6	406	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
15	cB	826	CLA	C3C-C4C-NC	-2.47	107.80	110.57
18	b6	402	BCR	C15-C16-C17	-2.47	118.41	123.47
15	a2	413	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
15	b6	406	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
15	cA	836	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
18	a4	420	BCR	C29-C30-C25	2.47	114.28	110.48
15	aB	822	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
15	bA	829	CLA	C2A-C1A-CHA	2.47	128.18	123.86
15	cA	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	bB	846	BCR	C7-C8-C9	-2.47	122.50	126.23
14	aA	801	CL0	O2A-CGA-CBA	2.47	119.65	111.91
15	b3	410	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
15	a4	409	CLA	CHB-C4A-NA	2.47	127.92	124.51
15	a2	404	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
15	cA	828	CLA	CHB-C4A-NA	2.47	127.92	124.51
15	a5	411	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
15	a3	412	CLA	CMC-C2C-C3C	2.47	132.81	126.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	414	CLA	C2D-C1D-ND	-2.47	108.29	110.10
15	bL	202	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
15	c2	422	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	cF	205	BCR	C11-C10-C9	-2.47	123.79	127.31
15	a2	408	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
18	cA	850	BCR	C10-C11-C12	-2.47	115.52	123.22
15	c6	416	CLA	O2A-CGA-O1A	-2.47	117.15	123.30
15	c5	420	CLA	C11-C10-C8	-2.47	107.95	115.92
18	b5	419	BCR	C29-C30-C25	2.47	114.28	110.48
18	aA	851	BCR	C10-C11-C12	-2.47	115.52	123.22
15	b3	407	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
15	cA	826	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
15	aL	203	CLA	O2D-CGD-CBD	2.46	115.65	111.27
15	bB	833	CLA	C6-C7-C8	-2.46	107.95	115.92
15	a1	409	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
18	bM	101	BCR	C7-C8-C9	-2.46	122.51	126.23
15	a6	413	CLA	CMC-C2C-C3C	2.46	132.81	126.12
15	c4	409	CLA	CHB-C4A-NA	2.46	127.92	124.51
15	b2	408	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
15	a3	416	CLA	C3C-C4C-NC	-2.46	107.81	110.57
15	b4	412	CLA	C1D-ND-C4D	2.46	108.08	106.33
15	bB	841	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	aB	801	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
15	aB	841	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	b6	417	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
15	c2	417	CLA	C3C-C4C-NC	-2.46	107.81	110.57
15	c2	404	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	a6	410	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
15	c3	412	CLA	CMC-C2C-C3C	2.46	132.80	126.12
15	b1	411	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	a6	407	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	c4	401	BCR	C15-C16-C17	-2.46	118.43	123.47
15	a4	409	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	b5	412	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	aB	833	CLA	C6-C7-C8	-2.46	107.97	115.92
15	bA	832	CLA	CMB-C2B-C3B	2.46	129.28	124.68
15	aB	802	CLA	O2D-CGD-CBD	2.46	115.64	111.27
15	aL	201	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	b6	416	CLA	O2A-CGA-O1A	-2.46	117.17	123.30
15	bA	841	CLA	C4-C3-C5	2.46	119.41	115.27
18	cB	846	BCR	C7-C8-C9	-2.46	122.52	126.23
15	b5	416	CLA	C3C-C4C-NC	-2.46	107.81	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	420	CLA	C11-C10-C8	-2.46	107.97	115.92
15	b4	415	CLA	CBA-CAA-C2A	2.46	121.12	113.86
15	b1	415	CLA	O2A-CGA-O1A	-2.46	117.17	123.30
15	c3	412	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	cB	833	CLA	CHD-C1D-ND	-2.46	122.20	124.45
15	bB	802	CLA	O2D-CGD-CBD	2.46	115.63	111.27
15	bA	835	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
14	bA	801	CL0	O2A-CGA-CBA	2.46	119.62	111.91
15	b3	412	CLA	CMC-C2C-C3C	2.46	132.78	126.12
18	c5	419	BCR	C24-C23-C22	-2.46	122.52	126.23
15	a6	416	CLA	O2A-CGA-O1A	-2.46	117.18	123.30
15	a5	412	CLA	CHA-C1A-NA	-2.46	120.78	126.40
15	c4	412	CLA	CHA-C1A-NA	-2.46	120.78	126.40
15	aB	833	CLA	CHD-C1D-ND	-2.45	122.20	124.45
15	cA	825	CLA	C2D-C1D-ND	-2.45	108.30	110.10
15	cK	102	CLA	CHB-C4A-NA	2.45	127.91	124.51
15	c4	406	CLA	CHB-C4A-NA	2.45	127.91	124.51
15	bK	101	CLA	O2A-CGA-O1A	-2.45	117.18	123.30
15	cA	841	CLA	C4-C3-C5	2.45	119.40	115.27
15	a1	413	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
15	b5	415	CLA	CBA-CAA-C2A	2.45	121.11	113.86
15	b1	416	CLA	C2A-C1A-CHA	2.45	128.15	123.86
15	aA	838	CLA	C2D-C1D-ND	-2.45	108.30	110.10
15	aK	102	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
15	c6	410	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
15	cB	806	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
15	bB	842	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
15	a4	412	CLA	C1D-ND-C4D	2.45	108.08	106.33
18	a2	421	BCR	C3-C4-C5	-2.45	109.70	114.08
15	a2	415	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
15	cA	835	CLA	C1-C2-C3	-2.45	121.80	126.04
15	aB	801	CLA	CHB-C4A-NA	2.45	127.90	124.51
15	aB	806	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
18	b6	421	BCR	C7-C8-C9	-2.45	122.53	126.23
15	cA	829	CLA	C6-C7-C8	-2.45	108.00	115.92
15	c3	416	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
15	a5	412	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
14	cA	801	CL0	O2A-CGA-CBA	2.45	119.60	111.91
15	cK	102	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
15	c1	415	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
15	b3	405	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
18	b1	420	BCR	C24-C23-C22	-2.45	122.53	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	422	CLA	CMB-C2B-C3B	2.45	129.26	124.68
18	aA	849	BCR	C30-C25-C26	-2.45	119.17	122.61
15	a1	415	CLA	C2A-C1A-CHA	2.45	128.14	123.86
15	aA	835	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	bA	826	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	b5	411	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	c1	411	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	c5	411	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
18	a5	419	BCR	C29-C30-C25	2.45	114.25	110.48
15	b1	414	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	c6	413	CLA	CMC-C2C-C3C	2.45	132.76	126.12
15	c5	415	CLA	CBA-CAA-C2A	2.45	121.08	113.86
15	c6	406	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	cB	802	CLA	O2D-CGD-CBD	2.45	115.61	111.27
15	a5	417	CLA	CHD-C1D-ND	-2.45	122.21	124.45
15	b2	422	CLA	C11-C10-C8	-2.44	108.02	115.92
18	b6	420	BCR	C15-C16-C17	-2.44	118.47	123.47
15	aA	829	CLA	C6-C7-C8	-2.44	108.02	115.92
15	b4	409	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	cL	201	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	b2	417	CLA	C3C-C4C-NC	-2.44	107.83	110.57
15	bA	829	CLA	C6-C7-C8	-2.44	108.02	115.92
15	c1	412	CLA	C1D-ND-C4D	2.44	108.07	106.33
15	b5	412	CLA	CHA-C1A-NA	-2.44	120.80	126.40
15	a2	405	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
15	c3	404	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	c5	407	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
18	cF	202	BCR	C1-C6-C5	-2.44	119.17	122.61
15	b2	404	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	c1	414	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
18	b6	402	BCR	C24-C23-C22	-2.44	122.55	126.23
15	a1	411	CLA	CMC-C2C-C3C	2.44	132.75	126.12
15	a6	417	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	aB	804	CLA	C1C-C2C-C3C	2.44	109.52	106.96
15	b5	420	CLA	C11-C10-C8	-2.44	108.03	115.92
15	a3	407	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	b2	407	CLA	O2A-CGA-O1A	-2.44	117.21	123.30
15	c6	405	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	aA	821	CLA	CMB-C2B-C3B	2.44	129.25	124.68
15	c6	417	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	b1	410	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
15	cA	835	CLA	C1B-CHB-C4A	-2.44	125.28	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	835	CLA	C1-C2-C3	-2.44	121.82	126.04
15	bB	842	CLA	CHB-C4A-NA	2.44	127.89	124.51
15	bB	833	CLA	CHD-C1D-ND	-2.44	122.21	124.45
15	cA	829	CLA	C2A-C1A-CHA	2.44	128.12	123.86
15	aA	828	CLA	CHB-C4A-NA	2.44	127.88	124.51
15	aA	841	CLA	C4-C3-C5	2.44	119.37	115.27
15	bB	808	CLA	O2D-CGD-CBD	2.44	115.60	111.27
15	cA	807	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
15	a2	405	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
15	bA	813	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
18	aB	846	BCR	C7-C8-C9	-2.44	122.55	126.23
18	c6	420	BCR	C15-C16-C17	-2.44	118.48	123.47
15	cJ	102	CLA	CMB-C2B-C3B	2.44	129.24	124.68
15	cA	823	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
15	c3	411	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
18	c5	401	BCR	C15-C16-C17	-2.44	118.48	123.47
15	bB	814	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
15	cA	815	CLA	C2D-C1D-ND	-2.44	108.31	110.10
15	aA	835	CLA	C1-C2-C3	-2.44	121.83	126.04
15	bB	806	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
18	bA	850	BCR	C30-C25-C26	-2.44	119.18	122.61
18	b2	420	BCR	C27-C26-C25	2.44	126.27	122.73
18	a5	419	BCR	C24-C23-C22	-2.44	122.55	126.23
18	c2	421	BCR	C3-C4-C5	-2.44	109.73	114.08
15	c1	409	CLA	CHB-C4A-NA	2.44	127.88	124.51
15	c2	415	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
15	b1	405	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
15	c2	405	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
18	bB	849	BCR	C1-C6-C5	-2.43	119.18	122.61
15	b3	411	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
15	cA	832	CLA	CMB-C2B-C3B	2.43	129.23	124.68
15	c5	412	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	b6	408	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
15	a2	409	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
18	cM	101	BCR	C24-C23-C22	-2.43	122.56	126.23
15	aA	832	CLA	CMB-C2B-C3B	2.43	129.23	124.68
15	cB	814	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
15	cA	821	CLA	CMB-C2B-C3B	2.43	129.23	124.68
15	bB	804	CLA	C1C-C2C-C3C	2.43	109.51	106.96
18	b2	421	BCR	C3-C4-C5	-2.43	109.73	114.08
15	c3	405	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
15	bB	801	CLA	CHB-C4A-NA	2.43	127.88	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	422	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	b4	409	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	c5	412	CLA	CHA-C1A-NA	-2.43	120.83	126.40
15	b5	406	CLA	O2A-CGA-O1A	-2.43	117.24	123.30
18	b5	401	BCR	C15-C16-C17	-2.43	118.49	123.47
15	b4	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	aA	813	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
15	c1	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	c2	413	CLA	CHA-C1A-NA	-2.43	120.83	126.40
15	b5	407	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
15	bK	101	CLA	O2D-CGD-CBD	2.43	115.59	111.27
15	c3	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	cB	814	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	bA	823	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	b1	420	BCR	C29-C30-C25	2.43	114.22	110.48
15	b2	413	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
15	a2	417	CLA	C3C-C4C-NC	-2.43	107.85	110.57
15	b3	417	CLA	CHD-C1D-ND	-2.43	122.22	124.45
15	c5	417	CLA	CHD-C1D-ND	-2.43	122.22	124.45
15	c3	421	CLA	CMB-C2B-C3B	2.43	129.22	124.68
15	b6	405	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	bK	101	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	a1	421	BCR	C24-C23-C22	-2.43	122.57	126.23
15	cA	813	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	c2	422	CLA	C11-C10-C8	-2.43	108.07	115.92
15	b2	405	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	b2	405	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
15	a1	404	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	a4	402	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	a4	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	aM	101	BCR	C24-C23-C22	-2.43	122.57	126.23
15	aB	808	CLA	O2D-CGD-CBD	2.43	115.58	111.27
15	a1	408	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	b1	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	aA	829	CLA	C2A-C1A-CHA	2.43	128.10	123.86
15	a5	415	CLA	CBA-CAA-C2A	2.43	121.02	113.86
18	c6	401	BCR	C15-C14-C13	-2.43	123.85	127.31
15	cA	804	CLA	C1-C2-C3	-2.42	121.85	126.04
18	b6	421	BCR	C24-C23-C22	-2.42	122.57	126.23
15	aB	842	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	cB	842	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	a6	408	CLA	C1B-CHB-C4A	-2.42	125.31	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	407	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
15	bB	815	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
15	a4	415	CLA	O2A-CGA-O1A	-2.42	117.26	123.30
15	c5	404	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	a3	406	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	aB	814	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
15	c6	415	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	b2	409	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	cJ	103	BCR	C30-C25-C26	-2.42	119.20	122.61
15	a1	410	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	c4	416	CLA	C2A-C1A-CHA	2.42	128.09	123.86
18	cA	848	BCR	C30-C25-C26	-2.42	119.20	122.61
15	a2	412	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
15	bA	828	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	a6	420	BCR	C15-C16-C17	-2.42	118.52	123.47
15	aA	834	CLA	C2D-C1D-ND	-2.42	108.32	110.10
15	bJ	102	CLA	CMB-C2B-C3B	2.42	129.21	124.68
15	b3	416	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
18	aF	201	BCR	C1-C6-C5	-2.42	119.20	122.61
15	a6	405	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
15	b2	415	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
15	c2	412	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
18	bJ	103	BCR	C30-C25-C26	-2.42	119.21	122.61
15	b4	412	CLA	CHA-C1A-NA	-2.42	120.86	126.40
15	bB	839	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
15	bB	803	CLA	C2A-C1A-CHA	2.42	128.09	123.86
15	c4	412	CLA	C1D-ND-C4D	2.42	108.05	106.33
15	aJ	203	CLA	CMB-C2B-C3B	2.42	129.20	124.68
15	aA	823	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
15	aK	102	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	a5	412	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	cB	815	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
15	b2	406	CLA	C11-C10-C8	-2.42	108.11	115.92
15	c1	412	CLA	CMC-C2C-C3C	2.42	132.68	126.12
15	cB	808	CLA	O2D-CGD-CBD	2.42	115.56	111.27
18	c3	401	BCR	C24-C23-C22	-2.42	122.58	126.23
15	cB	839	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
15	aJ	202	CLA	CAA-CBA-CGA	-2.42	106.10	112.51
18	b1	420	BCR	C3-C4-C5	-2.42	109.76	114.08
15	cB	832	CLA	C2D-C1D-ND	-2.42	108.32	110.10
15	a6	413	CLA	CHB-C4A-NA	2.42	127.85	124.51
15	bA	807	CLA	O2D-CGD-O1D	-2.42	119.12	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a6	422	CLA	CHA-C4D-ND	2.41	137.55	132.50
15	aB	804	CLA	CHC-C1C-NC	2.41	127.87	124.20
15	bA	821	CLA	CMB-C2B-C3B	2.41	129.19	124.68
15	a3	412	CLA	CHB-C4A-NA	2.41	127.85	124.51
15	a1	409	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
18	c3	420	BCR	C24-C23-C22	-2.41	122.59	126.23
18	cA	851	BCR	C1-C6-C5	-2.41	119.22	122.61
15	c5	406	CLA	O2A-CGA-O1A	-2.41	117.29	123.30
18	a6	402	BCR	C24-C23-C22	-2.41	122.59	126.23
18	bM	101	BCR	C24-C23-C22	-2.41	122.59	126.23
15	aA	804	CLA	C1-C2-C3	-2.41	121.87	126.04
18	b4	401	BCR	C1-C6-C5	-2.41	119.22	122.61
15	cK	102	CLA	O2D-CGD-CBD	2.41	115.55	111.27
15	aK	102	CLA	O2D-CGD-CBD	2.41	115.55	111.27
18	a2	420	BCR	C27-C26-C25	2.41	126.23	122.73
15	b5	406	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	c2	414	CLA	C2D-C1D-ND	-2.41	108.33	110.10
15	cB	804	CLA	CHC-C1C-NC	2.41	127.86	124.20
15	b2	414	CLA	CMB-C2B-C3B	2.41	129.19	124.68
15	aB	803	CLA	C2A-C1A-CHA	2.41	128.07	123.86
18	bA	853	BCR	C1-C6-C5	-2.41	119.22	122.61
15	bA	804	CLA	C1-C2-C3	-2.41	121.88	126.04
15	a5	406	CLA	O2A-CGA-O1A	-2.41	117.30	123.30
18	b1	401	BCR	C27-C26-C25	2.41	126.23	122.73
18	aJ	204	BCR	C30-C25-C26	-2.41	119.22	122.61
15	a2	418	CLA	C2A-C1A-CHA	2.41	128.07	123.86
15	a3	417	CLA	CHD-C1D-ND	-2.41	122.24	124.45
18	b3	420	BCR	C24-C23-C22	-2.41	122.60	126.23
15	aB	815	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
15	b6	413	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	aA	842	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	cF	201	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	c5	406	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	bB	803	CLA	O2D-CGD-CBD	2.40	115.54	111.27
15	bA	842	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	bB	812	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	a6	415	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	bB	840	CLA	C2A-C1A-CHA	2.40	128.06	123.86
18	a1	419	BCR	C29-C30-C25	2.40	114.18	110.48
15	c2	414	CLA	CMB-C2B-C3B	2.40	129.18	124.68
15	cB	806	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
15	a2	413	CLA	CHA-C1A-NA	-2.40	120.89	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a3	420	BCR	C24-C23-C22	-2.40	122.60	126.23
18	c4	418	BCR	C7-C8-C9	-2.40	122.60	126.23
18	a1	420	BCR	C34-C9-C10	-2.40	119.56	122.92
18	c1	420	BCR	C29-C30-C25	2.40	114.18	110.48
15	c6	408	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	c2	420	BCR	C27-C26-C25	2.40	126.22	122.73
18	aA	852	BCR	C1-C6-C5	-2.40	119.23	122.61
15	bB	804	CLA	CHC-C1C-NC	2.40	127.85	124.20
15	aA	813	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
15	c5	411	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
15	aB	814	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	b6	413	CLA	CMC-C2C-C3C	2.40	132.64	126.12
15	b2	408	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	cA	813	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
15	c1	416	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	a3	421	CLA	CHA-C4D-ND	2.40	137.52	132.50
15	aA	807	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
15	bA	838	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
15	a3	416	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
15	b4	416	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	bA	815	CLA	C2D-C1D-ND	-2.40	108.34	110.10
15	c2	405	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
15	b3	403	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	cB	840	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	aA	823	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	b1	401	BCR	C7-C8-C9	-2.40	122.61	126.23
15	b3	421	CLA	CMB-C2B-C3B	2.40	129.16	124.68
18	cI	102	BCR	C16-C15-C14	-2.40	118.57	123.47
15	a3	411	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
15	b6	415	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
15	b4	412	CLA	CMC-C2C-C3C	2.40	132.62	126.12
15	c4	412	CLA	CMC-C2C-C3C	2.40	132.62	126.12
15	c6	414	CLA	CMB-C2B-C3B	2.40	129.16	124.68
15	cA	814	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
15	bJ	101	CLA	CAA-CBA-CGA	-2.39	106.15	112.51
15	a5	404	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
18	c5	419	BCR	C3-C4-C5	-2.39	109.80	114.08
15	a5	406	CLA	CHB-C4A-NA	2.39	127.82	124.51
18	cI	102	BCR	C16-C17-C18	-2.39	123.89	127.31
15	aB	803	CLA	O2D-CGD-CBD	2.39	115.52	111.27
18	bL	206	BCR	C15-C14-C13	-2.39	123.90	127.31
15	a2	406	CLA	O2A-CGA-CBA	-2.39	104.40	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	813	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
15	aB	806	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
15	aB	840	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	b6	404	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	c3	403	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	c5	415	CLA	O2A-CGA-O1A	-2.39	117.34	123.30
15	a5	416	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
15	c6	418	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	a6	414	CLA	CMB-C2B-C3B	2.39	129.15	124.68
15	bB	834	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
15	a4	416	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	cJ	101	CLA	CAA-CBA-CGA	-2.39	106.17	112.51
18	c4	401	BCR	C1-C6-C5	-2.39	119.25	122.61
15	c3	412	CLA	CHA-C1A-NA	-2.39	120.93	126.40
15	a5	412	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	b4	416	CLA	C3C-C4C-NC	-2.39	107.89	110.57
15	c2	422	CLA	CMB-C2B-C3B	2.39	129.15	124.68
15	cA	823	CLA	CHB-C4A-NA	2.39	127.81	124.51
15	b2	413	CLA	CHA-C1A-NA	-2.39	120.93	126.40
15	bA	824	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
15	cA	835	CLA	CMB-C2B-C3B	2.39	129.15	124.68
15	a4	412	CLA	CHA-C1A-NA	-2.39	120.93	126.40
18	b4	418	BCR	C7-C8-C9	-2.39	122.63	126.23
15	c1	405	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
15	cB	834	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
15	bB	814	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
18	aL	205	BCR	C15-C14-C13	-2.39	123.90	127.31
15	bA	828	CLA	CMB-C2B-C3B	2.39	129.14	124.68
15	cA	843	CLA	CHD-C1D-ND	-2.39	122.26	124.45
18	aA	849	BCR	C38-C26-C27	-2.39	109.03	113.62
15	c4	416	CLA	C3C-C4C-NC	-2.39	107.90	110.57
18	bF	202	BCR	C38-C26-C27	-2.39	109.03	113.62
18	a4	401	BCR	C15-C16-C17	-2.38	118.59	123.47
18	c3	419	BCR	C3-C4-C5	-2.38	109.82	114.08
15	a3	415	CLA	CBA-CAA-C2A	2.38	120.90	113.86
15	b2	406	CLA	O2A-CGA-CBA	-2.38	104.42	111.91
15	c5	410	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
15	bA	829	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
15	cA	844	CLA	CAA-CBA-CGA	2.38	120.22	113.25
15	b4	421	CLA	CHA-C4D-ND	2.38	137.49	132.50
18	c1	401	BCR	C3-C4-C5	-2.38	109.82	114.08
15	aA	829	CLA	O2A-CGA-O1A	-2.38	117.58	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	403	CLA	C2A-C1A-CHA	2.38	128.03	123.86
15	cB	803	CLA	C2A-C1A-CHA	2.38	128.03	123.86
18	aI	103	BCR	C39-C30-C25	2.38	114.17	110.30
15	cB	803	CLA	O2D-CGD-CBD	2.38	115.50	111.27
18	aI	101	BCR	C38-C26-C27	-2.38	109.04	113.62
15	b3	415	CLA	O2A-CGA-O1A	-2.38	117.36	123.30
18	cI	101	BCR	C38-C26-C27	-2.38	109.04	113.62
15	cA	838	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	a3	401	BCR	C24-C23-C22	-2.38	122.64	126.23
15	aB	839	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
15	c5	416	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
18	c6	401	BCR	C27-C26-C25	2.38	126.19	122.73
18	b1	420	BCR	C1-C6-C5	-2.38	119.26	122.61
15	cK	102	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	cF	204	BCR	C38-C26-C27	-2.38	109.04	113.62
18	a1	419	BCR	C15-C16-C17	-2.38	118.60	123.47
18	cL	204	BCR	C39-C30-C25	2.38	114.16	110.30
18	bA	850	BCR	C38-C26-C27	-2.38	109.04	113.62
18	bI	102	BCR	C16-C15-C14	-2.38	118.60	123.47
18	b4	420	BCR	C15-C16-C17	-2.38	118.60	123.47
15	aB	808	CLA	CAC-C3C-C4C	2.38	127.90	124.81
15	c3	421	CLA	CHA-C4D-ND	2.38	137.48	132.50
15	cA	829	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	cB	845	BCR	C7-C8-C9	-2.38	122.64	126.23
15	c2	407	CLA	O2A-CGA-O1A	-2.38	117.37	123.30
18	b6	401	BCR	C15-C14-C13	-2.38	123.91	127.31
15	aB	832	CLA	C2D-C1D-ND	-2.38	108.35	110.10
18	c1	401	BCR	C27-C26-C25	2.38	126.19	122.73
15	cB	821	CLA	CMB-C2B-C3B	2.38	129.13	124.68
15	bB	806	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	cB	812	CLA	CHB-C4A-NA	2.38	127.80	124.51
15	aA	803	CLA	CMD-C2D-C3D	2.38	133.09	127.61
15	b6	411	CLA	C1D-ND-C4D	2.38	108.03	106.33
15	bA	835	CLA	CMB-C2B-C3B	2.38	129.13	124.68
15	c2	418	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	bB	806	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
15	c6	404	CLA	C2A-C1A-CHA	2.38	128.02	123.86
18	aI	102	BCR	C16-C17-C18	-2.38	123.92	127.31
15	a6	404	CLA	C2A-C1A-CHA	2.38	128.02	123.86
18	a3	420	BCR	C15-C16-C17	-2.38	118.60	123.47
15	b3	412	CLA	CHA-C1A-NA	-2.38	120.95	126.40
15	c5	410	CLA	C1D-ND-C4D	2.38	108.02	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	843	CLA	CMB-C2B-C3B	2.38	129.13	124.68
15	bA	821	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	a5	402	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
18	bI	101	BCR	C38-C26-C27	-2.38	109.05	113.62
15	cA	842	CLA	CMB-C2B-C3B	2.38	129.12	124.68
15	aA	845	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	cA	824	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
15	b6	414	CLA	CHC-C1C-NC	2.38	127.81	124.20
15	b6	418	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	cB	814	CLA	CHD-C1D-ND	-2.38	122.27	124.45
18	aI	102	BCR	C16-C15-C14	-2.38	118.61	123.47
15	bA	803	CLA	CMD-C2D-C3D	2.38	133.08	127.61
15	bB	821	CLA	CMB-C2B-C3B	2.37	129.12	124.68
15	aB	834	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
15	c6	413	CLA	CHA-C1A-NA	-2.37	120.96	126.40
15	aB	814	CLA	CHD-C1D-ND	-2.37	122.27	124.45
15	aA	824	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
15	bA	820	CLA	C2A-C1A-CHA	2.37	128.01	123.86
15	c5	403	CLA	C2A-C1A-CHA	2.37	128.01	123.86
15	a2	408	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	cB	823	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	a1	407	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	b5	412	CLA	C2A-C1A-CHA	2.37	128.01	123.86
15	b1	410	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
18	b3	419	BCR	C3-C4-C5	-2.37	109.84	114.08
15	a5	411	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	c2	412	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
15	cA	803	CLA	CMD-C2D-C3D	2.37	133.07	127.61
15	cA	834	CLA	C2D-C1D-ND	-2.37	108.36	110.10
15	b3	412	CLA	C1D-ND-C4D	2.37	108.02	106.33
15	bA	814	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	a2	414	CLA	CMB-C2B-C3B	2.37	129.11	124.68
15	aB	821	CLA	CMB-C2B-C3B	2.37	129.11	124.68
15	b1	405	CLA	O1D-CGD-CBD	2.37	129.33	124.48
15	aA	821	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	a5	410	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	c4	413	CLA	C2D-C1D-ND	-2.37	108.36	110.10
15	aA	814	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	aB	823	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	b2	403	CLA	C2A-C1A-CHA	2.37	128.00	123.86
15	b3	421	CLA	CHA-C4D-ND	2.37	137.45	132.50
15	aB	806	CLA	O2A-CGA-O1A	-2.37	117.62	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	404	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
15	a4	412	CLA	CMC-C2C-C3C	2.37	132.54	126.12
15	c3	410	CLA	C2A-C1A-CHA	2.37	128.00	123.86
18	aA	849	BCR	C11-C10-C9	-2.37	123.93	127.31
18	a4	401	BCR	C1-C6-C5	-2.37	119.28	122.61
15	cB	806	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
15	bB	823	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
15	c4	415	CLA	O2A-CGA-O1A	-2.37	117.40	123.30
15	aA	843	CLA	CMB-C2B-C3B	2.37	129.10	124.68
18	aF	202	BCR	C38-C26-C27	-2.36	109.07	113.62
18	a1	420	BCR	C3-C4-C5	-2.36	109.86	114.08
15	b3	404	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
15	bA	823	CLA	CHB-C4A-NA	2.36	127.78	124.51
15	c1	410	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
15	a4	416	CLA	C3C-C4C-NC	-2.36	107.92	110.57
15	a6	418	CLA	C2A-C1A-CHA	2.36	127.99	123.86
15	aA	844	CLA	CHD-C1D-ND	-2.36	122.28	124.45
18	a6	401	BCR	C15-C14-C13	-2.36	123.94	127.31
18	cA	848	BCR	C38-C26-C27	-2.36	109.08	113.62
18	bB	845	BCR	C7-C8-C9	-2.36	122.66	126.23
15	aA	838	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
15	b1	417	CLA	C3A-C2A-C1A	2.36	104.88	101.34
15	b6	414	CLA	C2D-C1D-ND	-2.36	108.36	110.10
18	a1	420	BCR	C27-C26-C25	2.36	126.16	122.73
18	a1	419	BCR	C3-C4-C5	-2.36	109.86	114.08
18	bI	102	BCR	C3-C4-C5	-2.36	109.86	114.08
15	c2	406	CLA	O2A-CGA-CBA	-2.36	104.50	111.91
15	aA	828	CLA	CMB-C2B-C3B	2.36	129.10	124.68
15	aA	845	CLA	CAA-CBA-CGA	2.36	120.15	113.25
15	bA	845	CLA	CAA-CBA-CGA	2.36	120.15	113.25
15	aK	102	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
15	a6	411	CLA	C1D-ND-C4D	2.36	108.01	106.33
15	c6	413	CLA	CHB-C4A-NA	2.36	127.78	124.51
15	a1	414	CLA	O2A-CGA-O1A	-2.36	117.42	123.30
15	a6	413	CLA	CHA-C1A-NA	-2.36	120.99	126.40
15	bB	809	CLA	CMB-C2B-C3B	2.36	129.09	124.68
16	cA	845	PQN	C21-C20-C18	-2.36	108.29	115.92
15	c3	412	CLA	C1D-ND-C4D	2.36	108.01	106.33
15	aA	835	CLA	CMB-C2B-C3B	2.36	129.09	124.68
15	b3	416	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	b6	418	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	c2	413	CLA	C2A-C1A-CHA	2.36	127.98	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a5	401	BCR	C15-C16-C17	-2.36	118.64	123.47
15	a4	421	CLA	CHA-C4D-ND	2.36	137.43	132.50
15	aB	809	CLA	CMB-C2B-C3B	2.36	129.09	124.68
15	cA	828	CLA	CMB-C2B-C3B	2.36	129.09	124.68
15	c5	413	CLA	C2D-C1D-ND	-2.36	108.37	110.10
18	c1	419	BCR	C27-C26-C25	2.36	126.15	122.73
15	a1	422	CLA	O2D-CGD-CBD	2.36	115.46	111.27
15	aA	807	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	c6	413	CLA	C1D-ND-C4D	2.36	108.01	106.33
15	b4	415	CLA	O2A-CGA-O1A	-2.36	117.43	123.30
15	b5	416	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
15	aA	802	CLA	C11-C10-C8	-2.36	108.30	115.92
15	aB	812	CLA	CHB-C4A-NA	2.36	127.77	124.51
15	cA	842	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
18	bI	102	BCR	C16-C17-C18	-2.36	123.95	127.31
15	bA	834	CLA	C2D-C1D-ND	-2.36	108.37	110.10
15	c6	417	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	b6	413	CLA	CHA-C1A-NA	-2.36	121.00	126.40
15	bA	810	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
15	b3	410	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	c5	412	CLA	C2A-C1A-CHA	2.35	127.98	123.86
15	b6	422	CLA	CMB-C2B-C3B	2.35	129.08	124.68
18	a6	401	BCR	C34-C9-C10	-2.35	119.62	122.92
18	bL	201	BCR	C15-C14-C13	-2.35	123.95	127.31
15	b5	416	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	aA	816	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
15	b5	402	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
18	b6	401	BCR	C27-C26-C25	2.35	126.15	122.73
15	b2	413	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	c1	408	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
16	bA	846	PQN	C21-C20-C18	-2.35	108.31	115.92
15	c2	411	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	bA	816	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
18	c6	402	BCR	C24-C23-C22	-2.35	122.68	126.23
15	b2	416	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
15	a3	416	CLA	C2A-C1A-CHA	2.35	127.97	123.86
16	aA	846	PQN	C21-C20-C18	-2.35	108.32	115.92
15	a2	407	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
15	cB	808	CLA	CAC-C3C-C4C	2.35	127.86	124.81
18	bL	205	BCR	C39-C30-C25	2.35	114.11	110.30
15	aX	102	CLA	O1A-CGA-CBA	2.35	130.63	123.08
15	aB	821	CLA	O2D-CGD-O1D	-2.35	119.24	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	821	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	a5	415	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
15	bB	814	CLA	CHD-C1D-ND	-2.35	122.29	124.45
18	cA	848	BCR	C11-C10-C9	-2.35	123.96	127.31
18	aB	845	BCR	C7-C8-C9	-2.35	122.68	126.23
15	a2	413	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	b5	403	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	c5	402	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
15	c4	421	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	cA	820	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	a6	412	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
15	a5	413	CLA	C2D-C1D-ND	-2.35	108.37	110.10
15	a3	412	CLA	CHA-C1A-NA	-2.35	121.02	126.40
15	b4	404	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
15	c5	416	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	bL	204	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	b3	401	BCR	C24-C23-C22	-2.35	122.69	126.23
15	c2	416	CLA	O2A-CGA-O1A	-2.35	117.45	123.30
15	aA	810	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
15	aA	843	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
15	bA	807	CLA	C2A-C1A-CHA	2.35	127.96	123.86
15	bB	839	CLA	C3A-C2A-C1A	2.35	104.86	101.34
15	aA	827	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
15	cB	821	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	c1	405	CLA	CMA-C3A-C2A	-2.35	104.36	113.83
15	c2	408	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
15	cX	102	CLA	O1A-CGA-CBA	2.35	130.62	123.08
15	b3	412	CLA	C2A-C1A-CHA	2.35	127.96	123.86
18	a3	419	BCR	C3-C4-C5	-2.35	109.89	114.08
18	b3	419	BCR	C27-C26-C25	2.35	126.14	122.73
15	b3	412	CLA	CHB-C4A-NA	2.35	127.76	124.51
15	bB	817	CLA	C2A-C1A-CHA	2.35	127.96	123.86
15	c2	418	CLA	C2A-C1A-CHA	2.35	127.96	123.86
15	cA	827	CLA	CAA-C2A-C3A	-2.35	106.36	112.78
15	b5	415	CLA	O2A-CGA-O1A	-2.35	117.45	123.30
15	aL	203	CLA	CHB-C4A-NA	2.35	127.75	124.51
15	c3	412	CLA	CHB-C4A-NA	2.35	127.75	124.51
18	a4	420	BCR	C15-C16-C17	-2.35	118.67	123.47
15	b1	412	CLA	CMC-C2C-C3C	2.34	132.48	126.12
15	a5	420	CLA	CHA-C1A-NA	-2.34	121.03	126.40
15	b2	416	CLA	CBA-CAA-C2A	2.34	120.78	113.86
15	c3	416	CLA	C2A-C1A-CHA	2.34	127.96	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	844	CLA	CHD-C1D-ND	-2.34	122.30	124.45
15	bX	102	CLA	O1A-CGA-CBA	2.34	130.61	123.08
15	cA	802	CLA	C11-C10-C8	-2.34	108.34	115.92
15	c6	411	CLA	C1D-ND-C4D	2.34	108.00	106.33
15	bB	808	CLA	CAC-C3C-C4C	2.34	127.85	124.81
15	bK	101	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	c6	412	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	aB	804	CLA	C2C-C1C-NC	-2.34	107.78	109.97
15	bA	827	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
15	bA	802	CLA	C11-C10-C8	-2.34	108.35	115.92
15	a3	415	CLA	O2A-CGA-O1A	-2.34	117.46	123.30
15	b3	415	CLA	CBA-CAA-C2A	2.34	120.78	113.86
15	b1	412	CLA	C1D-ND-C4D	2.34	108.00	106.33
18	b6	420	BCR	C24-C23-C22	-2.34	122.70	126.23
15	cB	809	CLA	CMB-C2B-C3B	2.34	129.06	124.68
15	cA	821	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
15	b5	410	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	cB	839	CLA	C3A-C2A-C1A	2.34	104.85	101.34
15	aA	820	CLA	C2A-C1A-CHA	2.34	127.95	123.86
18	b5	419	BCR	C15-C16-C17	-2.34	118.68	123.47
18	c1	420	BCR	C15-C16-C17	-2.34	118.68	123.47
15	b6	417	CLA	C2A-C1A-CHA	2.34	127.95	123.86
15	cA	828	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
15	c2	406	CLA	C11-C10-C8	-2.34	108.36	115.92
15	b5	420	CLA	CHA-C1A-NA	-2.34	121.04	126.40
15	aB	827	CLA	O2D-CGD-CBD	2.34	115.43	111.27
15	cB	804	CLA	C2C-C1C-NC	-2.34	107.78	109.97
18	b1	420	BCR	C15-C16-C17	-2.34	118.68	123.47
18	bA	850	BCR	C11-C10-C9	-2.34	123.97	127.31
15	aA	807	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	a6	417	CLA	C2A-C1A-CHA	2.34	127.95	123.86
15	aA	845	CLA	CMC-C2C-C3C	2.34	132.47	126.12
18	a1	418	BCR	C27-C26-C25	2.34	126.12	122.73
15	c5	412	CLA	CHB-C4A-NA	2.34	127.74	124.51
18	a5	419	BCR	C3-C4-C5	-2.34	109.90	114.08
15	c1	404	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
15	bA	842	CLA	O2D-CGD-CBD	2.34	115.42	111.27
15	bB	813	CLA	CHB-C4A-NA	2.34	127.74	124.51
15	cA	838	CLA	C1-C2-C3	-2.34	122.00	126.04
15	cA	807	CLA	C2A-C1A-CHA	2.34	127.94	123.86
15	cB	818	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
15	bA	845	CLA	CMC-C2C-C3C	2.34	132.46	126.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	816	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
15	a1	404	CLA	CMA-C3A-C2A	-2.33	104.41	113.83
15	aA	838	CLA	C1-C2-C3	-2.33	122.00	126.04
15	a4	417	CLA	CMA-C3A-C2A	-2.33	104.41	113.83
15	b1	404	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
15	aA	815	CLA	C2D-C1D-ND	-2.33	108.38	110.10
15	bB	832	CLA	C2D-C1D-ND	-2.33	108.38	110.10
15	cB	834	CLA	C2A-C1A-CHA	2.33	127.94	123.86
18	cI	102	BCR	C3-C4-C5	-2.33	109.91	114.08
15	a2	422	CLA	CMB-C2B-C3B	2.33	129.04	124.68
15	bA	828	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
18	c1	420	BCR	C3-C4-C5	-2.33	109.91	114.08
15	c2	405	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
15	c3	415	CLA	CBA-CAA-C2A	2.33	120.75	113.86
15	a2	416	CLA	O2A-CGA-O1A	-2.33	117.49	123.30
15	a3	417	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
15	cL	202	CLA	C3A-C2A-C1A	2.33	104.83	101.34
15	cB	827	CLA	O2D-CGD-CBD	2.33	115.41	111.27
18	a4	419	BCR	C27-C26-C25	2.33	126.11	122.73
15	bL	203	CLA	C3A-C2A-C1A	2.33	104.83	101.34
15	aL	202	CLA	C3A-C2A-C1A	2.33	104.83	101.34
15	cA	844	CLA	CMC-C2C-C3C	2.33	132.44	126.12
15	cL	203	CLA	CHB-C4A-NA	2.33	127.73	124.51
15	c3	415	CLA	O2A-CGA-O1A	-2.33	117.50	123.30
15	bA	807	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
15	a2	406	CLA	C11-C10-C8	-2.33	108.39	115.92
15	a3	412	CLA	C1D-ND-C4D	2.33	107.99	106.33
15	a3	412	CLA	C2A-C1A-CHA	2.33	127.93	123.86
15	cB	817	CLA	C2A-C1A-CHA	2.33	127.93	123.86
18	c6	420	BCR	C24-C23-C22	-2.33	122.72	126.23
15	bA	843	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	b5	401	BCR	C35-C13-C14	-2.33	119.66	122.92
18	c3	420	BCR	C15-C16-C17	-2.33	118.71	123.47
15	c5	420	CLA	CHA-C1A-NA	-2.33	121.07	126.40
15	a6	418	CLA	CHD-C1D-ND	-2.33	122.32	124.45
15	aA	828	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
15	bA	845	CLA	CHD-C1D-ND	-2.33	122.32	124.45
15	b6	414	CLA	CMB-C2B-C3B	2.32	129.03	124.68
15	cA	810	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
15	c3	412	CLA	C2A-C1A-CHA	2.32	127.92	123.86
15	cF	203	CLA	CAC-C3C-C4C	2.32	127.83	124.81
15	c6	418	CLA	CHD-C1D-ND	-2.32	122.32	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	412	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
15	bB	827	CLA	O2D-CGD-CBD	2.32	115.40	111.27
15	cF	201	CLA	O2D-CGD-CBD	2.32	115.40	111.27
15	a3	403	CLA	C2A-C1A-CHA	2.32	127.92	123.86
18	c5	419	BCR	C15-C16-C17	-2.32	118.72	123.47
15	aB	839	CLA	C3A-C2A-C1A	2.32	104.82	101.34
15	cA	844	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	b4	413	CLA	C2D-C1D-ND	-2.32	108.39	110.10
15	c1	417	CLA	C3A-C2A-C1A	2.32	104.82	101.34
18	b3	420	BCR	C15-C16-C17	-2.32	118.72	123.47
15	aA	845	CLA	CMC-C2C-C1C	-2.32	121.50	125.04
15	cA	807	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	a5	419	BCR	C15-C16-C17	-2.32	118.72	123.47
15	b6	410	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
15	c4	404	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
15	b5	413	CLA	C2D-C1D-ND	-2.32	108.39	110.10
15	bA	802	CLA	CHD-C1D-ND	-2.32	122.32	124.45
18	c4	419	BCR	C27-C26-C25	2.32	126.10	122.73
15	a2	411	CLA	C2A-C1A-CHA	2.32	127.92	123.86
15	b1	417	CLA	C2A-C1A-CHA	2.32	127.92	123.86
18	bI	101	BCR	C1-C6-C5	-2.32	119.35	122.61
15	c6	410	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
15	b2	418	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	cA	825	CLA	CHD-C1D-ND	-2.32	122.32	124.45
18	a1	419	BCR	C1-C6-C5	-2.32	119.35	122.61
18	b1	419	BCR	C27-C26-C25	2.32	126.10	122.73
15	bB	818	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
18	b5	419	BCR	C3-C4-C5	-2.32	109.94	114.08
15	aA	825	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	a4	407	CLA	CHA-C1A-NA	-2.32	121.09	126.40
18	a6	420	BCR	C24-C23-C22	-2.32	122.73	126.23
15	aB	840	CLA	CAC-C3C-C2C	-2.32	123.56	127.53
15	c2	408	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
15	bA	838	CLA	C1-C2-C3	-2.32	122.03	126.04
15	c1	412	CLA	CHA-C1A-NA	-2.32	121.09	126.40
15	a5	416	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	b3	417	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	c4	406	CLA	O2A-CGA-O1A	-2.32	117.52	123.30
15	bF	201	CLA	CAC-C3C-C4C	2.32	127.82	124.81
15	bB	805	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
15	c1	417	CLA	C2D-C1D-ND	-2.32	108.40	110.10
15	c1	403	CLA	C2A-C1A-CHA	2.32	127.91	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	403	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
15	aA	802	CLA	CHD-C1D-ND	-2.32	122.33	124.45
15	a1	411	CLA	CHA-C1A-NA	-2.32	121.09	126.40
15	aB	818	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
15	bB	831	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
15	aA	842	CLA	O2D-CGD-CBD	2.32	115.38	111.27
14	aA	801	CL0	C1-O2A-CGA	2.31	122.52	116.44
15	cB	813	CLA	CHB-C4A-NA	2.31	127.71	124.51
15	cF	201	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
15	cB	805	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
18	aB	849	BCR	C16-C15-C14	-2.31	118.73	123.47
15	cB	831	CLA	O2A-CGA-O1A	-2.31	117.53	123.30
15	a2	416	CLA	CBA-CAA-C2A	2.31	120.69	113.86
15	b2	418	CLA	CHD-C1D-ND	-2.31	122.33	124.45
15	bB	840	CLA	CAC-C3C-C2C	-2.31	123.57	127.53
18	b4	401	BCR	C15-C14-C13	-2.31	124.01	127.31
18	bF	202	BCR	C34-C9-C10	-2.31	119.68	122.92
15	a2	412	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
15	aB	817	CLA	C2A-C1A-CHA	2.31	127.90	123.86
14	bA	801	CL0	CMC-C2C-C1C	2.31	128.56	125.04
15	aB	805	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
15	bB	831	CLA	O2A-CGA-O1A	-2.31	117.54	123.30
18	c6	401	BCR	C34-C9-C10	-2.31	119.69	122.92
18	bB	846	BCR	C30-C25-C26	-2.31	119.36	122.61
14	aA	801	CL0	CMC-C2C-C1C	2.31	128.56	125.04
18	c4	420	BCR	C15-C16-C17	-2.31	118.75	123.47
18	aJ	204	BCR	C33-C5-C6	-2.31	121.94	124.53
18	a4	418	BCR	C7-C8-C9	-2.31	122.75	126.23
18	b4	419	BCR	C27-C26-C25	2.31	126.08	122.73
15	bA	842	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	bB	848	BCR	C7-C8-C9	-2.31	122.75	126.23
18	aI	102	BCR	C3-C4-C5	-2.31	109.96	114.08
18	cA	849	BCR	C40-C30-C25	2.31	114.04	110.30
15	b4	407	CLA	CHA-C1A-NA	-2.31	121.12	126.40
15	cF	203	CLA	O2A-CGA-O1A	-2.31	117.55	123.30
15	a2	403	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	b1	412	CLA	CHA-C1A-NA	-2.30	121.12	126.40
15	b5	411	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	a5	403	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	b2	411	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	b4	412	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	aA	830	CLA	O2A-CGA-O1A	-2.30	117.78	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	402	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
15	aB	831	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	cB	831	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	a1	416	CLA	C3A-C2A-C1A	2.30	104.79	101.34
15	aB	831	CLA	O2A-CGA-O1A	-2.30	117.56	123.30
15	c4	412	CLA	C2A-C1A-CHA	2.30	127.89	123.86
14	bA	801	CL0	C1-O2A-CGA	2.30	122.48	116.44
15	b4	410	CLA	C2A-C1A-CHA	2.30	127.89	123.86
18	aI	101	BCR	C1-C6-C5	-2.30	119.37	122.61
15	a2	405	CLA	CMA-C3A-C2A	-2.30	104.54	113.83
18	a6	401	BCR	C27-C26-C25	2.30	126.07	122.73
15	a4	404	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
15	c2	413	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	c1	415	CLA	CBA-CAA-C2A	2.30	120.65	113.86
14	cA	801	CL0	CMC-C2C-C1C	2.30	128.54	125.04
18	cF	202	BCR	C40-C30-C25	2.30	114.03	110.30
18	a4	401	BCR	C15-C14-C13	-2.30	124.03	127.31
18	b3	401	BCR	C2-C1-C6	2.30	114.02	110.48
15	a6	410	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
18	c2	421	BCR	C35-C13-C14	-2.30	119.70	122.92
15	a5	410	CLA	C2A-C1A-CHA	2.30	127.88	123.86
18	cI	101	BCR	C1-C6-C5	-2.30	119.38	122.61
15	bA	837	CLA	O2A-CGA-O1A	-2.30	117.57	123.30
15	aA	814	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
15	a3	410	CLA	C2A-C1A-CHA	2.30	127.88	123.86
15	a1	414	CLA	CBA-CAA-C2A	2.30	120.64	113.86
18	cB	849	BCR	C16-C15-C14	-2.30	118.77	123.47
15	aB	813	CLA	CHB-C4A-NA	2.30	127.69	124.51
15	aJ	201	CLA	O2A-CGA-O1A	-2.30	117.58	123.30
15	bA	845	CLA	CMC-C2C-C1C	-2.30	121.54	125.04
15	bA	830	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
15	c1	405	CLA	O1D-CGD-CBD	2.30	129.18	124.48
15	c4	407	CLA	CHA-C1A-NA	-2.29	121.14	126.40
15	cA	830	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
18	a4	420	BCR	C3-C4-C5	-2.29	109.98	114.08
15	aA	802	CLA	C4D-C3D-CAD	-2.29	105.39	108.10
15	aA	842	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
18	a5	401	BCR	C35-C13-C14	-2.29	119.71	122.92
15	cA	813	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
15	bB	835	CLA	CAA-C2A-C1A	2.29	119.49	111.97
14	cA	801	CL0	C1-O2A-CGA	2.29	122.46	116.44
15	c5	412	CLA	CHC-C1C-NC	2.29	127.68	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bB	849	BCR	C40-C30-C25	2.29	114.02	110.30
15	a4	406	CLA	O2A-CGA-O1A	-2.29	117.59	123.30
18	c3	419	BCR	C27-C26-C25	2.29	126.06	122.73
18	cB	846	BCR	C30-C25-C26	-2.29	119.39	122.61
18	c1	420	BCR	C1-C6-C5	-2.29	119.39	122.61
18	c3	401	BCR	C2-C1-C6	2.29	114.01	110.48
18	bB	850	BCR	C30-C25-C26	-2.29	119.39	122.61
18	bB	850	BCR	C16-C15-C14	-2.29	118.78	123.47
15	a3	417	CLA	C2A-C1A-CHA	2.29	127.86	123.86
15	c4	417	CLA	CMA-C3A-C2A	-2.29	104.59	113.83
18	a3	419	BCR	C27-C26-C25	2.29	126.05	122.73
15	bB	804	CLA	C2C-C1C-NC	-2.29	107.83	109.97
18	bA	851	BCR	C40-C30-C25	2.29	114.01	110.30
15	cB	835	CLA	CAA-C2A-C1A	2.29	119.47	111.97
15	c5	410	CLA	C2A-C1A-CHA	2.29	127.86	123.86
15	cA	807	CLA	CHA-C1A-NA	-2.29	121.16	126.40
18	cF	204	BCR	C34-C9-C10	-2.29	119.72	122.92
15	aB	834	CLA	C2A-C1A-CHA	2.29	127.86	123.86
15	b6	412	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
18	b6	401	BCR	C34-C9-C10	-2.29	119.72	122.92
15	a4	413	CLA	C2D-C1D-ND	-2.29	108.42	110.10
15	aB	835	CLA	CAA-C2A-C1A	2.29	119.47	111.97
18	a6	421	BCR	C7-C8-C9	-2.29	122.78	126.23
15	cB	806	CLA	C2D-C1D-ND	-2.29	108.42	110.10
15	aB	822	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
15	bA	807	CLA	CHA-C1A-NA	-2.28	121.17	126.40
15	aB	841	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
15	a1	402	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	cB	822	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
18	a3	401	BCR	C2-C1-C6	2.28	114.00	110.48
18	cJ	103	BCR	C33-C5-C6	-2.28	121.96	124.53
15	b3	407	CLA	CHA-C1A-NA	-2.28	121.17	126.40
15	cB	840	CLA	CAC-C3C-C2C	-2.28	123.62	127.53
15	aA	837	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
15	a6	411	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	b1	412	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	b5	405	CLA	CMA-C3A-C2A	-2.28	104.62	113.83
15	b2	405	CLA	CMA-C3A-C2A	-2.28	104.62	113.83
15	c6	414	CLA	CAC-C3C-C4C	2.28	127.77	124.81
15	bB	834	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	bB	822	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
15	b3	417	CLA	O2A-CGA-O1A	-2.28	117.84	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	813	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
15	bB	806	CLA	C2D-C1D-ND	-2.28	108.42	110.10
15	a1	401	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
15	b2	403	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
15	b1	405	CLA	CMA-C3A-C2A	-2.28	104.64	113.83
18	aB	848	BCR	C7-C8-C9	-2.28	122.80	126.23
15	cB	830	CLA	C7-C6-C5	-2.28	107.18	113.36
15	bB	841	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
15	a3	415	CLA	CHA-C4D-ND	2.28	137.26	132.50
18	aB	846	BCR	C30-C25-C26	-2.28	119.41	122.61
15	bB	830	CLA	C7-C6-C5	-2.28	107.18	113.36
15	bA	835	CLA	C3C-C4C-NC	-2.28	108.02	110.57
15	aB	830	CLA	C7-C6-C5	-2.28	107.18	113.36
15	a4	412	CLA	CHB-C4A-NA	2.28	127.66	124.51
15	b4	412	CLA	CHB-C4A-NA	2.28	127.66	124.51
15	a1	416	CLA	C2A-C1A-CHA	2.27	127.84	123.86
15	c1	409	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
15	b4	406	CLA	O2A-CGA-O1A	-2.27	117.63	123.30
18	b4	420	BCR	C3-C4-C5	-2.27	110.02	114.08
15	bA	813	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
15	c2	416	CLA	CBA-CAA-C2A	2.27	120.57	113.86
18	cB	848	BCR	C7-C8-C9	-2.27	122.80	126.23
15	cA	812	CLA	O1D-CGD-CBD	2.27	129.13	124.48
18	b6	419	BCR	C38-C26-C27	-2.27	109.25	113.62
15	aA	832	CLA	C1-C2-C3	-2.27	123.08	126.75
15	c2	409	CLA	O2A-CGA-O1A	-2.27	117.64	123.30
15	c3	417	CLA	C2A-C1A-CHA	2.27	127.83	123.86
15	cA	829	CLA	C3A-C2A-C1A	2.27	104.74	101.34
15	a2	418	CLA	CHD-C1D-ND	-2.27	122.37	124.45
15	c1	416	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
15	aA	835	CLA	C3C-C4C-NC	-2.27	108.03	110.57
15	aA	807	CLA	CHA-C1A-NA	-2.27	121.20	126.40
15	b3	415	CLA	CHA-C4D-ND	2.27	137.25	132.50
15	a2	402	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
15	bF	201	CLA	O2A-CGA-O1A	-2.27	117.64	123.30
18	aA	850	BCR	C40-C30-C25	2.27	113.98	110.30
18	aF	201	BCR	C40-C30-C25	2.27	113.98	110.30
15	bA	814	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
15	a5	405	CLA	CHC-C1C-NC	2.27	127.64	124.20
18	b2	421	BCR	C35-C13-C14	-2.27	119.75	122.92
15	b4	417	CLA	CMA-C3A-C2A	-2.27	104.68	113.83
15	a1	408	CLA	O2A-CGA-O1A	-2.27	117.87	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bI	102	BCR	C11-C10-C9	-2.27	124.07	127.31
15	cA	844	CLA	CMC-C2C-C1C	-2.27	121.59	125.04
15	c2	403	CLA	C2A-C1A-CHA	2.27	127.82	123.86
15	bA	812	CLA	O1D-CGD-CBD	2.27	129.12	124.48
15	bB	817	CLA	CHA-C1A-NA	-2.27	121.21	126.40
18	c4	401	BCR	C15-C14-C13	-2.27	124.08	127.31
15	a4	412	CLA	C2A-C1A-CHA	2.27	127.82	123.86
15	b6	411	CLA	C2A-C1A-CHA	2.27	127.82	123.86
15	b5	405	CLA	CHC-C1C-NC	2.26	127.64	124.20
15	c4	417	CLA	C3A-C2A-C1A	2.26	104.73	101.34
15	a3	404	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
15	a4	405	CLA	CMA-C3A-C2A	-2.26	104.70	113.83
15	bA	813	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	b3	413	CLA	C2D-C1D-ND	-2.26	108.44	110.10
15	c3	417	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	cB	849	BCR	C30-C25-C26	-2.26	119.43	122.61
18	bJ	105	BCR	C31-C1-C6	2.26	113.97	110.30
18	bL	201	BCR	C40-C30-C25	2.26	113.97	110.30
15	cB	819	CLA	C4-C3-C5	2.26	119.08	115.27
15	a2	403	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	a6	419	BCR	C38-C26-C27	-2.26	109.27	113.62
15	cA	822	CLA	C16-C15-C13	-2.26	108.61	115.92
15	b5	410	CLA	C1D-ND-C4D	2.26	107.94	106.33
15	cA	814	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
15	c2	403	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	a4	410	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	aA	813	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	aA	829	CLA	C3A-C2A-C1A	2.26	104.73	101.34
18	cF	205	BCR	C31-C1-C6	2.26	113.97	110.30
15	cA	839	CLA	C6-C7-C8	-2.26	108.61	115.92
15	b1	409	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
15	c1	403	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
15	aB	802	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
15	c6	411	CLA	C2A-C1A-CHA	2.26	127.81	123.86
18	cB	847	BCR	C35-C13-C12	2.26	119.59	114.60
15	c3	415	CLA	CHA-C4D-ND	2.26	137.22	132.50
15	cA	837	CLA	O2A-CGA-O1A	-2.26	117.67	123.30
18	aB	847	BCR	C35-C13-C12	2.26	119.59	114.60
18	b3	420	BCR	C3-C4-C5	-2.26	110.05	114.08
15	cA	802	CLA	CHD-C1D-ND	-2.26	122.38	124.45
15	aA	812	CLA	O1D-CGD-CBD	2.26	129.10	124.48
18	aI	102	BCR	C11-C10-C9	-2.26	124.09	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	829	CLA	C3A-C2A-C1A	2.26	104.72	101.34
18	aL	205	BCR	C40-C30-C25	2.26	113.96	110.30
15	b6	411	CLA	CHA-C1A-NA	-2.26	121.23	126.40
19	cA	852	LHG	O8-C23-O10	-2.26	117.90	123.59
15	b5	410	CLA	C2A-C1A-CHA	2.25	127.80	123.86
15	a6	411	CLA	CHA-C1A-NA	-2.25	121.23	126.40
18	aF	203	BCR	C31-C1-C6	2.25	113.95	110.30
15	a3	407	CLA	CHA-C1A-NA	-2.25	121.24	126.40
15	bJ	102	CLA	C2D-C1D-ND	-2.25	108.44	110.10
15	a5	412	CLA	C1D-ND-C4D	2.25	107.94	106.33
18	a2	421	BCR	C24-C23-C22	-2.25	122.83	126.23
18	c4	420	BCR	C3-C4-C5	-2.25	110.05	114.08
18	aF	202	BCR	C34-C9-C10	-2.25	119.77	122.92
18	cJ	104	BCR	C24-C23-C22	-2.25	122.83	126.23
15	cB	802	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
15	cB	817	CLA	CHA-C1A-NA	-2.25	121.24	126.40
18	aB	849	BCR	C30-C25-C26	-2.25	119.44	122.61
15	aB	817	CLA	CHA-C1A-NA	-2.25	121.24	126.40
15	b6	406	CLA	CMA-C3A-C2A	-2.25	104.75	113.83
15	aA	821	CLA	CMC-C2C-C3C	2.25	132.23	126.12
15	bA	805	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
15	cB	833	CLA	C16-C17-C18	-2.25	105.38	115.98
15	aA	822	CLA	C16-C15-C13	-2.25	108.64	115.92
15	cA	832	CLA	C1-C2-C3	-2.25	123.11	126.75
15	bA	802	CLA	C4D-C3D-CAD	-2.25	105.44	108.10
15	aB	806	CLA	C2D-C1D-ND	-2.25	108.45	110.10
18	bL	206	BCR	C40-C30-C25	2.25	113.95	110.30
18	cM	101	BCR	C16-C15-C14	-2.25	118.87	123.47
15	a5	410	CLA	C1D-ND-C4D	2.25	107.93	106.33
15	a1	411	CLA	C2A-C1A-CHA	2.25	127.79	123.86
15	c4	411	CLA	CHD-C1D-ND	-2.25	122.39	124.45
15	c2	408	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	cA	828	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
18	b4	419	BCR	C3-C4-C5	-2.25	110.06	114.08
15	a2	408	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	cB	803	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
18	cA	850	BCR	C27-C26-C25	2.25	126.00	122.73
15	c3	407	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	bB	819	CLA	C4-C3-C5	2.25	119.05	115.27
15	bA	839	CLA	C6-C7-C8	-2.25	108.65	115.92
19	aA	853	LHG	O8-C23-O10	-2.25	117.92	123.59
18	c4	418	BCR	C38-C26-C27	-2.25	109.30	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	409	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
19	bA	854	LHG	O8-C23-O10	-2.25	117.92	123.59
15	cA	813	CLA	CHB-C4A-NA	2.25	127.62	124.51
15	cB	826	CLA	OBD-CAD-C3D	2.25	133.93	128.52
15	bA	821	CLA	CMC-C2C-C3C	2.25	132.22	126.12
15	aB	803	CLA	CAA-CBA-CGA	-2.25	106.69	113.25
15	aB	819	CLA	C4-C3-C5	2.25	119.05	115.27
15	c1	412	CLA	C2A-C1A-CHA	2.25	127.79	123.86
15	cA	805	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
15	aB	804	CLA	CMD-C2D-C1D	-2.25	120.76	124.71
15	cA	821	CLA	CMC-C2C-C3C	2.25	132.21	126.12
15	bB	804	CLA	CMD-C2D-C1D	-2.24	120.76	124.71
18	bB	847	BCR	C35-C13-C12	2.24	119.56	114.60
15	cJ	102	CLA	C2D-C1D-ND	-2.24	108.45	110.10
15	aJ	201	CLA	CAC-C3C-C4C	2.24	127.72	124.81
15	b3	402	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
15	b2	408	CLA	CHA-C1A-NA	-2.24	121.26	126.40
15	bB	826	CLA	OBD-CAD-C3D	2.24	133.92	128.52
15	aA	839	CLA	C6-C7-C8	-2.24	108.67	115.92
15	aB	833	CLA	C16-C17-C18	-2.24	105.41	115.98
18	c5	418	BCR	C7-C8-C9	-2.24	122.84	126.23
18	aA	851	BCR	C27-C26-C25	2.24	125.99	122.73
15	aA	823	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
18	c4	419	BCR	C3-C4-C5	-2.24	110.07	114.08
15	bB	833	CLA	C16-C17-C18	-2.24	105.42	115.98
18	b5	401	BCR	C7-C8-C9	-2.24	122.85	126.23
15	bA	823	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
15	bA	822	CLA	C16-C15-C13	-2.24	108.67	115.92
15	b6	413	CLA	C1D-ND-C4D	2.24	107.93	106.33
15	aB	826	CLA	OBD-CAD-C3D	2.24	133.91	128.52
18	cI	102	BCR	C11-C10-C9	-2.24	124.11	127.31
18	bM	101	BCR	C16-C15-C14	-2.24	118.88	123.47
15	cA	807	CLA	C2D-C1D-ND	-2.24	108.45	110.10
18	b5	418	BCR	C7-C8-C9	-2.24	122.85	126.23
18	bA	852	BCR	C27-C26-C25	2.24	125.98	122.73
15	a2	413	CLA	CHC-C1C-NC	2.24	127.60	124.20
15	b2	411	CLA	C1D-ND-C4D	2.24	107.93	106.33
15	c2	411	CLA	C1D-ND-C4D	2.24	107.93	106.33
15	c6	411	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	cA	823	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
15	c4	416	CLA	CHC-C1C-NC	2.24	127.60	124.20
15	cA	835	CLA	C3C-C4C-NC	-2.24	108.06	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	803	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
18	c5	401	BCR	C35-C13-C14	-2.24	119.79	122.92
15	b4	421	CLA	CMB-C2B-C3B	2.24	128.87	124.68
15	c4	410	CLA	C2A-C1A-CHA	2.24	127.77	123.86
15	bB	802	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
15	c5	405	CLA	CHC-C1C-NC	2.24	127.60	124.20
15	a6	413	CLA	C1D-ND-C4D	2.24	107.92	106.33
15	aA	805	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
15	cB	841	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
18	bJ	103	BCR	C33-C5-C6	-2.24	122.02	124.53
18	aM	101	BCR	C15-C14-C13	-2.24	124.12	127.31
15	bA	825	CLA	CHD-C1D-ND	-2.24	122.40	124.45
15	b4	410	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
18	cM	101	BCR	C27-C26-C25	2.24	125.98	122.73
18	c2	421	BCR	C24-C23-C22	-2.23	122.86	126.23
18	aM	101	BCR	C16-C15-C14	-2.23	118.90	123.47
18	aI	102	BCR	C27-C26-C25	2.23	125.97	122.73
18	cL	204	BCR	C33-C5-C6	-2.23	122.02	124.53
15	cA	833	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
18	a3	420	BCR	C3-C4-C5	-2.23	110.09	114.08
15	b4	405	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
15	b2	413	CLA	CHC-C1C-NC	2.23	127.59	124.20
15	b5	412	CLA	CHC-C1C-NC	2.23	127.59	124.20
15	a5	405	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
15	c1	413	CLA	C2D-C1D-ND	-2.23	108.46	110.10
15	a1	402	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
15	a5	412	CLA	CHC-C1C-NC	2.23	127.59	124.20
15	b5	415	CLA	CHA-C4D-ND	2.23	137.17	132.50
15	aA	810	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
15	bA	832	CLA	C1-C2-C3	-2.23	123.14	126.75
18	c5	401	BCR	C7-C8-C9	-2.23	122.86	126.23
18	aM	101	BCR	C15-C16-C17	-2.23	118.90	123.47
15	a1	403	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
15	aA	826	CLA	CHA-C1A-NA	-2.23	121.29	126.40
15	a4	416	CLA	CHC-C1C-NC	2.23	127.59	124.20
18	c2	420	BCR	C40-C30-C25	2.23	113.92	110.30
18	bL	205	BCR	C33-C5-C6	-2.23	122.02	124.53
19	bA	854	LHG	C18-C17-C16	-2.23	103.11	114.42
15	cA	826	CLA	CHA-C1A-NA	-2.23	121.29	126.40
15	cA	810	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
18	a2	421	BCR	C35-C13-C14	-2.23	119.80	122.92
15	a4	405	CLA	CHD-C4C-C3C	2.23	128.12	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	410	CLA	C2A-C1A-CHA	2.23	127.76	123.86
19	aA	853	LHG	C18-C17-C16	-2.23	103.11	114.42
15	aA	828	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	bM	101	BCR	C27-C26-C25	2.23	125.97	122.73
15	c4	403	CLA	C2A-C1A-CHA	2.23	127.76	123.86
15	bA	833	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
15	cB	818	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	cM	101	BCR	C15-C14-C13	-2.23	124.13	127.31
18	bI	102	BCR	C27-C26-C25	2.23	125.97	122.73
15	b1	417	CLA	C2D-C1D-ND	-2.23	108.46	110.10
15	b2	413	CLA	CHB-C4A-NA	2.23	127.59	124.51
15	a3	402	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
15	bA	828	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	b4	418	BCR	C38-C26-C27	-2.23	109.34	113.62
15	b2	402	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
15	aA	812	CLA	O2A-C1-C2	-2.23	102.78	108.64
15	bA	806	CLA	CAC-C3C-C4C	2.23	127.70	124.81
15	cB	801	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
15	c2	406	CLA	CED-O2D-CGD	2.23	120.97	115.94
15	bB	809	CLA	C1-C2-C3	-2.23	122.19	126.04
19	cA	852	LHG	C18-C17-C16	-2.23	103.13	114.42
15	c5	415	CLA	CHA-C4D-ND	2.22	137.15	132.50
15	a3	409	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
15	a2	405	CLA	CHC-C1C-NC	2.22	127.58	124.20
15	b1	415	CLA	CBA-CAA-C2A	2.22	120.43	113.86
15	a6	406	CLA	CMA-C3A-C2A	-2.22	104.86	113.83
15	a6	413	CLA	C2A-C1A-CHA	2.22	127.75	123.86
15	bA	830	CLA	O2D-CGD-CBD	2.22	115.22	111.27
18	aM	101	BCR	C27-C26-C25	2.22	125.96	122.73
18	cM	101	BCR	C15-C16-C17	-2.22	118.92	123.47
15	aB	818	CLA	CHD-C1D-ND	-2.22	122.41	124.45
15	c3	409	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
18	b2	419	BCR	C38-C26-C27	-2.22	109.35	113.62
18	aI	103	BCR	C33-C5-C6	-2.22	122.03	124.53
15	a2	411	CLA	C1D-ND-C4D	2.22	107.91	106.33
15	a2	409	CLA	O2A-CGA-O1A	-2.22	117.76	123.30
18	cB	846	BCR	C29-C30-C25	2.22	113.90	110.48
15	bB	838	CLA	CHD-C1D-ND	-2.22	122.41	124.45
15	aB	801	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
15	b4	405	CLA	CHC-C1C-NC	2.22	127.57	124.20
15	b4	403	CLA	C2A-C1A-CHA	2.22	127.74	123.86
15	c1	417	CLA	C2A-C1A-CHA	2.22	127.74	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c6	413	CLA	C2A-C1A-CHA	2.22	127.74	123.86
18	aJ	205	BCR	C24-C23-C22	-2.22	122.88	126.23
15	c4	405	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
15	a1	416	CLA	C2D-C1D-ND	-2.22	108.47	110.10
18	b2	421	BCR	C24-C23-C22	-2.22	122.88	126.23
15	aB	827	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
15	aB	818	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
15	bA	803	CLA	O2A-CGA-CBA	2.22	118.88	111.91
15	cA	840	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
15	b4	403	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
15	b4	405	CLA	CHD-C4C-C3C	2.22	128.10	124.84
18	c6	419	BCR	C38-C26-C27	-2.22	109.35	113.62
15	b3	409	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
15	cB	809	CLA	C1-C2-C3	-2.22	122.21	126.04
15	c4	410	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
15	c3	413	CLA	C2D-C1D-ND	-2.22	108.47	110.10
15	bA	810	CLA	CAA-CBA-CGA	-2.22	106.77	113.25
15	cA	812	CLA	O2A-C1-C2	-2.22	102.81	108.64
15	c1	403	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
15	cB	806	CLA	CAC-C3C-C4C	2.22	127.69	124.81
15	aA	833	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
15	bB	827	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
18	a4	401	BCR	C7-C8-C9	-2.22	122.89	126.23
15	cB	804	CLA	CMD-C2D-C1D	-2.22	120.81	124.71
15	b6	416	CLA	CHA-C4D-ND	2.22	137.13	132.50
18	bM	101	BCR	C15-C14-C13	-2.22	124.15	127.31
18	a4	418	BCR	C38-C26-C27	-2.21	109.36	113.62
15	cB	827	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
15	b2	422	CLA	CHA-C4D-ND	2.21	137.13	132.50
15	bA	814	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	cB	802	CLA	C11-C10-C8	-2.21	108.76	115.92
15	b2	406	CLA	CED-O2D-CGD	2.21	120.94	115.94
15	bA	826	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	c4	412	CLA	CHB-C4A-NA	2.21	127.57	124.51
15	bB	806	CLA	CAC-C3C-C4C	2.21	127.68	124.81
15	c4	421	CLA	CMB-C2B-C3B	2.21	128.82	124.68
18	bB	846	BCR	C29-C30-C25	2.21	113.89	110.48
18	bJ	104	BCR	C24-C23-C22	-2.21	122.89	126.23
15	bA	810	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
15	bB	801	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
18	b2	420	BCR	C40-C30-C25	2.21	113.89	110.30
15	bA	812	CLA	O2A-C1-C2	-2.21	102.82	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	803	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
18	aF	201	BCR	C30-C25-C26	-2.21	119.50	122.61
15	c3	405	CLA	CMA-C3A-C2A	-2.21	104.91	113.83
15	a2	405	CLA	CHD-C4C-C3C	2.21	128.09	124.84
18	b2	401	BCR	C24-C23-C22	-2.21	122.89	126.23
18	cK	101	BCR	C7-C8-C9	-2.21	122.89	126.23
15	b1	416	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
15	c4	405	CLA	CHD-C4C-C3C	2.21	128.09	124.84
15	c4	403	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
18	aB	846	BCR	C29-C30-C25	2.21	113.88	110.48
15	cA	828	CLA	CHD-C4C-NC	2.21	127.69	124.20
15	aA	814	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	a5	415	CLA	CHA-C4D-ND	2.21	137.12	132.50
18	b4	401	BCR	C7-C8-C9	-2.21	122.90	126.23
18	a3	401	BCR	C16-C15-C14	-2.21	118.95	123.47
15	b4	409	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aA	833	CLA	O2D-CGD-CBD	2.21	115.19	111.27
15	b1	413	CLA	C2D-C1D-ND	-2.21	108.48	110.10
15	cB	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	bB	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aB	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aB	802	CLA	C11-C10-C8	-2.21	108.78	115.92
18	bM	101	BCR	C15-C16-C17	-2.21	118.95	123.47
15	bX	102	CLA	O2A-CGA-O1A	-2.21	117.80	123.30
15	cA	832	CLA	C2D-C1D-ND	-2.21	108.48	110.10
15	aA	825	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aA	840	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	c5	405	CLA	CMA-C3A-C2A	-2.21	104.93	113.83
15	bA	814	CLA	C2A-C1A-CHA	2.21	127.72	123.86
15	cA	802	CLA	C4D-C3D-CAD	-2.21	105.50	108.10
15	aA	810	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
15	cJ	102	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
15	c3	403	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
15	c4	417	CLA	C3C-C4C-NC	-2.21	108.10	110.57
15	cB	824	CLA	O2A-CGA-O1A	-2.21	117.80	123.30
15	a3	412	CLA	CHC-C1C-NC	2.20	127.55	124.20
15	b4	416	CLA	CHC-C1C-NC	2.20	127.55	124.20
15	bB	803	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
15	c4	421	CLA	C11-C10-C8	-2.20	108.79	115.92
15	cX	102	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
15	cA	803	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
18	cJ	104	BCR	C38-C26-C25	-2.20	122.05	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	810	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
15	c1	402	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
15	b2	412	CLA	CHD-C1D-ND	-2.20	122.43	124.45
15	c3	405	CLA	CHC-C1C-NC	2.20	127.55	124.20
15	b6	408	CLA	CHA-C1A-NA	-2.20	121.35	126.40
15	b2	411	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
15	cA	814	CLA	C2A-C1A-CHA	2.20	127.71	123.86
15	aB	809	CLA	C1-C2-C3	-2.20	122.23	126.04
15	cA	814	CLA	CHA-C1A-NA	-2.20	121.35	126.40
18	bA	848	BCR	C7-C8-C9	-2.20	122.91	126.23
15	a4	403	CLA	C2A-C1A-CHA	2.20	127.71	123.86
18	c5	419	BCR	C11-C10-C9	-2.20	124.17	127.31
15	bA	825	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
15	c6	404	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
15	bB	802	CLA	C11-C10-C8	-2.20	108.80	115.92
15	bA	832	CLA	C2D-C1D-ND	-2.20	108.48	110.10
15	cA	803	CLA	O2A-CGA-CBA	2.20	118.81	111.91
14	cA	801	CL0	C11-C12-C13	-2.20	108.81	115.92
14	aA	801	CL0	C11-C12-C13	-2.20	108.81	115.92
15	aB	827	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	cA	825	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	a6	411	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
15	a1	412	CLA	C2D-C1D-ND	-2.20	108.48	110.10
15	aA	814	CLA	C2A-C1A-CHA	2.20	127.70	123.86
18	a2	420	BCR	C40-C30-C25	2.20	113.87	110.30
15	a2	411	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
15	bB	839	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
15	cB	827	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	c6	411	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
15	a1	404	CLA	O1D-CGD-CBD	2.20	128.98	124.48
15	c3	402	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
15	a6	408	CLA	CHA-C1A-NA	-2.20	121.37	126.40
15	b1	403	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
15	cF	203	CLA	C3A-C2A-C1A	2.20	104.63	101.34
18	c2	420	BCR	C3-C4-C5	-2.20	110.15	114.08
15	aA	830	CLA	O2D-CGD-CBD	2.20	115.17	111.27
15	aJ	203	CLA	C2D-C1D-ND	-2.20	108.48	110.10
15	aA	803	CLA	O2A-CGA-CBA	2.20	118.80	111.91
15	a1	416	CLA	CHD-C1D-ND	-2.20	122.44	124.45
15	bB	818	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
15	a6	416	CLA	CHA-C4D-ND	2.20	137.09	132.50
15	a3	405	CLA	CHC-C1C-NC	2.20	127.53	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	819	CLA	O2D-CGD-CBD	2.20	115.17	111.27
15	cA	806	CLA	CAC-C3C-C4C	2.20	127.66	124.81
15	b2	405	CLA	CHC-C1C-NC	2.19	127.53	124.20
15	bB	827	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
18	cK	101	BCR	C20-C21-C22	-2.19	124.18	127.31
15	cB	803	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
18	cF	202	BCR	C30-C25-C26	-2.19	119.52	122.61
15	aB	803	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
15	bB	804	CLA	O1D-CGD-CBD	2.19	128.97	124.48
18	cB	844	BCR	C7-C8-C9	-2.19	122.92	126.23
15	cA	834	CLA	C7-C6-C5	-2.19	107.40	113.36
15	aB	839	CLA	CAA-CBA-CGA	-2.19	106.84	113.25
15	c6	406	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
15	b1	411	CLA	C2A-C1A-CHA	2.19	127.69	123.86
15	c6	408	CLA	CHA-C1A-NA	-2.19	121.38	126.40
15	a2	422	CLA	CHA-C4D-ND	2.19	137.09	132.50
14	bA	801	CL0	C11-C12-C13	-2.19	108.83	115.92
15	aB	818	CLA	CGD-CBD-CAD	-2.19	103.63	110.73
15	cB	804	CLA	O1D-CGD-CBD	2.19	128.97	124.48
15	b2	416	CLA	CHA-C4D-ND	2.19	137.08	132.50
15	b5	412	CLA	C1D-ND-C4D	2.19	107.89	106.33
18	c3	419	BCR	C40-C30-C25	2.19	113.85	110.30
15	bA	834	CLA	C7-C6-C5	-2.19	107.41	113.36
15	aB	824	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	bA	819	CLA	O2D-CGD-CBD	2.19	115.16	111.27
18	aB	844	BCR	C7-C8-C9	-2.19	122.92	126.23
15	a2	406	CLA	CED-O2D-CGD	2.19	120.89	115.94
15	cA	830	CLA	O2D-CGD-CBD	2.19	115.16	111.27
15	bJ	102	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
18	aK	101	BCR	C20-C21-C22	-2.19	124.18	127.31
15	bB	824	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	b2	408	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	a1	404	CLA	CMA-C3A-C4A	2.19	117.66	111.77
15	bA	836	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
15	a6	414	CLA	CHC-C1C-NC	2.19	127.53	124.20
15	aA	806	CLA	CAC-C3C-C4C	2.19	127.65	124.81
15	bB	801	CLA	CAC-C3C-C4C	2.19	127.65	124.81
15	c1	405	CLA	CMA-C3A-C4A	2.19	117.66	111.77
15	a4	409	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
15	cB	839	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
15	aB	804	CLA	O1D-CGD-CBD	2.19	128.96	124.48
15	aA	828	CLA	CHD-C4C-NC	2.19	127.65	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c6	419	BCR	C15-C16-C17	-2.19	118.99	123.47
15	aA	826	CLA	C7-C6-C5	-2.19	107.41	113.36
15	aJ	203	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
15	bF	201	CLA	C3A-C2A-C1A	2.19	104.62	101.34
15	aB	840	CLA	C1-C2-C3	-2.19	122.26	126.04
18	b1	419	BCR	C15-C14-C13	-2.19	124.19	127.31
15	aX	102	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	c2	405	CLA	CHC-C1C-NC	2.19	127.52	124.20
15	a4	421	CLA	CMB-C2B-C3B	2.19	128.77	124.68
18	a1	418	BCR	C15-C14-C13	-2.19	124.19	127.31
18	a4	419	BCR	C3-C4-C5	-2.19	110.17	114.08
15	a3	413	CLA	C2D-C1D-ND	-2.19	108.49	110.10
18	aK	101	BCR	C7-C8-C9	-2.19	122.93	126.23
18	aJ	205	BCR	C38-C26-C25	-2.19	122.07	124.53
15	cA	833	CLA	O2D-CGD-CBD	2.19	115.15	111.27
18	a3	418	BCR	C38-C26-C27	-2.19	109.42	113.62
15	bA	840	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
15	c4	409	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
15	bB	825	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
15	c2	417	CLA	CMD-C2D-C3D	2.19	132.64	127.61
15	aA	832	CLA	C2D-C1D-ND	-2.19	108.49	110.10
15	aB	825	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
15	b6	406	CLA	CMA-C3A-C4A	2.19	117.65	111.77
15	cB	818	CLA	CGD-CBD-CAD	-2.19	103.66	110.73
15	cB	810	CLA	C11-C12-C13	-2.19	108.86	115.92
15	c2	418	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
15	c5	412	CLA	C1D-ND-C4D	2.18	107.89	106.33
15	cA	822	CLA	C2D-C1D-ND	-2.18	108.49	110.10
15	c4	415	CLA	CHA-C4D-ND	2.18	137.07	132.50
15	a4	403	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
15	aA	834	CLA	C7-C6-C5	-2.18	107.43	113.36
15	bA	843	CLA	CBC-CAC-C3C	2.18	118.45	112.43
18	c1	419	BCR	C16-C15-C14	-2.18	119.00	123.47
15	b3	403	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
15	cA	827	CLA	C2D-C1D-ND	-2.18	108.50	110.10
18	b5	419	BCR	C11-C10-C9	-2.18	124.19	127.31
15	b4	405	CLA	CHB-C4A-NA	2.18	127.53	124.51
15	a3	405	CLA	CMA-C3A-C2A	-2.18	105.02	113.83
18	b5	401	BCR	C27-C26-C25	2.18	125.90	122.73
18	cI	102	BCR	C27-C26-C25	2.18	125.90	122.73
18	a4	420	BCR	C24-C23-C22	-2.18	122.94	126.23
15	a2	416	CLA	CHA-C4D-ND	2.18	137.06	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	840	CLA	C1-C2-C3	-2.18	122.27	126.04
15	cB	825	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
18	c5	401	BCR	C24-C23-C22	-2.18	122.94	126.23
15	aB	824	CLA	CHB-C4A-NA	2.18	127.53	124.51
15	bX	102	CLA	CMD-C2D-C3D	2.18	132.63	127.61
16	cA	845	PQN	C2M-C2-C3	-2.18	120.84	124.40
15	cB	801	CLA	CAC-C3C-C4C	2.18	127.64	124.81
15	c2	413	CLA	CHC-C1C-NC	2.18	127.51	124.20
15	c3	412	CLA	CHC-C1C-NC	2.18	127.51	124.20
15	a2	413	CLA	CHB-C4A-NA	2.18	127.53	124.51
18	b1	420	BCR	C11-C10-C9	-2.18	124.20	127.31
15	bA	826	CLA	C7-C6-C5	-2.18	107.44	113.36
18	c3	420	BCR	C3-C4-C5	-2.18	110.19	114.08
15	aX	102	CLA	CMD-C2D-C3D	2.18	132.63	127.61
15	aB	820	CLA	C2D-C1D-ND	-2.18	108.50	110.10
15	c2	416	CLA	CHA-C4D-ND	2.18	137.06	132.50
15	aA	836	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
15	cJ	101	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
15	b1	409	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
15	bB	818	CLA	CGD-CBD-CAD	-2.18	103.68	110.73
15	bA	831	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
15	b4	411	CLA	CHD-C1D-ND	-2.18	122.45	124.45
15	aA	818	CLA	O2D-CGD-CBD	2.18	115.14	111.27
15	bA	840	CLA	C2A-C1A-CHA	2.18	127.67	123.86
15	a3	410	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	b6	413	CLA	C2A-C1A-CHA	2.18	127.67	123.86
15	aA	831	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
15	a4	402	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
15	b6	411	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
15	c5	405	CLA	CED-O2D-CGD	-2.18	111.02	115.94
15	cA	826	CLA	C7-C6-C5	-2.18	107.45	113.36
15	cA	842	CLA	CBC-CAC-C3C	2.18	118.43	112.43
15	bJ	101	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
18	c3	401	BCR	C16-C15-C14	-2.18	119.02	123.47
15	a4	421	CLA	C3A-C2A-C1A	2.18	104.60	101.34
18	bB	849	BCR	C30-C25-C26	-2.18	119.55	122.61
15	c4	402	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
18	aA	848	BCR	C29-C30-C25	2.17	113.83	110.48
15	a1	410	CLA	C2A-C1A-CHA	2.17	127.66	123.86
18	a3	420	BCR	C1-C6-C5	-2.17	119.55	122.61
15	bB	810	CLA	C11-C12-C13	-2.17	108.89	115.92
15	aB	801	CLA	CAC-C3C-C4C	2.17	127.63	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	830	CLA	C1-C2-C3	-2.17	122.28	126.04
15	a3	403	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
15	a6	406	CLA	O1D-CGD-CBD	2.17	128.93	124.48
15	b4	410	CLA	C1D-ND-C4D	2.17	107.88	106.33
15	bA	830	CLA	C1-C2-C3	-2.17	122.28	126.04
15	cA	839	CLA	O1D-CGD-CBD	2.17	128.93	124.48
15	cB	840	CLA	C3A-C2A-C1A	2.17	104.59	101.34
15	a3	410	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
15	cA	836	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
18	bA	848	BCR	C20-C21-C22	-2.17	124.21	127.31
15	aJ	201	CLA	C3A-C2A-C1A	2.17	104.59	101.34
15	cA	831	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
15	c6	412	CLA	C2A-C1A-CHA	2.17	127.66	123.86
18	c2	401	BCR	C24-C23-C22	-2.17	122.95	126.23
18	c6	402	BCR	C16-C15-C14	-2.17	119.03	123.47
15	c6	416	CLA	CHA-C4D-ND	2.17	137.04	132.50
15	c1	411	CLA	C2A-C1A-CHA	2.17	127.66	123.86
18	a5	401	BCR	C7-C8-C9	-2.17	122.95	126.23
15	c4	412	CLA	CHC-C1C-NC	2.17	127.50	124.20
15	bB	810	CLA	C2A-C1A-CHA	2.17	127.66	123.86
15	bA	834	CLA	C1-C2-C3	-2.17	122.29	126.04
15	cB	833	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	aA	850	BCR	C20-C21-C22	-2.17	124.21	127.31
15	bA	833	CLA	O2D-CGD-CBD	2.17	115.12	111.27
18	b3	401	BCR	C16-C15-C14	-2.17	119.03	123.47
15	a6	406	CLA	CMA-C3A-C4A	2.17	117.61	111.77
15	bA	807	CLA	C2D-C1D-ND	-2.17	108.50	110.10
15	bA	827	CLA	C2D-C1D-ND	-2.17	108.50	110.10
15	cX	102	CLA	CMD-C2D-C3D	2.17	132.60	127.61
15	b6	403	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
18	a5	418	BCR	C7-C8-C9	-2.17	122.96	126.23
15	b4	421	CLA	C11-C10-C8	-2.17	108.91	115.92
15	aB	840	CLA	C3A-C2A-C1A	2.17	104.59	101.34
15	bB	840	CLA	C3A-C2A-C1A	2.17	104.59	101.34
16	aA	846	PQN	C2M-C2-C3	-2.17	120.86	124.40
15	aA	803	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
15	aA	819	CLA	O2D-CGD-CBD	2.17	115.12	111.27
15	c4	405	CLA	CHB-C4A-NA	2.17	127.51	124.51
15	a6	404	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
15	c5	405	CLA	CHD-C4C-C3C	2.17	128.03	124.84
15	b6	406	CLA	O1D-CGD-CBD	2.17	128.92	124.48
15	c3	410	CLA	CHA-C1A-NA	-2.17	121.43	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	833	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	b2	420	BCR	C3-C4-C5	-2.17	110.21	114.08
15	a6	410	CLA	O1D-CGD-CBD	2.17	128.92	124.48
15	aJ	202	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
15	b1	408	CLA	C3C-C4C-NC	-2.17	108.14	110.57
15	bA	828	CLA	CHD-C4C-NC	2.17	127.62	124.20
15	b2	411	CLA	CHA-C1A-NA	-2.17	121.44	126.40
18	bJ	104	BCR	C38-C26-C25	-2.17	122.09	124.53
15	b3	410	CLA	C1D-ND-C4D	2.17	107.87	106.33
18	aL	205	BCR	C27-C26-C25	2.17	125.88	122.73
18	a5	401	BCR	C27-C26-C25	2.17	125.88	122.73
18	a6	419	BCR	C15-C16-C17	-2.17	119.04	123.47
15	c6	414	CLA	CHC-C1C-NC	2.17	127.49	124.20
15	aA	843	CLA	CBC-CAC-C3C	2.17	118.40	112.43
18	c1	419	BCR	C15-C14-C13	-2.17	124.22	127.31
15	cB	836	CLA	CHA-C1A-NA	-2.17	121.44	126.40
15	a5	417	CLA	CMA-C3A-C2A	-2.17	105.09	113.83
15	bA	818	CLA	O2D-CGD-CBD	2.17	115.12	111.27
15	a6	403	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
15	a5	405	CLA	CHB-C4A-NA	2.17	127.51	124.51
15	c5	409	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
15	b5	417	CLA	CMA-C3A-C2A	-2.16	105.09	113.83
15	b3	405	CLA	CHC-C1C-NC	2.16	127.49	124.20
15	b2	409	CLA	O2A-CGA-O1A	-2.16	117.90	123.30
15	a4	417	CLA	C3A-C2A-C1A	2.16	104.58	101.34
15	b5	407	CLA	CHA-C1A-NA	-2.16	121.44	126.40
15	a3	421	CLA	C16-C15-C13	-2.16	108.92	115.92
15	a2	418	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
15	b2	405	CLA	CHD-C4C-C3C	2.16	128.02	124.84
15	c4	421	CLA	C3A-C2A-C1A	2.16	104.58	101.34
18	bL	201	BCR	C38-C26-C27	-2.16	109.46	113.62
18	bL	206	BCR	C38-C26-C27	-2.16	109.46	113.62
18	c5	401	BCR	C27-C26-C25	2.16	125.87	122.73
18	c6	401	BCR	C40-C30-C25	2.16	113.81	110.30
15	bB	818	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	bA	806	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
15	bA	839	CLA	O1D-CGD-CBD	2.16	128.91	124.48
15	b2	417	CLA	CMD-C2D-C3D	2.16	132.59	127.61
15	b4	417	CLA	C3A-C2A-C1A	2.16	104.58	101.34
18	a2	419	BCR	C38-C26-C27	-2.16	109.46	113.62
18	cA	849	BCR	C20-C21-C22	-2.16	124.22	127.31
15	aB	810	CLA	C11-C12-C13	-2.16	108.93	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	824	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
15	c4	408	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
15	b6	413	CLA	CHC-C1C-NC	2.16	127.48	124.20
18	cA	847	BCR	C29-C30-C25	2.16	113.81	110.48
15	b1	402	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
18	cA	850	BCR	C8-C7-C6	-2.16	121.13	127.20
15	a5	410	CLA	CHA-C1A-NA	-2.16	121.45	126.40
15	b4	402	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
15	b3	412	CLA	CHC-C1C-NC	2.16	127.48	124.20
15	aB	838	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	cB	830	CLA	CMA-C3A-C2A	-2.16	105.11	113.83
15	c5	417	CLA	C3A-C2A-C1A	2.16	104.57	101.34
15	aB	824	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
15	cA	840	CLA	C2A-C1A-CHA	2.16	127.64	123.86
15	bB	824	CLA	CHB-C4A-NA	2.16	127.50	124.51
15	cB	824	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
15	aA	840	CLA	C2A-C1A-CHA	2.16	127.63	123.86
15	a2	408	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
15	a2	412	CLA	C2A-C1A-CHA	2.16	127.63	123.86
15	a2	411	CLA	CHA-C1A-NA	-2.16	121.46	126.40
18	a5	419	BCR	C11-C10-C9	-2.16	124.23	127.31
18	cF	205	BCR	C3-C4-C5	-2.16	110.22	114.08
15	c6	406	CLA	O1D-CGD-CBD	2.16	128.90	124.48
18	b3	419	BCR	C40-C30-C25	2.16	113.80	110.30
15	c2	413	CLA	CHB-C4A-NA	2.16	127.50	124.51
15	bB	830	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
15	a4	405	CLA	CHC-C1C-NC	2.16	127.47	124.20
15	bB	833	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
15	c2	411	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	c4	410	CLA	C1D-ND-C4D	2.16	107.87	106.33
15	c2	405	CLA	CHD-C4C-C3C	2.16	128.01	124.84
15	cB	811	CLA	CAC-C3C-C4C	2.16	127.61	124.81
15	cA	805	CLA	CAA-C2A-C1A	-2.16	104.91	111.97
15	aA	805	CLA	CAA-C2A-C1A	-2.16	104.91	111.97
18	bJ	105	BCR	C3-C4-C5	-2.16	110.23	114.08
15	c2	408	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
15	cB	820	CLA	C2D-C1D-ND	-2.15	108.52	110.10
18	c4	401	BCR	C7-C8-C9	-2.15	122.98	126.23
15	b4	417	CLA	C3C-C4C-NC	-2.15	108.16	110.57
15	aA	803	CLA	CMD-C2D-C1D	-2.15	120.92	124.71
15	bA	805	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
18	aF	203	BCR	C3-C4-C5	-2.15	110.23	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	830	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
15	cB	836	CLA	CBC-CAC-C3C	2.15	118.37	112.43
15	a4	421	CLA	C11-C10-C8	-2.15	108.96	115.92
18	aL	205	BCR	C38-C26-C27	-2.15	109.48	113.62
15	b4	421	CLA	C3A-C2A-C1A	2.15	104.56	101.34
18	b5	401	BCR	C24-C23-C22	-2.15	122.98	126.23
15	a6	412	CLA	C2A-C1A-CHA	2.15	127.62	123.86
15	c6	406	CLA	CMA-C3A-C4A	2.15	117.56	111.77
15	b5	405	CLA	CHD-C4C-C3C	2.15	128.00	124.84
18	bA	851	BCR	C20-C21-C22	-2.15	124.24	127.31
15	a4	415	CLA	CHA-C4D-ND	2.15	137.00	132.50
18	a2	420	BCR	C3-C4-C5	-2.15	110.23	114.08
15	a4	405	CLA	CHB-C4A-NA	2.15	127.49	124.51
15	c2	412	CLA	CHD-C1D-ND	-2.15	122.48	124.45
15	cB	833	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
15	aB	806	CLA	CAC-C3C-C4C	2.15	127.60	124.81
15	bA	803	CLA	CMD-C2D-C1D	-2.15	120.92	124.71
18	aA	851	BCR	C8-C7-C6	-2.15	121.16	127.20
15	a4	410	CLA	C1D-ND-C4D	2.15	107.86	106.33
15	cB	810	CLA	C2A-C1A-CHA	2.15	127.62	123.86
15	a6	413	CLA	CHC-C1C-NC	2.15	127.47	124.20
15	cB	814	CLA	CHB-C4A-NA	2.15	127.49	124.51
15	bA	843	CLA	O2A-C1-C2	2.15	114.29	108.64
15	a5	407	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	bB	836	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	a6	401	BCR	C40-C30-C25	2.15	113.79	110.30
15	aA	839	CLA	O1D-CGD-CBD	2.15	128.88	124.48
15	cA	838	CLA	C2A-C1A-CHA	2.15	127.62	123.86
15	a4	411	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	aF	201	BCR	C24-C23-C22	-2.15	122.99	126.23
18	a6	420	BCR	C7-C8-C9	-2.15	122.99	126.23
15	a5	420	CLA	O2D-CGD-CBD	2.15	115.09	111.27
15	a1	404	CLA	CHC-C1C-NC	2.15	127.46	124.20
15	c5	420	CLA	O2D-CGD-CBD	2.15	115.09	111.27
18	b3	418	BCR	C38-C26-C27	-2.15	109.49	113.62
15	aA	838	CLA	C2A-C1A-CHA	2.15	127.62	123.86
18	a3	419	BCR	C40-C30-C25	2.15	113.78	110.30
15	cA	830	CLA	C1-C2-C3	-2.15	122.33	126.04
15	b3	405	CLA	CMA-C3A-C2A	-2.15	105.16	113.83
15	bA	822	CLA	C2D-C1D-ND	-2.15	108.52	110.10
15	cL	202	CLA	C2A-C1A-CHA	2.15	127.61	123.86
18	aK	101	BCR	C33-C5-C6	-2.15	122.12	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c5	410	CLA	CHA-C1A-NA	-2.15	121.48	126.40
18	bA	852	BCR	C8-C7-C6	-2.15	121.17	127.20
15	cB	824	CLA	CHB-C4A-NA	2.15	127.48	124.51
15	b3	417	CLA	C2D-C1D-ND	-2.15	108.52	110.10
15	b5	405	CLA	CHB-C4A-NA	2.15	127.48	124.51
15	a1	409	CLA	C2A-C1A-CHA	2.15	127.61	123.86
18	cK	101	BCR	C33-C5-C6	-2.15	122.12	124.53
15	b4	415	CLA	CHA-C4D-ND	2.15	136.99	132.50
18	cF	204	BCR	C2-C1-C6	2.14	113.78	110.48
15	cA	842	CLA	O2A-C1-C2	2.14	114.27	108.64
15	bA	838	CLA	C2A-C1A-CHA	2.14	127.61	123.86
15	c2	422	CLA	CHA-C4D-ND	2.14	136.99	132.50
18	b6	402	BCR	C16-C15-C14	-2.14	119.08	123.47
15	aB	836	CLA	CHA-C1A-NA	-2.14	121.49	126.40
18	bB	844	BCR	C7-C8-C9	-2.14	123.00	126.23
15	c6	403	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
18	a3	418	BCR	C16-C15-C14	-2.14	119.08	123.47
15	c6	410	CLA	O1D-CGD-CBD	2.14	128.87	124.48
15	a2	417	CLA	CMD-C2D-C3D	2.14	132.54	127.61
15	c5	407	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	aL	202	CLA	C2A-C1A-CHA	2.14	127.61	123.86
15	cA	821	CLA	C2A-C1A-CHA	2.14	127.61	123.86
18	b2	419	BCR	C11-C10-C9	-2.14	124.25	127.31
15	c1	410	CLA	CHA-C1A-NA	-2.14	121.49	126.40
18	bL	201	BCR	C27-C26-C25	2.14	125.84	122.73
18	bB	850	BCR	C16-C17-C18	-2.14	124.25	127.31
15	cA	806	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
15	cA	818	CLA	O2D-CGD-CBD	2.14	115.07	111.27
15	bB	840	CLA	C1-C2-C3	-2.14	122.34	126.04
15	aA	822	CLA	C2D-C1D-ND	-2.14	108.53	110.10
15	bJ	101	CLA	O2D-CGD-CBD	2.14	115.07	111.27
15	c3	405	CLA	CHB-C4A-NA	2.14	127.47	124.51
18	a1	418	BCR	C40-C30-C25	2.14	113.77	110.30
16	bA	846	PQN	C2M-C2-C3	-2.14	120.91	124.40
15	aA	806	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
15	b5	410	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	c6	407	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
15	a2	412	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	aF	202	BCR	C2-C1-C6	2.14	113.78	110.48
18	b4	420	BCR	C1-C6-C5	-2.14	119.60	122.61
18	a6	402	BCR	C16-C15-C14	-2.14	119.09	123.47
15	aB	819	CLA	C2A-C1A-CHA	2.14	127.60	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b3	401	BCR	C29-C30-C25	2.14	113.78	110.48
16	bA	846	PQN	C14-C13-C15	2.14	118.87	115.27
15	aB	836	CLA	CBC-CAC-C3C	2.14	118.33	112.43
15	bB	841	CLA	O2D-CGD-CBD	2.14	115.07	111.27
18	b6	419	BCR	C7-C8-C9	-2.14	123.00	126.23
15	bB	804	CLA	C2A-C1A-CHA	2.14	127.60	123.86
15	aA	843	CLA	O2A-C1-C2	2.14	114.26	108.64
15	b3	410	CLA	CHA-C1A-NA	-2.14	121.50	126.40
18	bL	206	BCR	C27-C26-C25	2.14	125.84	122.73
18	aF	201	BCR	C32-C1-C2	-2.14	100.35	108.91
15	b4	408	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
15	aA	834	CLA	C1-C2-C3	-2.14	122.34	126.04
18	c3	418	BCR	C1-C6-C5	-2.14	119.60	122.61
18	aB	846	BCR	C35-C13-C14	-2.14	119.93	122.92
15	cB	838	CLA	O2D-CGD-CBD	2.14	115.07	111.27
15	a5	409	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	c6	419	BCR	C7-C8-C9	-2.14	123.00	126.23
15	a5	405	CLA	CHD-C4C-C3C	2.14	127.98	124.84
15	cA	803	CLA	CMD-C2D-C1D	-2.14	120.95	124.71
18	b3	420	BCR	C1-C6-C5	-2.14	119.60	122.61
18	c5	418	BCR	C38-C26-C27	-2.14	109.51	113.62
18	cA	849	BCR	C27-C26-C25	2.14	125.83	122.73
18	bA	849	BCR	C29-C30-C25	2.14	113.77	110.48
15	aB	810	CLA	C2A-C1A-CHA	2.14	127.59	123.86
18	aF	201	BCR	C7-C8-C9	-2.14	123.01	126.23
15	a1	411	CLA	CHC-C1C-NC	2.14	127.44	124.20
15	aB	841	CLA	O2D-CGD-CBD	2.14	115.06	111.27
15	b6	404	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
15	bB	833	CLA	C3C-C4C-NC	-2.14	108.18	110.57
15	a1	402	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
15	bA	821	CLA	C2A-C1A-CHA	2.14	127.59	123.86
18	bB	849	BCR	C32-C1-C2	-2.14	100.36	108.91
15	aB	834	CLA	CHD-C1D-ND	-2.13	122.49	124.45
18	b6	419	BCR	C15-C16-C17	-2.13	119.10	123.47
15	c4	417	CLA	C2D-C1D-ND	-2.13	108.53	110.10
18	c3	418	BCR	C16-C15-C14	-2.13	119.10	123.47
15	c6	413	CLA	CHC-C1C-NC	2.13	127.44	124.20
18	cF	202	BCR	C32-C1-C2	-2.13	100.37	108.91
18	bA	848	BCR	C33-C5-C6	-2.13	122.13	124.53
18	b1	418	BCR	C15-C14-C13	-2.13	124.27	127.31
15	b6	412	CLA	C2A-C1A-CHA	2.13	127.59	123.86
15	a3	417	CLA	C2D-C1D-ND	-2.13	108.53	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a5	401	BCR	C24-C23-C22	-2.13	123.01	126.23
15	c1	405	CLA	CHC-C1C-NC	2.13	127.44	124.20
15	cB	818	CLA	CHD-C1D-ND	-2.13	122.49	124.45
15	c3	421	CLA	C16-C15-C13	-2.13	109.03	115.92
18	a4	420	BCR	C1-C6-C5	-2.13	119.61	122.61
15	aB	829	CLA	O2D-CGD-CBD	2.13	115.06	111.27
15	bB	820	CLA	C2D-C1D-ND	-2.13	108.53	110.10
16	cA	845	PQN	C14-C13-C15	2.13	118.86	115.27
15	b3	410	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
15	a1	404	CLA	CHB-C4A-NA	2.13	127.46	124.51
15	a4	417	CLA	C2D-C1D-ND	-2.13	108.53	110.10
15	a3	417	CLA	C3C-C4C-NC	-2.13	108.18	110.57
15	c5	408	CLA	CAA-CBA-CGA	2.13	118.16	112.51
15	cA	834	CLA	C1-C2-C3	-2.13	122.36	126.04
15	c5	417	CLA	CMA-C3A-C2A	-2.13	105.24	113.83
15	aB	838	CLA	O2D-CGD-CBD	2.13	115.05	111.27
15	aA	821	CLA	C2A-C1A-CHA	2.13	127.58	123.86
18	cF	202	BCR	C24-C23-C22	-2.13	123.02	126.23
15	aB	811	CLA	C7-C6-C5	-2.13	107.58	113.36
15	b6	407	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
15	bL	203	CLA	C2A-C1A-CHA	2.13	127.58	123.86
15	aB	808	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	c3	418	BCR	C38-C26-C27	-2.13	109.53	113.62
15	a3	411	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	a6	419	BCR	C7-C8-C9	-2.13	123.02	126.23
18	bM	101	BCR	C40-C30-C25	2.13	113.75	110.30
15	b5	408	CLA	CAA-CBA-CGA	2.13	118.16	112.51
18	a3	401	BCR	C29-C30-C25	2.13	113.76	110.48
15	aA	834	CLA	C2A-C1A-CHA	2.13	127.58	123.86
18	cB	849	BCR	C16-C17-C18	-2.13	124.27	127.31
15	cX	102	CLA	O1D-CGD-CBD	2.13	128.84	124.48
15	aA	827	CLA	C2D-C1D-ND	-2.13	108.54	110.10
18	a2	401	BCR	C28-C27-C26	-2.13	110.28	114.08
15	b2	412	CLA	C2A-C1A-CHA	2.13	127.58	123.86
18	c1	418	BCR	C15-C14-C13	-2.13	124.27	127.31
15	aA	807	CLA	C2D-C1D-ND	-2.13	108.54	110.10
18	bB	849	BCR	C7-C8-C9	-2.13	123.02	126.23
15	b2	410	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
15	c3	417	CLA	C3C-C4C-NC	-2.13	108.19	110.57
15	b3	411	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
15	bB	836	CLA	CBC-CAC-C3C	2.13	118.29	112.43
15	a6	407	CLA	O2A-CGA-O1A	-2.13	118.00	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b1	419	BCR	C16-C15-C14	-2.13	119.12	123.47
15	bB	811	CLA	CAC-C3C-C4C	2.12	127.57	124.81
18	c1	401	BCR	C34-C9-C10	-2.12	119.95	122.92
15	cB	841	CLA	O2D-CGD-CBD	2.12	115.04	111.27
15	cJ	101	CLA	O2D-CGD-CBD	2.12	115.04	111.27
15	b4	412	CLA	CHC-C1C-NC	2.12	127.43	124.20
18	a2	401	BCR	C24-C23-C22	-2.12	123.03	126.23
15	b2	413	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	a3	405	CLA	CHB-C4A-NA	2.12	127.45	124.51
15	aK	102	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	cK	102	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	c2	412	CLA	C2A-C1A-CHA	2.12	127.57	123.86
18	cB	846	BCR	C35-C13-C14	-2.12	119.95	122.92
15	cB	830	CLA	O2A-C1-C2	-2.12	103.06	108.64
15	cB	838	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
15	bA	803	CLA	O1D-CGD-CBD	2.12	128.83	124.48
15	aB	814	CLA	CHB-C4A-NA	2.12	127.45	124.51
15	c1	410	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	aB	833	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	a1	407	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	a4	412	CLA	CHC-C1C-NC	2.12	127.42	124.20
18	b4	420	BCR	C24-C23-C22	-2.12	123.03	126.23
15	cA	827	CLA	O2D-CGD-CBD	2.12	115.04	111.27
15	b1	405	CLA	CMA-C3A-C4A	2.12	117.47	111.77
18	b5	418	BCR	C38-C26-C27	-2.12	109.54	113.62
15	aJ	202	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	cJ	101	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	b6	417	CLA	CMD-C2D-C3D	2.12	132.49	127.61
18	b6	420	BCR	C7-C8-C9	-2.12	123.03	126.23
18	b2	421	BCR	C1-C6-C5	-2.12	119.63	122.61
15	aB	805	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
15	c2	411	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
15	cB	838	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	c2	419	BCR	C38-C26-C27	-2.12	109.54	113.62
18	c3	401	BCR	C29-C30-C25	2.12	113.74	110.48
18	bB	846	BCR	C35-C13-C14	-2.12	119.95	122.92
15	a4	417	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	aB	804	CLA	C2A-C1A-CHA	2.12	127.56	123.86
15	aA	823	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
15	a1	416	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
15	c1	412	CLA	CHC-C1C-NC	2.12	127.42	124.20
18	cF	202	BCR	C7-C8-C9	-2.12	123.03	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	838	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
15	bA	827	CLA	O2D-CGD-CBD	2.12	115.03	111.27
15	bB	825	CLA	C2D-C1D-ND	-2.12	108.54	110.10
15	c3	410	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
18	bF	202	BCR	C2-C1-C6	2.12	113.74	110.48
15	cB	830	CLA	CMC-C2C-C3C	2.12	131.87	126.12
15	b2	413	CLA	CHD-C4C-C3C	2.12	127.95	124.84
15	bA	834	CLA	C2A-C1A-CHA	2.12	127.56	123.86
18	bB	845	BCR	C39-C30-C25	2.12	113.73	110.30
15	a5	417	CLA	C3A-C2A-C1A	2.12	104.51	101.34
15	a1	411	CLA	C3C-C4C-NC	-2.12	108.20	110.57
15	cA	834	CLA	C2A-C1A-CHA	2.12	127.56	123.86
18	bJ	103	BCR	C38-C26-C27	-2.12	109.55	113.62
15	bB	830	CLA	CMC-C2C-C3C	2.12	131.86	126.12
18	aJ	204	BCR	C38-C26-C27	-2.12	109.55	113.62
15	bB	808	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
15	c5	407	CLA	O2A-CGA-O1A	-2.12	118.03	123.30
15	b1	410	CLA	C2A-C1A-CHA	2.12	127.56	123.86
15	cA	812	CLA	O1A-CGA-CBA	2.12	131.99	123.73
18	a6	420	BCR	C1-C6-C5	-2.12	119.63	122.61
15	aA	815	CLA	CHD-C1D-ND	-2.12	122.51	124.45
15	bX	102	CLA	O1D-CGD-CBD	2.11	128.81	124.48
18	aM	101	BCR	C16-C17-C18	-2.11	124.29	127.31
15	bB	814	CLA	CHB-C4A-NA	2.11	127.44	124.51
18	b6	401	BCR	C40-C30-C25	2.11	113.73	110.30
18	c5	401	BCR	C40-C30-C25	2.11	113.73	110.30
15	c2	410	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	c5	405	CLA	CHB-C4A-NA	2.11	127.44	124.51
18	cM	101	BCR	C40-C30-C25	2.11	113.73	110.30
15	a5	405	CLA	CMA-C3A-C4A	2.11	117.45	111.77
18	a2	421	BCR	C1-C6-C5	-2.11	119.64	122.61
15	b5	403	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
18	a5	401	BCR	C16-C15-C14	-2.11	119.15	123.47
15	aA	815	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
15	a4	416	CLA	C1C-C2C-C3C	-2.11	104.73	106.96
15	cB	804	CLA	C2A-C1A-CHA	2.11	127.55	123.86
18	c3	420	BCR	C1-C6-C5	-2.11	119.64	122.61
15	a1	409	CLA	CHA-C1A-NA	-2.11	121.56	126.40
15	a6	412	CLA	CHD-C1D-ND	-2.11	122.51	124.45
15	b3	411	CLA	CHD-C1D-ND	-2.11	122.51	124.45
15	aB	827	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
15	c3	408	CLA	CAA-C2A-C3A	-2.11	106.99	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a6	422	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	cB	805	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
15	cA	823	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	cB	825	CLA	C2D-C1D-ND	-2.11	108.55	110.10
15	aB	830	CLA	O2A-C1-C2	-2.11	103.09	108.64
15	b3	405	CLA	CMA-C3A-C4A	2.11	117.45	111.77
18	aA	850	BCR	C27-C26-C25	2.11	125.80	122.73
18	a6	421	BCR	C2-C3-C4	2.11	116.09	111.38
18	cJ	103	BCR	C38-C26-C27	-2.11	109.56	113.62
15	aA	827	CLA	O2D-CGD-CBD	2.11	115.02	111.27
15	cB	829	CLA	O2D-CGD-CBD	2.11	115.02	111.27
15	c1	417	CLA	CHD-C1D-ND	-2.11	122.52	124.45
15	b4	405	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
15	cB	803	CLA	CMD-C2D-C3D	2.11	132.47	127.61
15	c6	417	CLA	CMD-C2D-C3D	2.11	132.47	127.61
15	aA	813	CLA	CHA-C1A-NA	-2.11	121.57	126.40
15	bB	830	CLA	CHB-C4A-NA	2.11	127.43	124.51
15	bA	808	CLA	O2D-CGD-CBD	2.11	115.02	111.27
14	aA	801	CL0	C2A-C1A-CHA	-2.11	120.17	123.86
15	cA	807	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
15	cB	808	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	b4	401	BCR	C27-C26-C25	2.11	125.79	122.73
18	b4	420	BCR	C11-C10-C9	-2.11	124.30	127.31
15	bB	830	CLA	O2A-C1-C2	-2.11	103.09	108.64
18	c4	420	BCR	C1-C6-C5	-2.11	119.64	122.61
15	a3	405	CLA	CMA-C3A-C4A	2.11	117.44	111.77
15	bB	829	CLA	O2D-CGD-CBD	2.11	115.01	111.27
15	bK	101	CLA	C2A-C1A-CHA	2.11	127.55	123.86
15	cB	819	CLA	C2A-C1A-CHA	2.11	127.55	123.86
15	bA	812	CLA	O1A-CGA-CBA	2.11	131.96	123.73
15	aA	803	CLA	O1D-CGD-CBD	2.11	128.80	124.48
15	aB	830	CLA	CMC-C2C-C3C	2.11	131.84	126.12
15	bA	815	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
15	bL	202	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
15	b3	421	CLA	C16-C15-C13	-2.11	109.11	115.92
15	a4	416	CLA	CMD-C2D-C3D	2.11	132.46	127.61
18	a6	401	BCR	C3-C4-C5	-2.11	110.31	114.08
15	c4	404	CLA	O1D-CGD-CBD	2.11	128.80	124.48
16	aA	846	PQN	C14-C13-C15	2.11	118.82	115.27
15	c3	403	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
15	aB	838	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
18	aM	101	BCR	C40-C30-C25	2.11	113.72	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	405	CLA	CHB-C4A-NA	2.11	127.42	124.51
15	aX	102	CLA	O1D-CGD-CBD	2.11	128.79	124.48
15	cB	841	CLA	C2A-C1A-CHA	2.11	127.54	123.86
18	bA	851	BCR	C27-C26-C25	2.11	125.79	122.73
15	cA	803	CLA	C11-C12-C13	-2.11	109.11	115.92
15	a5	408	CLA	CAA-CBA-CGA	2.11	118.10	112.51
15	aA	803	CLA	C11-C12-C13	-2.11	109.11	115.92
15	bB	805	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
15	cB	834	CLA	CHD-C1D-ND	-2.11	122.52	124.45
15	cA	815	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
15	aA	812	CLA	O1A-CGA-CBA	2.11	131.95	123.73
15	c6	406	CLA	CHC-C1C-NC	2.11	127.40	124.20
15	c5	411	CLA	C2A-C1A-CHA	2.11	127.54	123.86
15	bB	838	CLA	O2D-CGD-CBD	2.10	115.01	111.27
18	b6	401	BCR	C3-C4-C5	-2.10	110.32	114.08
15	bA	815	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	a1	417	BCR	C15-C14-C13	-2.10	124.31	127.31
15	b4	412	CLA	C3C-C4C-NC	-2.10	108.21	110.57
15	bB	819	CLA	C2A-C1A-CHA	2.10	127.54	123.86
14	cA	801	CL0	C2A-C1A-CHA	-2.10	120.18	123.86
15	cB	812	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	a2	410	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
15	cA	803	CLA	O1D-CGD-CBD	2.10	128.79	124.48
15	a5	415	CLA	O2D-CGD-CBD	2.10	115.00	111.27
15	bB	841	CLA	C2A-C1A-CHA	2.10	127.53	123.86
15	aB	812	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	b2	404	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
15	b1	417	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
18	bB	849	BCR	C24-C23-C22	-2.10	123.06	126.23
18	b1	419	BCR	C40-C30-C25	2.10	113.71	110.30
15	b1	417	CLA	C3C-C4C-NC	-2.10	108.21	110.57
15	a1	405	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
15	c4	405	CLA	CHC-C1C-NC	2.10	127.39	124.20
18	c1	419	BCR	C40-C30-C25	2.10	113.71	110.30
15	aB	811	CLA	CAC-C3C-C4C	2.10	127.54	124.81
15	bB	803	CLA	CMD-C2D-C3D	2.10	132.45	127.61
15	cB	811	CLA	C7-C6-C5	-2.10	107.65	113.36
15	c3	411	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	a3	406	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
15	c5	403	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	cB	827	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	a5	411	CLA	C2A-C1A-CHA	2.10	127.53	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c6	420	BCR	C7-C8-C9	-2.10	123.06	126.23
15	a4	408	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
15	c1	412	CLA	C3C-C4C-NC	-2.10	108.22	110.57
15	c2	405	CLA	CMA-C3A-C4A	2.10	117.41	111.77
18	cJ	103	BCR	C40-C30-C25	2.10	113.70	110.30
15	a3	421	CLA	C11-C10-C8	-2.10	109.14	115.92
15	bA	803	CLA	C11-C12-C13	-2.10	109.14	115.92
15	c5	417	CLA	C3C-C4C-NC	-2.10	108.22	110.57
15	b1	410	CLA	CHA-C1A-NA	-2.10	121.59	126.40
18	aI	101	BCR	C27-C26-C25	2.10	125.78	122.73
18	b6	401	BCR	C7-C8-C9	-2.10	123.06	126.23
15	b2	418	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	c5	403	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
15	a4	404	CLA	O1D-CGD-CBD	2.10	128.78	124.48
15	aB	827	CLA	C16-C15-C13	-2.10	109.14	115.92
15	c4	416	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
18	bJ	103	BCR	C40-C30-C25	2.10	113.70	110.30
15	cA	844	CLA	O2D-CGD-CBD	2.10	115.00	111.27
15	a5	403	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
15	a5	404	CLA	C2A-C1A-CHA	2.10	127.53	123.86
15	bA	807	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	c6	401	BCR	C3-C4-C5	-2.10	110.33	114.08
15	a6	412	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
15	a6	406	CLA	CHC-C1C-NC	2.10	127.38	124.20
15	a3	409	CLA	O1D-CGD-CBD	2.10	128.77	124.48
18	a6	401	BCR	C7-C8-C9	-2.10	123.07	126.23
15	c6	414	CLA	CHD-C1D-C2D	2.10	129.88	125.48
15	cA	808	CLA	O2D-CGD-CBD	2.10	114.99	111.27
18	b2	401	BCR	C28-C27-C26	-2.10	110.33	114.08
18	b6	402	BCR	C28-C27-C26	-2.10	110.33	114.08
18	c6	402	BCR	C28-C27-C26	-2.10	110.33	114.08
18	a1	418	BCR	C16-C15-C14	-2.10	119.18	123.47
15	aJ	202	CLA	O2D-CGD-CBD	2.10	114.99	111.27
15	b3	421	CLA	O2D-CGD-CBD	2.10	114.99	111.27
18	a6	402	BCR	C28-C27-C26	-2.10	110.33	114.08
15	a5	405	CLA	CED-O2D-CGD	-2.10	111.20	115.94
15	a3	408	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
18	aF	203	BCR	C15-C16-C17	-2.10	119.18	123.47
18	b3	418	BCR	C16-C15-C14	-2.09	119.18	123.47
15	a5	411	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	bB	827	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
15	a1	408	CLA	O2D-CGD-O1D	-2.09	119.74	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	405	CLA	CMA-C3A-C4A	2.09	117.40	111.77
18	aB	849	BCR	C16-C17-C18	-2.09	124.32	127.31
15	bB	811	CLA	C7-C6-C5	-2.09	107.67	113.36
15	cA	813	CLA	CHA-C1A-NA	-2.09	121.60	126.40
18	cF	204	BCR	C31-C1-C6	2.09	113.69	110.30
15	cK	102	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	a6	412	CLA	CAA-CBA-CGA	2.09	118.06	112.51
15	c1	417	CLA	C3C-C4C-NC	-2.09	108.22	110.57
15	aA	845	CLA	O2D-CGD-CBD	2.09	114.99	111.27
18	bJ	105	BCR	C15-C16-C17	-2.09	119.19	123.47
15	aA	807	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
15	bB	833	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
18	bM	101	BCR	C16-C17-C18	-2.09	124.33	127.31
18	c4	420	BCR	C11-C10-C9	-2.09	124.33	127.31
15	b5	411	CLA	C2A-C1A-CHA	2.09	127.52	123.86
15	a6	417	CLA	CMD-C2D-C3D	2.09	132.43	127.61
15	c1	417	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
15	b5	405	CLA	CMA-C3A-C4A	2.09	117.39	111.77
15	c3	405	CLA	CMA-C3A-C4A	2.09	117.39	111.77
18	cM	101	BCR	C16-C17-C18	-2.09	124.33	127.31
15	bJ	101	CLA	C2A-C1A-CHA	2.09	127.51	123.86
15	b5	405	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
15	b3	406	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
18	aB	845	BCR	C39-C30-C25	2.09	113.69	110.30
15	b3	417	CLA	C3C-C4C-NC	-2.09	108.23	110.57
15	b1	412	CLA	CHC-C1C-NC	2.09	127.37	124.20
18	bA	848	BCR	C11-C10-C9	-2.09	124.33	127.31
15	c1	406	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
15	aB	834	CLA	C3C-C4C-NC	-2.09	108.23	110.57
15	b5	411	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	cL	201	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	bA	802	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	b4	410	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	aA	808	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
15	bA	823	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	a3	412	CLA	C3C-C4C-NC	-2.09	108.23	110.57
15	b5	409	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	c2	417	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	bB	812	CLA	CHA-C1A-NA	-2.09	121.62	126.40
18	aK	101	BCR	C29-C30-C25	2.09	113.69	110.48
15	b6	412	CLA	CHD-C1D-ND	-2.09	122.54	124.45
18	c2	421	BCR	C1-C6-C5	-2.09	119.67	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bF	202	BCR	C23-C22-C21	-2.09	115.74	118.94
15	aB	803	CLA	CMD-C2D-C3D	2.09	132.41	127.61
15	b4	405	CLA	CMA-C3A-C4A	2.09	117.38	111.77
15	b1	404	CLA	O1D-CGD-CBD	2.09	128.75	124.48
18	a1	418	BCR	C7-C8-C9	-2.09	123.08	126.23
19	cX	101	LHG	O8-C23-C24	2.09	121.48	112.38
15	b6	410	CLA	O1D-CGD-CBD	2.09	128.75	124.48
15	bB	803	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	c4	411	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
15	b2	405	CLA	CMA-C3A-C4A	2.09	117.38	111.77
15	a3	403	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
18	a3	418	BCR	C1-C6-C5	-2.09	119.68	122.61
15	cB	803	CLA	C6-C7-C8	-2.09	109.18	115.92
15	b1	406	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
18	cF	205	BCR	C15-C16-C17	-2.09	119.20	123.47
15	bA	813	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	bB	834	CLA	CHD-C1D-ND	-2.08	122.54	124.45
15	bL	204	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
15	bB	827	CLA	C16-C15-C13	-2.08	109.18	115.92
15	b5	407	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
15	b5	420	CLA	O2D-CGD-CBD	2.08	114.97	111.27
18	aJ	204	BCR	C40-C30-C25	2.08	113.68	110.30
15	b3	416	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	b6	412	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
15	c3	404	CLA	C2A-C1A-CHA	2.08	127.50	123.86
15	aA	841	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	bA	808	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
18	b3	418	BCR	C7-C8-C9	-2.08	123.09	126.23
15	cB	833	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
15	aK	102	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	cA	841	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	b3	421	CLA	C11-C10-C8	-2.08	109.19	115.92
15	b3	408	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
15	a5	405	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
15	aB	841	CLA	C2A-C1A-CHA	2.08	127.50	123.86
18	bF	202	BCR	C31-C1-C6	2.08	113.68	110.30
15	c3	408	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
15	c6	412	CLA	CAA-CBA-CGA	2.08	118.03	112.51
15	aB	814	CLA	O1D-CGD-CBD	2.08	128.74	124.48
15	a1	422	CLA	C16-C15-C13	-2.08	109.19	115.92
15	c5	405	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
18	c4	418	BCR	C1-C6-C5	-2.08	119.68	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	405	CLA	CHB-C4A-NA	2.08	127.39	124.51
15	cA	802	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	aL	201	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
18	b6	420	BCR	C1-C6-C5	-2.08	119.68	122.61
18	c5	401	BCR	C16-C15-C14	-2.08	119.21	123.47
15	c5	405	CLA	O1D-CGD-CBD	2.08	128.74	124.48
15	aB	825	CLA	C2D-C1D-ND	-2.08	108.57	110.10
15	aB	803	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	cA	808	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
15	c4	405	CLA	CED-O2D-CGD	-2.08	111.23	115.94
18	a5	418	BCR	C38-C26-C27	-2.08	109.62	113.62
15	aB	833	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
15	c6	412	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
15	a4	405	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
15	cB	827	CLA	C16-C15-C13	-2.08	109.20	115.92
15	b1	415	CLA	CHA-C4D-ND	2.08	136.85	132.50
15	b6	414	CLA	CHD-C1D-C2D	2.08	129.84	125.48
15	aB	803	CLA	C6-C7-C8	-2.08	109.20	115.92
15	a4	405	CLA	CMA-C3A-C4A	2.08	117.36	111.77
15	b5	405	CLA	CED-O2D-CGD	-2.08	111.24	115.94
15	b4	416	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
16	aA	846	PQN	C17-C16-C15	-2.08	107.72	113.36
18	b1	420	BCR	C16-C15-C14	-2.08	119.22	123.47
15	c4	405	CLA	CMA-C3A-C4A	2.08	117.36	111.77
19	bX	101	LHG	O8-C23-C24	2.08	121.44	112.38
15	aA	802	CLA	CHA-C1A-NA	-2.08	121.64	126.40
15	b5	420	CLA	O1D-CGD-CBD	2.08	128.73	124.48
15	c5	411	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
18	aF	202	BCR	C23-C22-C21	-2.08	115.75	118.94
15	b4	409	CLA	O1D-CGD-CBD	2.08	128.73	124.48
15	a3	411	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
15	bA	841	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	aA	851	BCR	C31-C1-C6	2.08	113.67	110.30
15	c4	416	CLA	CMD-C2D-C3D	2.08	132.39	127.61
15	a3	421	CLA	O2D-CGD-CBD	2.08	114.96	111.27
18	c1	419	BCR	C7-C8-C9	-2.08	123.10	126.23
18	a5	401	BCR	C40-C30-C25	2.08	113.67	110.30
15	b5	411	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
15	aB	807	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
15	bB	824	CLA	O1A-CGA-CBA	2.07	129.75	123.08
15	cB	824	CLA	O1A-CGA-CBA	2.07	129.75	123.08
15	aL	203	CLA	CAA-C2A-C3A	-2.07	107.10	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c2	419	BCR	C11-C10-C9	-2.07	124.35	127.31
15	c3	421	CLA	C11-C10-C8	-2.07	109.21	115.92
15	a6	405	CLA	C2A-C1A-CHA	2.07	127.49	123.86
15	b3	404	CLA	C2A-C1A-CHA	2.07	127.49	123.86
15	aB	823	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	c3	411	CLA	CHD-C1D-ND	-2.07	122.55	124.45
15	cB	813	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
18	c1	418	BCR	C16-C15-C14	-2.07	119.23	123.47
15	b4	416	CLA	CMD-C2D-C3D	2.07	132.38	127.61
15	c1	416	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	b4	417	CLA	C2D-C1D-ND	-2.07	108.58	110.10
18	cB	845	BCR	C39-C30-C25	2.07	113.66	110.30
18	c4	420	BCR	C24-C23-C22	-2.07	123.10	126.23
18	a6	421	BCR	C28-C27-C26	-2.07	110.38	114.08
19	aX	101	LHG	O8-C23-C24	2.07	121.42	112.38
15	b3	408	CLA	C3C-C4C-NC	-2.07	108.25	110.57
15	c6	413	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
15	a4	410	CLA	CHA-C1A-NA	-2.07	121.65	126.40
15	c4	412	CLA	C3C-C4C-NC	-2.07	108.25	110.57
15	b3	403	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	bB	813	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
15	aX	102	CLA	C2A-C1A-CHA	2.07	127.48	123.86
15	b5	409	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
15	aB	824	CLA	O1A-CGA-CBA	2.07	129.73	123.08
15	aB	813	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
15	bA	845	CLA	O2D-CGD-CBD	2.07	114.95	111.27
15	b3	408	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
15	cA	815	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	c2	401	BCR	C31-C1-C6	2.07	113.66	110.30
15	bB	803	CLA	C6-C7-C8	-2.07	109.23	115.92
18	a4	401	BCR	C27-C26-C25	2.07	125.73	122.73
15	a1	414	CLA	CHA-C4D-ND	2.07	136.83	132.50
15	cB	830	CLA	CHB-C4A-NA	2.07	127.37	124.51
15	b5	415	CLA	O2D-CGD-CBD	2.07	114.94	111.27
15	c3	406	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
18	b1	418	BCR	C1-C6-C5	-2.07	119.70	122.61
15	a2	405	CLA	CHA-C4D-ND	2.07	136.83	132.50
15	c3	405	CLA	CHA-C4D-ND	2.07	136.82	132.50
15	bB	814	CLA	O1D-CGD-CBD	2.07	128.72	124.48
18	a4	420	BCR	C11-C10-C9	-2.07	124.36	127.31
18	aF	201	BCR	C38-C26-C27	-2.07	109.64	113.62
15	cA	821	CLA	CHC-C1C-NC	2.07	127.34	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	413	CLA	CHD-C4C-C3C	2.07	127.88	124.84
18	bA	852	BCR	C16-C15-C14	-2.07	119.24	123.47
15	a5	405	CLA	O1D-CGD-CBD	2.07	128.71	124.48
14	bA	801	CL0	C2A-C1A-CHA	-2.07	120.25	123.86
15	a6	414	CLA	CHD-C4C-C3C	2.07	127.88	124.84
16	bA	846	PQN	C17-C16-C15	-2.07	107.75	113.36
18	c6	420	BCR	C1-C6-C5	-2.07	119.70	122.61
18	b1	419	BCR	C7-C8-C9	-2.07	123.11	126.23
18	b5	401	BCR	C16-C15-C14	-2.07	119.24	123.47
15	c4	410	CLA	CHA-C1A-NA	-2.07	121.67	126.40
15	b5	404	CLA	C2A-C1A-CHA	2.07	127.47	123.86
15	bK	101	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	b1	416	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
18	aF	202	BCR	C31-C1-C6	2.06	113.65	110.30
15	aA	832	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
18	c2	401	BCR	C28-C27-C26	-2.06	110.39	114.08
15	b5	403	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
18	b5	419	BCR	C1-C6-C5	-2.06	119.71	122.61
15	cA	832	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
15	b5	416	CLA	CMD-C2D-C3D	2.06	132.36	127.61
15	a3	403	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
16	cA	845	PQN	C17-C16-C15	-2.06	107.76	113.36
18	bA	852	BCR	C31-C1-C6	2.06	113.64	110.30
15	c2	403	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
15	a1	406	CLA	CHA-C1A-NA	-2.06	121.67	126.40
18	cF	202	BCR	C38-C26-C27	-2.06	109.65	113.62
15	cA	815	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	aB	810	CLA	CAC-C3C-C4C	2.06	127.48	124.81
15	b5	417	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	a1	421	BCR	C28-C27-C26	-2.06	110.40	114.08
18	c4	401	BCR	C27-C26-C25	2.06	125.72	122.73
18	aL	205	BCR	C11-C10-C9	-2.06	124.37	127.31
15	c2	404	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
15	a5	416	CLA	CMD-C2D-C3D	2.06	132.35	127.61
15	c5	415	CLA	O2D-CGD-CBD	2.06	114.93	111.27
15	b1	405	CLA	CHC-C1C-NC	2.06	127.33	124.20
15	cB	803	CLA	CHA-C1A-NA	-2.06	121.68	126.40
15	bB	807	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
15	cA	819	CLA	CAC-C3C-C2C	-2.06	124.01	127.53
15	a5	411	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
15	a3	405	CLA	CHA-C4D-ND	2.06	136.81	132.50
18	cA	850	BCR	C31-C1-C6	2.06	113.64	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	403	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
15	cL	203	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
15	bX	102	CLA	C2A-C1A-CHA	2.06	127.46	123.86
18	cF	204	BCR	C23-C22-C21	-2.06	115.78	118.94
15	a3	404	CLA	C2A-C1A-CHA	2.06	127.46	123.86
15	a5	407	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
18	bI	101	BCR	C27-C26-C25	2.06	125.72	122.73
15	bB	834	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	a4	418	BCR	C1-C6-C5	-2.06	119.72	122.61
15	a5	408	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
15	cA	821	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
15	bA	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	b2	409	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	a1	413	CLA	CMA-C3A-C2A	-2.06	111.30	116.10
15	bA	832	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	bB	823	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	c1	404	CLA	O1D-CGD-CBD	2.06	128.69	124.48
15	aA	808	CLA	O2D-CGD-CBD	2.06	114.92	111.27
15	b1	414	CLA	CMA-C3A-C2A	-2.06	111.30	116.10
15	bA	821	CLA	CHC-C1C-NC	2.06	127.32	124.20
18	c5	418	BCR	C15-C16-C17	-2.06	119.26	123.47
15	a4	409	CLA	O1D-CGD-CBD	2.06	128.69	124.48
15	c4	405	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
19	cA	852	LHG	C15-C14-C13	-2.06	103.98	114.42
15	c3	416	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	b2	403	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
15	a3	408	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
15	b5	403	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
15	a6	413	CLA	O2A-CGA-O1A	-2.06	118.18	123.30
15	aA	815	CLA	CHA-C1A-NA	-2.06	121.69	126.40
15	b3	405	CLA	CHA-C4D-ND	2.05	136.80	132.50
15	b1	408	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	c5	409	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
15	a2	413	CLA	C3C-C4C-NC	-2.05	108.27	110.57
15	aA	821	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
18	cA	850	BCR	C16-C15-C14	-2.05	119.27	123.47
18	cI	101	BCR	C27-C26-C25	2.05	125.71	122.73
15	b5	417	CLA	C3A-C2A-C1A	2.05	104.42	101.34
15	c4	409	CLA	O1D-CGD-CBD	2.05	128.69	124.48
15	aB	808	CLA	C7-C6-C5	-2.05	107.78	113.36
15	c5	411	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	bB	810	CLA	CAC-C3C-C4C	2.05	127.47	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	810	CLA	CAC-C3C-C4C	2.05	127.47	124.81
18	b5	401	BCR	C1-C6-C5	-2.05	119.72	122.61
15	c5	420	CLA	O1D-CGD-CBD	2.05	128.68	124.48
15	cB	841	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	c4	421	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
15	a3	410	CLA	C1D-ND-C4D	2.05	107.79	106.33
18	a1	421	BCR	C34-C9-C10	-2.05	120.05	122.92
15	cB	823	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
15	bB	818	CLA	C2A-C1A-CHA	2.05	127.44	123.86
15	a2	410	CLA	O1D-CGD-CBD	2.05	128.68	124.48
15	c1	407	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	aI	103	BCR	C7-C8-C9	-2.05	123.14	126.23
15	c1	403	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	b6	409	CLA	C3C-C4C-NC	-2.05	108.27	110.57
19	aA	853	LHG	C15-C14-C13	-2.05	104.02	114.42
18	a5	419	BCR	C1-C6-C5	-2.05	119.73	122.61
15	c3	417	CLA	C2D-C1D-ND	-2.05	108.59	110.10
15	c5	420	CLA	CHA-C4D-ND	2.05	136.78	132.50
18	bB	849	BCR	C38-C26-C27	-2.05	109.68	113.62
15	c1	405	CLA	CHB-C4A-NA	2.05	127.34	124.51
15	a4	415	CLA	O2D-CGD-CBD	2.05	114.91	111.27
15	b4	415	CLA	O2D-CGD-CBD	2.05	114.91	111.27
15	a5	403	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
15	a5	403	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
15	b6	406	CLA	CHC-C1C-NC	2.05	127.31	124.20
15	cA	831	CLA	CMC-C2C-C3C	2.05	131.68	126.12
15	aA	811	CLA	C2D-C1D-ND	-2.05	108.59	110.10
15	c3	411	CLA	C2A-C1A-CHA	2.05	127.44	123.86
15	a4	402	CLA	O1D-CGD-CBD	2.05	128.67	124.48
15	a5	420	CLA	O1D-CGD-CBD	2.05	128.67	124.48
15	b3	412	CLA	C3C-C4C-NC	-2.05	108.28	110.57
15	b3	404	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
15	a4	415	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
18	c2	419	BCR	C15-C16-C17	-2.05	119.28	123.47
15	c5	414	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	a1	417	BCR	C1-C6-C5	-2.05	119.73	122.61
15	a4	412	CLA	C3C-C4C-NC	-2.05	108.28	110.57
15	b2	410	CLA	O1D-CGD-CBD	2.05	128.67	124.48
18	bL	206	BCR	C11-C10-C9	-2.05	124.39	127.31
15	c5	405	CLA	CMA-C3A-C4A	2.05	117.27	111.77
15	b2	404	CLA	O1D-CGD-CBD	2.05	128.67	124.48
15	b1	405	CLA	CMD-C2D-C3D	-2.05	122.91	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	402	CLA	O1D-CGD-CBD	2.05	128.67	124.48
18	aK	101	BCR	C11-C10-C9	-2.05	124.39	127.31
18	a1	419	BCR	C11-C10-C9	-2.05	124.39	127.31
15	aA	842	CLA	CHA-C4D-ND	2.05	136.78	132.50
15	c4	415	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
18	aA	851	BCR	C16-C15-C14	-2.04	119.28	123.47
15	cB	808	CLA	C7-C6-C5	-2.04	107.81	113.36
15	c1	411	CLA	CHD-C1D-ND	-2.04	122.58	124.45
15	b6	405	CLA	C2A-C1A-CHA	2.04	127.43	123.86
15	b2	417	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
15	c3	410	CLA	C1D-ND-C4D	2.04	107.79	106.33
15	cB	814	CLA	O1D-CGD-CBD	2.04	128.67	124.48
18	c3	418	BCR	C7-C8-C9	-2.04	123.15	126.23
18	cK	101	BCR	C29-C30-C25	2.04	113.63	110.48
15	bA	808	CLA	CHD-C1D-ND	-2.04	122.58	124.45
15	c5	403	CLA	CHA-C1A-NA	-2.04	121.72	126.40
18	c1	420	BCR	C16-C15-C14	-2.04	119.29	123.47
15	b5	405	CLA	O1D-CGD-CBD	2.04	128.66	124.48
19	bA	854	LHG	C15-C14-C13	-2.04	104.06	114.42
15	aA	831	CLA	CMC-C2C-C3C	2.04	131.66	126.12
15	bB	836	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	c6	405	CLA	C2A-C1A-CHA	2.04	127.43	123.86
15	bA	815	CLA	CHA-C1A-NA	-2.04	121.72	126.40
18	bB	845	BCR	C15-C16-C17	-2.04	119.29	123.47
18	a2	419	BCR	C11-C10-C9	-2.04	124.40	127.31
18	cB	845	BCR	C15-C16-C17	-2.04	119.29	123.47
15	bB	841	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	aA	821	CLA	CHC-C1C-NC	2.04	127.30	124.20
15	c2	417	CLA	O2D-CGD-CBD	2.04	114.89	111.27
15	c3	405	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
18	a2	419	BCR	C15-C16-C17	-2.04	119.30	123.47
15	a1	415	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	b6	408	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
18	cK	101	BCR	C11-C10-C9	-2.04	124.40	127.31
15	aB	841	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	a5	404	CLA	O1D-CGD-CBD	2.04	128.66	124.48
18	c5	419	BCR	C1-C6-C5	-2.04	119.74	122.61
15	cA	829	CLA	C7-C6-C5	-2.04	107.82	113.36
15	aA	813	CLA	C1-C2-C3	-2.04	122.52	126.04
18	bA	848	BCR	C29-C30-C25	2.04	113.62	110.48
15	a3	405	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
15	c3	403	CLA	O2A-CGA-O1A	-2.04	118.45	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	408	CLA	C3C-C4C-NC	-2.04	108.28	110.57
15	cX	102	CLA	C2A-C1A-CHA	2.04	127.42	123.86
15	a1	402	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	cB	828	CLA	C2A-C1A-CHA	2.04	127.42	123.86
18	b3	420	BCR	C16-C15-C14	-2.04	119.30	123.47
15	c2	413	CLA	CHD-C4C-C3C	2.04	127.83	124.84
15	cB	807	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
18	aA	850	BCR	C33-C5-C6	-2.04	122.24	124.53
18	cA	849	BCR	C28-C27-C26	-2.04	110.44	114.08
15	a3	404	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	c6	419	BCR	C1-C6-C5	-2.04	119.74	122.61
15	bB	812	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
15	c2	405	CLA	CHA-C4D-ND	2.04	136.76	132.50
18	c1	418	BCR	C11-C10-C9	-2.04	124.40	127.31
18	bA	851	BCR	C33-C5-C6	-2.04	122.24	124.53
15	b2	405	CLA	CHA-C4D-ND	2.04	136.76	132.50
15	c6	404	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
18	cB	849	BCR	C38-C26-C27	-2.04	109.70	113.62
15	b6	404	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
15	cB	818	CLA	C2A-C1A-CHA	2.04	127.42	123.86
15	c5	404	CLA	C2A-C1A-CHA	2.04	127.42	123.86
18	b2	419	BCR	C1-C6-C5	-2.04	119.75	122.61
15	aA	819	CLA	CAC-C3C-C2C	-2.04	124.05	127.53
18	aA	850	BCR	C28-C27-C26	-2.04	110.44	114.08
15	a1	406	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
18	cL	204	BCR	C7-C8-C9	-2.04	123.16	126.23
15	b6	406	CLA	CHB-C4A-NA	2.04	127.33	124.51
18	a1	419	BCR	C16-C15-C14	-2.04	119.30	123.47
15	c3	409	CLA	O1D-CGD-CBD	2.04	128.65	124.48
18	b5	401	BCR	C40-C30-C25	2.04	113.60	110.30
15	cF	201	CLA	CHA-C4D-ND	2.04	136.76	132.50
15	b1	412	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	bJ	105	BCR	C1-C6-C5	-2.03	119.75	122.61
15	bA	829	CLA	C7-C6-C5	-2.03	107.83	113.36
15	b2	405	CLA	CHB-C4A-NA	2.03	127.33	124.51
15	b3	405	CLA	CHB-C4A-NA	2.03	127.33	124.51
15	aB	807	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	cB	824	CLA	C2D-C1D-ND	-2.03	108.61	110.10
18	c5	401	BCR	C1-C6-C5	-2.03	119.75	122.61
15	b3	405	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
15	b1	403	CLA	CHA-C1A-NA	-2.03	121.74	126.40
15	cA	806	CLA	O2A-CGA-O1A	-2.03	118.46	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	836	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
15	aB	824	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	cA	808	CLA	CHD-C1D-ND	-2.03	122.59	124.45
15	bA	821	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
18	a2	419	BCR	C1-C6-C5	-2.03	119.75	122.61
18	bL	201	BCR	C11-C10-C9	-2.03	124.41	127.31
15	c1	407	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
15	b3	409	CLA	O1D-CGD-CBD	2.03	128.64	124.48
15	a3	416	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	cB	807	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	bB	808	CLA	C7-C6-C5	-2.03	107.84	113.36
15	b5	403	CLA	CHA-C1A-NA	-2.03	121.75	126.40
15	b4	402	CLA	O1D-CGD-CBD	2.03	128.64	124.48
18	bL	205	BCR	C7-C8-C9	-2.03	123.17	126.23
18	a5	401	BCR	C1-C6-C5	-2.03	119.75	122.61
18	b3	418	BCR	C1-C6-C5	-2.03	119.75	122.61
18	b2	401	BCR	C31-C1-C6	2.03	113.59	110.30
15	bA	842	CLA	CHA-C4D-ND	2.03	136.75	132.50
18	b6	421	BCR	C28-C27-C26	-2.03	110.45	114.08
15	b6	406	CLA	CHA-C4D-ND	2.03	136.75	132.50
15	c1	410	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	bA	831	CLA	CMC-C2C-C3C	2.03	131.63	126.12
15	c3	421	CLA	O2D-CGD-CBD	2.03	114.88	111.27
18	bF	202	BCR	C33-C5-C6	-2.03	122.25	124.53
15	c2	409	CLA	CHD-C1D-ND	-2.03	122.59	124.45
15	b1	407	CLA	CHA-C1A-NA	-2.03	121.75	126.40
18	b1	401	BCR	C40-C30-C25	2.03	113.59	110.30
15	b6	413	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
15	c2	405	CLA	CHB-C4A-NA	2.03	127.32	124.51
18	a3	418	BCR	C7-C8-C9	-2.03	123.17	126.23
15	a2	404	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	b6	405	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	a5	419	BCR	C16-C15-C14	-2.03	119.32	123.47
15	a6	406	CLA	CHB-C4A-NA	2.03	127.32	124.51
15	a3	417	CLA	CHD-C4C-NC	2.03	127.40	124.20
15	a5	409	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
18	b2	401	BCR	C29-C30-C25	2.03	113.60	110.48
15	a5	414	CLA	CHD-C1D-ND	-2.03	122.59	124.45
15	aL	201	CLA	CHA-C1A-NA	-2.03	121.76	126.40
18	a5	418	BCR	C15-C16-C17	-2.03	119.32	123.47
15	aB	818	CLA	C2A-C1A-CHA	2.03	127.40	123.86
15	a3	411	CLA	C2A-C1A-CHA	2.03	127.40	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aI	101	BCR	C35-C13-C14	-2.03	120.08	122.92
15	a6	404	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
15	b1	411	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
15	aB	828	CLA	C2A-C1A-CHA	2.03	127.40	123.86
18	a6	419	BCR	C1-C6-C5	-2.03	119.76	122.61
15	c6	405	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	bB	828	CLA	C2A-C1A-CHA	2.03	127.40	123.86
18	a2	401	BCR	C29-C30-C25	2.03	113.60	110.48
15	cF	201	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
18	c6	401	BCR	C7-C8-C9	-2.03	123.17	126.23
15	cB	827	CLA	CHA-C4D-ND	2.03	136.74	132.50
15	c6	406	CLA	CHB-C4A-NA	2.02	127.31	124.51
15	a6	406	CLA	CHA-C4D-ND	2.02	136.73	132.50
15	aB	801	CLA	C3C-C4C-NC	-2.02	108.30	110.57
15	aB	836	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
15	a2	417	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
15	aA	829	CLA	C7-C6-C5	-2.02	107.86	113.36
18	bA	851	BCR	C28-C27-C26	-2.02	110.46	114.08
15	bL	202	CLA	CHA-C1A-NA	-2.02	121.76	126.40
15	cA	841	CLA	C11-C12-C13	-2.02	109.38	115.92
15	a1	416	CLA	C3C-C4C-NC	-2.02	108.30	110.57
15	cB	834	CLA	C3C-C4C-NC	-2.02	108.30	110.57
15	c5	416	CLA	CMD-C2D-C3D	2.02	132.27	127.61
15	aB	802	CLA	CMB-C2B-C3B	2.02	128.46	124.68
15	b3	417	CLA	CHD-C4C-NC	2.02	127.39	124.20
15	b6	417	CLA	O2D-CGD-CBD	2.02	114.86	111.27
15	aB	839	CLA	C7-C6-C5	-2.02	107.87	113.36
18	c1	418	BCR	C7-C8-C9	-2.02	123.18	126.23
15	a3	416	CLA	C3A-C2A-C1A	2.02	104.37	101.34
15	b4	415	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
15	a2	417	CLA	CHD-C4C-NC	-2.02	121.02	124.20
15	cA	811	CLA	C2D-C1D-ND	-2.02	108.61	110.10
15	cB	802	CLA	C1D-ND-C4D	-2.02	104.90	106.33
15	b5	404	CLA	O1D-CGD-CBD	2.02	128.62	124.48
15	a5	420	CLA	CHA-C4D-ND	2.02	136.73	132.50
18	a2	401	BCR	C31-C1-C6	2.02	113.58	110.30
15	cB	839	CLA	C7-C6-C5	-2.02	107.87	113.36
15	cL	201	CLA	CHA-C1A-NA	-2.02	121.77	126.40
18	aB	849	BCR	C38-C26-C27	-2.02	109.73	113.62
15	b5	406	CLA	O1A-CGA-CBA	2.02	129.57	123.08
15	bB	802	CLA	CMB-C2B-C3B	2.02	128.46	124.68
15	c6	412	CLA	CHD-C1D-ND	-2.02	122.60	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	420	CLA	CGD-CBD-CAD	-2.02	104.19	110.73
15	bA	819	CLA	CAC-C3C-C2C	-2.02	124.08	127.53
18	cB	847	BCR	C40-C30-C39	-2.02	102.33	108.53
18	a4	401	BCR	C16-C15-C14	-2.02	119.34	123.47
15	aB	821	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
15	cB	802	CLA	CMB-C2B-C3B	2.02	128.46	124.68
18	b5	418	BCR	C15-C14-C13	-2.02	124.43	127.31
18	aB	847	BCR	C40-C30-C39	-2.02	102.33	108.53
15	b5	408	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
15	bB	839	CLA	C7-C6-C5	-2.02	107.88	113.36
15	bB	821	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
15	c1	415	CLA	CHA-C4D-ND	2.02	136.72	132.50
15	c1	405	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
15	b2	403	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	cB	827	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
15	b6	414	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
15	b1	404	CLA	C2A-C1A-CHA	2.02	127.39	123.86
15	c2	410	CLA	O1D-CGD-CBD	2.02	128.61	124.48
18	aF	203	BCR	C1-C6-C5	-2.02	119.77	122.61
15	a4	421	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
15	a2	417	CLA	C3A-C2A-C1A	2.02	104.36	101.34
15	bA	812	CLA	CHB-C4A-NA	2.02	127.30	124.51
18	a4	401	BCR	C40-C30-C25	2.02	113.57	110.30
15	a1	404	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
15	aA	825	CLA	O1D-CGD-CBD	2.02	128.61	124.48
15	c6	406	CLA	CHD-C4C-C3C	2.02	127.80	124.84
15	bA	811	CLA	C2D-C1D-ND	-2.02	108.62	110.10
15	b5	417	CLA	C2D-C1D-ND	-2.02	108.62	110.10
15	cB	814	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	c1	417	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
15	bA	825	CLA	O1D-CGD-CBD	2.02	128.61	124.48
15	a4	403	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
15	aA	836	CLA	CMB-C2B-C3B	2.02	128.45	124.68
18	cA	849	BCR	C33-C5-C6	-2.02	122.27	124.53
18	cF	204	BCR	C33-C5-C6	-2.02	122.27	124.53
15	bA	841	CLA	C11-C12-C13	-2.01	109.41	115.92
15	b6	418	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
15	b6	412	CLA	CAA-CBA-CGA	2.01	117.85	112.51
15	aX	102	CLA	CHA-C1A-NA	-2.01	121.78	126.40
15	bB	814	CLA	CHA-C1A-NA	-2.01	121.78	126.40
18	c1	418	BCR	C1-C6-C5	-2.01	119.78	122.61
15	a5	406	CLA	O1A-CGA-CBA	2.01	129.55	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bF	201	CLA	C2A-C1A-CHA	2.01	127.38	123.86
15	c4	405	CLA	CHA-C4D-ND	2.01	136.71	132.50
15	c5	403	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
15	aB	830	CLA	CHB-C4A-NA	2.01	127.30	124.51
18	c1	420	BCR	C11-C10-C9	-2.01	124.44	127.31
15	b3	416	CLA	C3A-C2A-C1A	2.01	104.36	101.34
15	b5	420	CLA	CHA-C4D-ND	2.01	136.71	132.50
18	c4	419	BCR	C40-C30-C25	2.01	113.56	110.30
15	a4	411	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
15	c5	412	CLA	C3C-C4C-NC	-2.01	108.31	110.57
15	b1	410	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
15	c2	404	CLA	O1D-CGD-CBD	2.01	128.60	124.48
15	aJ	201	CLA	C2A-C1A-CHA	2.01	127.38	123.86
15	c3	412	CLA	C3C-C4C-NC	-2.01	108.31	110.57
15	c6	417	CLA	O2D-CGD-CBD	2.01	114.84	111.27
15	aB	827	CLA	CHA-C4D-ND	2.01	136.71	132.50
15	aB	837	CLA	C1-C2-C3	-2.01	122.56	126.04
15	aA	806	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	bB	850	BCR	C38-C26-C27	-2.01	109.75	113.62
18	bB	847	BCR	C40-C30-C39	-2.01	102.35	108.53
18	a1	420	BCR	C40-C30-C25	2.01	113.56	110.30
15	bA	842	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
15	b6	404	CLA	CHA-C1A-NA	-2.01	121.79	126.40
15	bA	820	CLA	C3A-C2A-C1A	2.01	104.35	101.34
18	c5	419	BCR	C16-C15-C14	-2.01	119.35	123.47
15	bB	827	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
18	c5	418	BCR	C1-C6-C5	-2.01	119.78	122.61
15	a4	405	CLA	CED-O2D-CGD	-2.01	111.39	115.94
15	bA	837	CLA	O1A-CGA-CBA	2.01	129.54	123.08
15	b2	406	CLA	CHA-C4D-ND	2.01	136.70	132.50
15	b4	411	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
15	a1	403	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	a5	420	CLA	CGD-CBD-CAD	-2.01	104.22	110.73
15	cB	822	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	aA	812	CLA	C6-C7-C8	-2.01	109.42	115.92
15	aA	808	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	aB	812	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
15	a4	405	CLA	CHA-C4D-ND	2.01	136.70	132.50
15	cF	203	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	bB	813	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	a1	403	CLA	O1D-CGD-CBD	2.01	128.59	124.48
15	aB	814	CLA	CHA-C1A-NA	-2.01	121.80	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c6	404	CLA	CHA-C1A-NA	-2.01	121.80	126.40
18	b4	418	BCR	C1-C6-C5	-2.01	119.78	122.61
18	b6	419	BCR	C1-C6-C5	-2.01	119.78	122.61
18	b4	419	BCR	C40-C30-C25	2.01	113.56	110.30
18	b5	418	BCR	C1-C6-C5	-2.01	119.78	122.61
15	aB	822	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	a6	404	CLA	CHA-C1A-NA	-2.01	121.80	126.40
15	b3	411	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	c1	408	CLA	C3C-C4C-NC	-2.01	108.32	110.57
15	c2	413	CLA	C3C-C4C-NC	-2.01	108.32	110.57
15	a1	415	CLA	C3A-C2A-C1A	2.01	104.34	101.34
15	bB	827	CLA	CHA-C4D-ND	2.01	136.70	132.50
15	c3	417	CLA	CHD-C4C-NC	2.01	127.37	124.20
15	aA	842	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
15	b1	405	CLA	CHA-C4D-ND	2.01	136.70	132.50
18	aB	845	BCR	C15-C16-C17	-2.01	119.36	123.47
15	a1	411	CLA	CHD-C4C-C3C	2.01	127.79	124.84
15	a5	417	CLA	C3C-C4C-NC	-2.01	108.32	110.57
15	c5	408	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
15	cA	812	CLA	CHB-C4A-NA	2.01	127.29	124.51
15	bB	837	CLA	C1-C2-C3	-2.01	122.57	126.04
15	aB	827	CLA	CAA-CBA-CGA	-2.01	107.39	113.25
18	bI	101	BCR	C35-C13-C14	-2.01	120.11	122.92
15	cA	813	CLA	C1-C2-C3	-2.01	122.58	126.04
15	bB	832	CLA	CHA-C1A-NA	-2.01	121.81	126.40
15	b4	421	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
18	aF	202	BCR	C40-C30-C25	2.00	113.55	110.30
15	a1	416	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
18	cB	849	BCR	C1-C6-C5	-2.00	119.79	122.61
15	a6	408	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
15	a6	414	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
18	bB	849	BCR	C16-C15-C14	-2.00	119.37	123.47
15	bB	817	CLA	C2D-C1D-ND	-2.00	108.63	110.10
18	a5	418	BCR	C1-C6-C5	-2.00	119.79	122.61
18	c4	401	BCR	C16-C15-C14	-2.00	119.37	123.47
15	c6	409	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
15	cA	820	CLA	C3A-C2A-C1A	2.00	104.34	101.34
15	aB	813	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
15	c5	404	CLA	O1D-CGD-CBD	2.00	128.58	124.48
15	aB	837	CLA	C3C-C4C-NC	-2.00	108.33	110.57
15	a2	404	CLA	O1D-CGD-CBD	2.00	128.58	124.48
15	c3	405	CLA	CHD-C4C-C3C	2.00	127.78	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	821	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
15	c3	416	CLA	C3A-C2A-C1A	2.00	104.34	101.34
15	bB	822	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
15	bA	836	CLA	CMB-C2B-C3B	2.00	128.42	124.68
15	aA	845	CLA	CHD-C4C-NC	2.00	127.36	124.20
15	b2	414	CLA	CHB-C4A-NA	2.00	127.28	124.51
15	b2	409	CLA	C3C-C4C-NC	-2.00	108.33	110.57
15	c5	420	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
15	bA	812	CLA	C6-C7-C8	-2.00	109.45	115.92
15	cA	818	CLA	C4-C3-C5	2.00	118.64	115.27
15	cB	813	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

All (560) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	aA	801	CL0	ND
14	aA	801	CL0	NC
14	aA	801	CL0	NA
14	bA	801	CL0	ND
14	bA	801	CL0	NC
14	bA	801	CL0	NA
14	cA	801	CL0	ND
14	cA	801	CL0	NC
14	cA	801	CL0	NA
15	aA	802	CLA	ND
15	aA	803	CLA	ND
15	aA	804	CLA	ND
15	aA	805	CLA	ND
15	aA	806	CLA	ND
15	aA	807	CLA	ND
15	aA	809	CLA	ND
15	aA	810	CLA	ND
15	aA	811	CLA	ND
15	aA	812	CLA	ND
15	aA	813	CLA	ND
15	aA	814	CLA	ND
15	aA	815	CLA	ND
15	aA	818	CLA	ND
15	aA	819	CLA	ND
15	aA	820	CLA	ND
15	aA	821	CLA	ND
15	aA	822	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	aA	823	CLA	ND
15	aA	824	CLA	ND
15	aA	825	CLA	ND
15	aA	826	CLA	ND
15	aA	827	CLA	ND
15	aA	828	CLA	ND
15	aA	829	CLA	ND
15	aA	830	CLA	ND
15	aA	831	CLA	ND
15	aA	832	CLA	ND
15	aA	833	CLA	ND
15	aA	834	CLA	ND
15	aA	835	CLA	ND
15	aA	836	CLA	ND
15	aA	838	CLA	ND
15	aA	839	CLA	ND
15	aA	840	CLA	ND
15	aA	841	CLA	ND
15	aA	842	CLA	ND
15	aA	843	CLA	ND
15	aA	844	CLA	ND
15	aA	845	CLA	ND
15	aB	801	CLA	ND
15	aB	802	CLA	ND
15	aB	803	CLA	ND
15	aB	804	CLA	ND
15	aB	805	CLA	ND
15	aB	806	CLA	ND
15	aB	807	CLA	ND
15	aB	809	CLA	ND
15	aB	810	CLA	ND
15	aB	811	CLA	ND
15	aB	812	CLA	ND
15	aB	813	CLA	ND
15	aB	814	CLA	ND
15	aB	815	CLA	ND
15	aB	816	CLA	ND
15	aB	817	CLA	ND
15	aB	818	CLA	ND
15	aB	819	CLA	ND
15	aB	820	CLA	ND
15	aB	821	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	aB	822	CLA	ND
15	aB	823	CLA	ND
15	aB	824	CLA	ND
15	aB	825	CLA	ND
15	aB	826	CLA	ND
15	aB	827	CLA	ND
15	aB	828	CLA	ND
15	aB	829	CLA	ND
15	aB	830	CLA	ND
15	aB	831	CLA	ND
15	aB	832	CLA	ND
15	aB	833	CLA	ND
15	aB	834	CLA	ND
15	aB	835	CLA	ND
15	aB	836	CLA	ND
15	aB	837	CLA	ND
15	aB	838	CLA	ND
15	aB	839	CLA	ND
15	aB	840	CLA	ND
15	aB	841	CLA	ND
15	aJ	201	CLA	ND
15	aJ	202	CLA	ND
15	aJ	203	CLA	ND
15	aK	102	CLA	ND
15	aL	201	CLA	ND
15	aL	202	CLA	ND
15	aL	203	CLA	ND
15	aX	102	CLA	ND
15	a1	401	CLA	ND
15	a1	402	CLA	ND
15	a1	403	CLA	ND
15	a1	404	CLA	ND
15	a1	405	CLA	ND
15	a1	406	CLA	ND
15	a1	407	CLA	ND
15	a1	408	CLA	ND
15	a1	409	CLA	ND
15	a1	410	CLA	ND
15	a1	411	CLA	ND
15	a1	412	CLA	ND
15	a1	413	CLA	ND
15	a1	415	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	a1	416	CLA	ND
15	a1	422	CLA	ND
15	a2	402	CLA	ND
15	a2	403	CLA	ND
15	a2	404	CLA	ND
15	a2	405	CLA	ND
15	a2	406	CLA	ND
15	a2	407	CLA	ND
15	a2	408	CLA	ND
15	a2	409	CLA	ND
15	a2	410	CLA	ND
15	a2	411	CLA	ND
15	a2	412	CLA	ND
15	a2	413	CLA	ND
15	a2	414	CLA	ND
15	a2	415	CLA	ND
15	a2	417	CLA	ND
15	a2	418	CLA	ND
15	a2	422	CLA	ND
15	a3	402	CLA	ND
15	a3	403	CLA	ND
15	a3	404	CLA	ND
15	a3	405	CLA	ND
15	a3	406	CLA	ND
15	a3	407	CLA	ND
15	a3	408	CLA	ND
15	a3	409	CLA	ND
15	a3	410	CLA	ND
15	a3	411	CLA	ND
15	a3	412	CLA	ND
15	a3	413	CLA	ND
15	a3	414	CLA	ND
15	a3	416	CLA	ND
15	a3	417	CLA	ND
15	a3	421	CLA	ND
15	a4	402	CLA	ND
15	a4	403	CLA	ND
15	a4	404	CLA	ND
15	a4	405	CLA	ND
15	a4	406	CLA	ND
15	a4	407	CLA	ND
15	a4	408	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	a4	409	CLA	ND
15	a4	410	CLA	ND
15	a4	411	CLA	ND
15	a4	412	CLA	ND
15	a4	413	CLA	ND
15	a4	414	CLA	ND
15	a4	416	CLA	ND
15	a4	417	CLA	ND
15	a4	421	CLA	ND
15	a5	402	CLA	ND
15	a5	403	CLA	ND
15	a5	404	CLA	ND
15	a5	405	CLA	ND
15	a5	406	CLA	ND
15	a5	407	CLA	ND
15	a5	408	CLA	ND
15	a5	409	CLA	ND
15	a5	410	CLA	ND
15	a5	411	CLA	ND
15	a5	412	CLA	ND
15	a5	413	CLA	ND
15	a5	414	CLA	ND
15	a5	416	CLA	ND
15	a5	417	CLA	ND
15	a5	420	CLA	ND
15	a6	403	CLA	ND
15	a6	404	CLA	ND
15	a6	405	CLA	ND
15	a6	406	CLA	ND
15	a6	407	CLA	ND
15	a6	408	CLA	ND
15	a6	409	CLA	ND
15	a6	410	CLA	ND
15	a6	411	CLA	ND
15	a6	412	CLA	ND
15	a6	413	CLA	ND
15	a6	414	CLA	ND
15	a6	415	CLA	ND
15	a6	417	CLA	ND
15	a6	418	CLA	ND
15	a6	422	CLA	ND
15	bA	802	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	bA	803	CLA	ND
15	bA	804	CLA	ND
15	bA	805	CLA	ND
15	bA	806	CLA	ND
15	bA	807	CLA	ND
15	bA	809	CLA	ND
15	bA	810	CLA	ND
15	bA	811	CLA	ND
15	bA	812	CLA	ND
15	bA	813	CLA	ND
15	bA	814	CLA	ND
15	bA	815	CLA	ND
15	bA	818	CLA	ND
15	bA	819	CLA	ND
15	bA	820	CLA	ND
15	bA	821	CLA	ND
15	bA	822	CLA	ND
15	bA	823	CLA	ND
15	bA	824	CLA	ND
15	bA	825	CLA	ND
15	bA	826	CLA	ND
15	bA	827	CLA	ND
15	bA	828	CLA	ND
15	bA	829	CLA	ND
15	bA	830	CLA	ND
15	bA	831	CLA	ND
15	bA	832	CLA	ND
15	bA	833	CLA	ND
15	bA	834	CLA	ND
15	bA	835	CLA	ND
15	bA	836	CLA	ND
15	bA	838	CLA	ND
15	bA	839	CLA	ND
15	bA	840	CLA	ND
15	bA	841	CLA	ND
15	bA	842	CLA	ND
15	bA	843	CLA	ND
15	bA	844	CLA	ND
15	bA	845	CLA	ND
15	bB	801	CLA	ND
15	bB	802	CLA	ND
15	bB	803	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	bB	804	CLA	ND
15	bB	805	CLA	ND
15	bB	806	CLA	ND
15	bB	807	CLA	ND
15	bB	809	CLA	ND
15	bB	810	CLA	ND
15	bB	811	CLA	ND
15	bB	812	CLA	ND
15	bB	813	CLA	ND
15	bB	814	CLA	ND
15	bB	815	CLA	ND
15	bB	816	CLA	ND
15	bB	817	CLA	ND
15	bB	818	CLA	ND
15	bB	819	CLA	ND
15	bB	820	CLA	ND
15	bB	821	CLA	ND
15	bB	822	CLA	ND
15	bB	823	CLA	ND
15	bB	824	CLA	ND
15	bB	825	CLA	ND
15	bB	826	CLA	ND
15	bB	827	CLA	ND
15	bB	828	CLA	ND
15	bB	829	CLA	ND
15	bB	830	CLA	ND
15	bB	831	CLA	ND
15	bB	832	CLA	ND
15	bB	833	CLA	ND
15	bB	834	CLA	ND
15	bB	835	CLA	ND
15	bB	836	CLA	ND
15	bB	837	CLA	ND
15	bB	838	CLA	ND
15	bB	839	CLA	ND
15	bB	840	CLA	ND
15	bB	841	CLA	ND
15	bF	201	CLA	ND
15	bJ	101	CLA	ND
15	bJ	102	CLA	ND
15	bK	101	CLA	ND
15	bL	202	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	bL	203	CLA	ND
15	bL	204	CLA	ND
15	bX	102	CLA	ND
15	b1	402	CLA	ND
15	b1	403	CLA	ND
15	b1	404	CLA	ND
15	b1	405	CLA	ND
15	b1	406	CLA	ND
15	b1	407	CLA	ND
15	b1	408	CLA	ND
15	b1	409	CLA	ND
15	b1	410	CLA	ND
15	b1	411	CLA	ND
15	b1	412	CLA	ND
15	b1	413	CLA	ND
15	b1	414	CLA	ND
15	b1	416	CLA	ND
15	b1	417	CLA	ND
15	b2	402	CLA	ND
15	b2	403	CLA	ND
15	b2	404	CLA	ND
15	b2	405	CLA	ND
15	b2	406	CLA	ND
15	b2	407	CLA	ND
15	b2	408	CLA	ND
15	b2	409	CLA	ND
15	b2	410	CLA	ND
15	b2	411	CLA	ND
15	b2	412	CLA	ND
15	b2	413	CLA	ND
15	b2	414	CLA	ND
15	b2	415	CLA	ND
15	b2	417	CLA	ND
15	b2	418	CLA	ND
15	b2	422	CLA	ND
15	b3	402	CLA	ND
15	b3	403	CLA	ND
15	b3	404	CLA	ND
15	b3	405	CLA	ND
15	b3	406	CLA	ND
15	b3	407	CLA	ND
15	b3	408	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	b3	409	CLA	ND
15	b3	410	CLA	ND
15	b3	411	CLA	ND
15	b3	412	CLA	ND
15	b3	413	CLA	ND
15	b3	414	CLA	ND
15	b3	416	CLA	ND
15	b3	417	CLA	ND
15	b3	421	CLA	ND
15	b4	402	CLA	ND
15	b4	403	CLA	ND
15	b4	404	CLA	ND
15	b4	405	CLA	ND
15	b4	406	CLA	ND
15	b4	407	CLA	ND
15	b4	408	CLA	ND
15	b4	409	CLA	ND
15	b4	410	CLA	ND
15	b4	411	CLA	ND
15	b4	412	CLA	ND
15	b4	413	CLA	ND
15	b4	414	CLA	ND
15	b4	416	CLA	ND
15	b4	417	CLA	ND
15	b4	421	CLA	ND
15	b5	402	CLA	ND
15	b5	403	CLA	ND
15	b5	404	CLA	ND
15	b5	405	CLA	ND
15	b5	406	CLA	ND
15	b5	407	CLA	ND
15	b5	408	CLA	ND
15	b5	409	CLA	ND
15	b5	410	CLA	ND
15	b5	411	CLA	ND
15	b5	412	CLA	ND
15	b5	413	CLA	ND
15	b5	414	CLA	ND
15	b5	416	CLA	ND
15	b5	417	CLA	ND
15	b5	420	CLA	ND
15	b6	403	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	b6	404	CLA	ND
15	b6	405	CLA	ND
15	b6	406	CLA	ND
15	b6	407	CLA	ND
15	b6	408	CLA	ND
15	b6	409	CLA	ND
15	b6	410	CLA	ND
15	b6	411	CLA	ND
15	b6	412	CLA	ND
15	b6	413	CLA	ND
15	b6	414	CLA	ND
15	b6	415	CLA	ND
15	b6	417	CLA	ND
15	b6	418	CLA	ND
15	b6	422	CLA	ND
15	cA	802	CLA	ND
15	cA	803	CLA	ND
15	cA	804	CLA	ND
15	cA	805	CLA	ND
15	cA	806	CLA	ND
15	cA	807	CLA	ND
15	cA	809	CLA	ND
15	cA	810	CLA	ND
15	cA	811	CLA	ND
15	cA	812	CLA	ND
15	cA	813	CLA	ND
15	cA	814	CLA	ND
15	cA	815	CLA	ND
15	cA	818	CLA	ND
15	cA	819	CLA	ND
15	cA	820	CLA	ND
15	cA	821	CLA	ND
15	cA	822	CLA	ND
15	cA	823	CLA	ND
15	cA	824	CLA	ND
15	cA	825	CLA	ND
15	cA	826	CLA	ND
15	cA	827	CLA	ND
15	cA	828	CLA	ND
15	cA	829	CLA	ND
15	cA	830	CLA	ND
15	cA	831	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	cA	832	CLA	ND
15	cA	833	CLA	ND
15	cA	834	CLA	ND
15	cA	835	CLA	ND
15	cA	836	CLA	ND
15	cA	838	CLA	ND
15	cA	839	CLA	ND
15	cA	840	CLA	ND
15	cA	841	CLA	ND
15	cA	842	CLA	ND
15	cA	843	CLA	ND
15	cA	844	CLA	ND
15	cB	801	CLA	ND
15	cB	802	CLA	ND
15	cB	803	CLA	ND
15	cB	804	CLA	ND
15	cB	805	CLA	ND
15	cB	806	CLA	ND
15	cB	807	CLA	ND
15	cB	809	CLA	ND
15	cB	810	CLA	ND
15	cB	811	CLA	ND
15	cB	812	CLA	ND
15	cB	813	CLA	ND
15	cB	814	CLA	ND
15	cB	815	CLA	ND
15	cB	816	CLA	ND
15	cB	817	CLA	ND
15	cB	818	CLA	ND
15	cB	819	CLA	ND
15	cB	820	CLA	ND
15	cB	821	CLA	ND
15	cB	822	CLA	ND
15	cB	823	CLA	ND
15	cB	824	CLA	ND
15	cB	825	CLA	ND
15	cB	826	CLA	ND
15	cB	827	CLA	ND
15	cB	828	CLA	ND
15	cB	829	CLA	ND
15	cB	830	CLA	ND
15	cB	831	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	cB	832	CLA	ND
15	cB	833	CLA	ND
15	cB	834	CLA	ND
15	cB	835	CLA	ND
15	cB	836	CLA	ND
15	cB	837	CLA	ND
15	cB	838	CLA	ND
15	cB	839	CLA	ND
15	cB	840	CLA	ND
15	cB	841	CLA	ND
15	cF	201	CLA	ND
15	cF	203	CLA	ND
15	cJ	101	CLA	ND
15	cJ	102	CLA	ND
15	cK	102	CLA	ND
15	cL	201	CLA	ND
15	cL	202	CLA	ND
15	cL	203	CLA	ND
15	cX	102	CLA	ND
15	c1	402	CLA	ND
15	c1	403	CLA	ND
15	c1	404	CLA	ND
15	c1	405	CLA	ND
15	c1	406	CLA	ND
15	c1	407	CLA	ND
15	c1	408	CLA	ND
15	c1	409	CLA	ND
15	c1	410	CLA	ND
15	c1	411	CLA	ND
15	c1	412	CLA	ND
15	c1	413	CLA	ND
15	c1	414	CLA	ND
15	c1	416	CLA	ND
15	c1	417	CLA	ND
15	c2	402	CLA	ND
15	c2	403	CLA	ND
15	c2	404	CLA	ND
15	c2	405	CLA	ND
15	c2	406	CLA	ND
15	c2	407	CLA	ND
15	c2	408	CLA	ND
15	c2	409	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	c2	410	CLA	ND
15	c2	411	CLA	ND
15	c2	412	CLA	ND
15	c2	413	CLA	ND
15	c2	414	CLA	ND
15	c2	415	CLA	ND
15	c2	417	CLA	ND
15	c2	418	CLA	ND
15	c2	422	CLA	ND
15	c3	402	CLA	ND
15	c3	403	CLA	ND
15	c3	404	CLA	ND
15	c3	405	CLA	ND
15	c3	406	CLA	ND
15	c3	407	CLA	ND
15	c3	408	CLA	ND
15	c3	410	CLA	ND
15	c3	411	CLA	ND
15	c3	412	CLA	ND
15	c3	413	CLA	ND
15	c3	414	CLA	ND
15	c3	416	CLA	ND
15	c3	417	CLA	ND
15	c3	421	CLA	ND
15	c4	402	CLA	ND
15	c4	403	CLA	ND
15	c4	404	CLA	ND
15	c4	405	CLA	ND
15	c4	406	CLA	ND
15	c4	407	CLA	ND
15	c4	408	CLA	ND
15	c4	409	CLA	ND
15	c4	410	CLA	ND
15	c4	411	CLA	ND
15	c4	412	CLA	ND
15	c4	413	CLA	ND
15	c4	414	CLA	ND
15	c4	416	CLA	ND
15	c4	417	CLA	ND
15	c4	421	CLA	ND
15	c5	402	CLA	ND
15	c5	403	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
15	c5	404	CLA	ND
15	c5	405	CLA	ND
15	c5	406	CLA	ND
15	c5	407	CLA	ND
15	c5	408	CLA	ND
15	c5	409	CLA	ND
15	c5	410	CLA	ND
15	c5	411	CLA	ND
15	c5	412	CLA	ND
15	c5	413	CLA	ND
15	c5	414	CLA	ND
15	c5	416	CLA	ND
15	c5	417	CLA	ND
15	c5	420	CLA	ND
15	c6	403	CLA	ND
15	c6	404	CLA	ND
15	c6	405	CLA	ND
15	c6	406	CLA	ND
15	c6	407	CLA	ND
15	c6	408	CLA	ND
15	c6	409	CLA	ND
15	c6	410	CLA	ND
15	c6	411	CLA	ND
15	c6	412	CLA	ND
15	c6	413	CLA	ND
15	c6	414	CLA	ND
15	c6	415	CLA	ND
15	c6	417	CLA	ND
15	c6	418	CLA	ND

All (7069) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	aA	803	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	C1A-C2A-CAA-CBA
15	aA	804	CLA	CHA-CBD-CGD-O1D
15	aA	804	CLA	CHA-CBD-CGD-O2D
15	aA	806	CLA	C1A-C2A-CAA-CBA
15	aA	806	CLA	C3A-C2A-CAA-CBA
15	aA	806	CLA	CHA-CBD-CGD-O1D
15	aA	806	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	806	CLA	CAD-CBD-CGD-O1D
15	aA	807	CLA	C1A-C2A-CAA-CBA
15	aA	809	CLA	C3A-C2A-CAA-CBA
15	aA	809	CLA	CHA-CBD-CGD-O1D
15	aA	809	CLA	CHA-CBD-CGD-O2D
15	aA	810	CLA	CBD-CGD-O2D-CED
15	aA	811	CLA	C1A-C2A-CAA-CBA
15	aA	811	CLA	C3A-C2A-CAA-CBA
15	aA	811	CLA	CHA-CBD-CGD-O1D
15	aA	811	CLA	CHA-CBD-CGD-O2D
15	aA	811	CLA	CBD-CGD-O2D-CED
15	aA	816	CLA	CAD-CBD-CGD-O1D
15	aA	816	CLA	CAD-CBD-CGD-O2D
15	aA	819	CLA	C3A-C2A-CAA-CBA
15	aA	820	CLA	C1A-C2A-CAA-CBA
15	aA	820	CLA	C3A-C2A-CAA-CBA
15	aA	820	CLA	CHA-CBD-CGD-O1D
15	aA	820	CLA	CHA-CBD-CGD-O2D
15	aA	821	CLA	C1A-C2A-CAA-CBA
15	aA	821	CLA	C3A-C2A-CAA-CBA
15	aA	824	CLA	CHA-CBD-CGD-O1D
15	aA	824	CLA	CHA-CBD-CGD-O2D
15	aA	824	CLA	C2-C3-C5-C6
15	aA	824	CLA	C4-C3-C5-C6
15	aA	825	CLA	CHA-CBD-CGD-O1D
15	aA	825	CLA	CHA-CBD-CGD-O2D
15	aA	829	CLA	C1A-C2A-CAA-CBA
15	aA	829	CLA	C3A-C2A-CAA-CBA
15	aA	830	CLA	CHA-CBD-CGD-O1D
15	aA	830	CLA	CHA-CBD-CGD-O2D
15	aA	831	CLA	CHA-CBD-CGD-O1D
15	aA	831	CLA	CHA-CBD-CGD-O2D
15	aA	839	CLA	CHA-CBD-CGD-O1D
15	aA	839	CLA	CHA-CBD-CGD-O2D
15	aA	839	CLA	CAD-CBD-CGD-O1D
15	aA	839	CLA	CBD-CGD-O2D-CED
15	aA	842	CLA	CHA-CBD-CGD-O2D
15	aA	842	CLA	CBD-CGD-O2D-CED
15	aA	842	CLA	C2-C3-C5-C6
15	aA	842	CLA	C4-C3-C5-C6
15	aA	843	CLA	C1A-C2A-CAA-CBA
15	aA	845	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	845	CLA	CHA-CBD-CGD-O2D
15	aA	845	CLA	CAD-CBD-CGD-O1D
15	aB	801	CLA	C4-C3-C5-C6
15	aB	802	CLA	CHA-CBD-CGD-O1D
15	aB	802	CLA	CHA-CBD-CGD-O2D
15	aB	802	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	C2-C3-C5-C6
15	aB	803	CLA	C4-C3-C5-C6
15	aB	806	CLA	C1A-C2A-CAA-CBA
15	aB	806	CLA	C3A-C2A-CAA-CBA
15	aB	806	CLA	CHA-CBD-CGD-O1D
15	aB	806	CLA	CHA-CBD-CGD-O2D
15	aB	806	CLA	C6-C7-C8-C9
15	aB	810	CLA	C1A-C2A-CAA-CBA
15	aB	810	CLA	C3A-C2A-CAA-CBA
15	aB	812	CLA	CBD-CGD-O2D-CED
15	aB	814	CLA	C1A-C2A-CAA-CBA
15	aB	814	CLA	C3A-C2A-CAA-CBA
15	aB	814	CLA	CHA-CBD-CGD-O1D
15	aB	814	CLA	CHA-CBD-CGD-O2D
15	aB	816	CLA	CHA-CBD-CGD-O1D
15	aB	816	CLA	CHA-CBD-CGD-O2D
15	aB	817	CLA	C1A-C2A-CAA-CBA
15	aB	819	CLA	C1A-C2A-CAA-CBA
15	aB	819	CLA	C3A-C2A-CAA-CBA
15	aB	821	CLA	C1A-C2A-CAA-CBA
15	aB	821	CLA	C3A-C2A-CAA-CBA
15	aB	825	CLA	C2-C3-C5-C6
15	aB	825	CLA	C4-C3-C5-C6
15	aB	826	CLA	C1A-C2A-CAA-CBA
15	aB	827	CLA	C1A-C2A-CAA-CBA
15	aB	827	CLA	C3A-C2A-CAA-CBA
15	aB	827	CLA	C11-C10-C8-C7
15	aB	828	CLA	CBD-CGD-O2D-CED
15	aB	829	CLA	C1A-C2A-CAA-CBA
15	aB	829	CLA	C3A-C2A-CAA-CBA
15	aB	829	CLA	CHA-CBD-CGD-O1D
15	aB	829	CLA	CHA-CBD-CGD-O2D
15	aB	831	CLA	C1A-C2A-CAA-CBA
15	aB	831	CLA	C3A-C2A-CAA-CBA
15	aB	834	CLA	C1A-C2A-CAA-CBA
15	aB	834	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	835	CLA	C1A-C2A-CAA-CBA
15	aB	835	CLA	C3A-C2A-CAA-CBA
15	aB	837	CLA	CHA-CBD-CGD-O1D
15	aB	837	CLA	CHA-CBD-CGD-O2D
15	aB	840	CLA	C1A-C2A-CAA-CBA
15	aB	840	CLA	C3A-C2A-CAA-CBA
15	aJ	201	CLA	CAD-CBD-CGD-O1D
15	aJ	201	CLA	CAD-CBD-CGD-O2D
15	aJ	201	CLA	CBD-CGD-O2D-CED
15	aJ	202	CLA	CHA-CBD-CGD-O1D
15	aJ	202	CLA	CAD-CBD-CGD-O1D
15	aJ	202	CLA	CAD-CBD-CGD-O2D
15	aJ	202	CLA	CBD-CGD-O2D-CED
15	aL	201	CLA	C1A-C2A-CAA-CBA
15	aL	201	CLA	C3A-C2A-CAA-CBA
15	aL	202	CLA	C2A-CAA-CBA-CGA
15	a1	407	CLA	C1A-C2A-CAA-CBA
15	a1	407	CLA	CBD-CGD-O2D-CED
15	a1	410	CLA	C1A-C2A-CAA-CBA
15	a1	413	CLA	CBD-CGD-O2D-CED
15	a1	414	CLA	CBD-CGD-O2D-CED
15	a1	415	CLA	C1A-C2A-CAA-CBA
15	a1	415	CLA	C3A-C2A-CAA-CBA
15	a1	415	CLA	C2A-CAA-CBA-CGA
15	a1	415	CLA	CBD-CGD-O2D-CED
15	a1	422	CLA	CBD-CGD-O2D-CED
15	a1	422	CLA	C11-C12-C13-C14
15	a2	406	CLA	C1A-C2A-CAA-CBA
15	a2	406	CLA	CBD-CGD-O2D-CED
15	a2	406	CLA	C11-C12-C13-C14
15	a2	409	CLA	C1A-C2A-CAA-CBA
15	a2	409	CLA	CBD-CGD-O2D-CED
15	a2	412	CLA	C1A-C2A-CAA-CBA
15	a2	413	CLA	CBD-CGD-O2D-CED
15	a2	415	CLA	CBD-CGD-O2D-CED
15	a2	416	CLA	CBD-CGD-O2D-CED
15	a2	417	CLA	C1A-C2A-CAA-CBA
15	a2	417	CLA	C3A-C2A-CAA-CBA
15	a2	417	CLA	C2A-CAA-CBA-CGA
15	a2	417	CLA	CBD-CGD-O2D-CED
15	a2	422	CLA	C1A-C2A-CAA-CBA
15	a2	422	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a3	408	CLA	C1A-C2A-CAA-CBA
15	a3	408	CLA	CBD-CGD-O2D-CED
15	a3	411	CLA	C1A-C2A-CAA-CBA
15	a3	412	CLA	CBD-CGD-O2D-CED
15	a3	414	CLA	CBD-CGD-O2D-CED
15	a3	415	CLA	CBD-CGD-O2D-CED
15	a3	416	CLA	C1A-C2A-CAA-CBA
15	a3	416	CLA	C3A-C2A-CAA-CBA
15	a3	416	CLA	C2A-CAA-CBA-CGA
15	a3	416	CLA	CBD-CGD-O2D-CED
15	a3	417	CLA	CBD-CGD-O2D-CED
15	a3	421	CLA	C1A-C2A-CAA-CBA
15	a3	421	CLA	CBD-CGD-O2D-CED
15	a4	408	CLA	CBD-CGD-O2D-CED
15	a4	411	CLA	C1A-C2A-CAA-CBA
15	a4	414	CLA	CBD-CGD-O2D-CED
15	a4	415	CLA	CBD-CGD-O2D-CED
15	a4	416	CLA	C1A-C2A-CAA-CBA
15	a4	416	CLA	C3A-C2A-CAA-CBA
15	a4	416	CLA	C2A-CAA-CBA-CGA
15	a4	416	CLA	CBD-CGD-O2D-CED
15	a4	417	CLA	CBD-CGD-O2D-CED
15	a4	421	CLA	C1A-C2A-CAA-CBA
15	a4	421	CLA	CBD-CGD-O2D-CED
15	a5	408	CLA	C1A-C2A-CAA-CBA
15	a5	408	CLA	CBD-CGD-O2D-CED
15	a5	411	CLA	C1A-C2A-CAA-CBA
15	a5	414	CLA	CBD-CGD-O2D-CED
15	a5	415	CLA	CBD-CGD-O2D-CED
15	a5	416	CLA	C1A-C2A-CAA-CBA
15	a5	416	CLA	C3A-C2A-CAA-CBA
15	a5	416	CLA	C2A-CAA-CBA-CGA
15	a5	416	CLA	CBD-CGD-O2D-CED
15	a5	417	CLA	CBD-CGD-O2D-CED
15	a5	420	CLA	CBD-CGD-O2D-CED
15	a6	406	CLA	CBD-CGD-O2D-CED
15	a6	409	CLA	CBD-CGD-O2D-CED
15	a6	412	CLA	C1A-C2A-CAA-CBA
15	a6	415	CLA	CBD-CGD-O2D-CED
15	a6	416	CLA	CBD-CGD-O2D-CED
15	a6	417	CLA	C1A-C2A-CAA-CBA
15	a6	417	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	417	CLA	C2A-CAA-CBA-CGA
15	a6	417	CLA	CBD-CGD-O2D-CED
15	a6	422	CLA	CBD-CGD-O2D-CED
15	bA	803	CLA	CBA-CGA-O2A-C1
15	bA	803	CLA	O1A-CGA-O2A-C1
15	bA	804	CLA	C1A-C2A-CAA-CBA
15	bA	804	CLA	CHA-CBD-CGD-O1D
15	bA	804	CLA	CHA-CBD-CGD-O2D
15	bA	806	CLA	C1A-C2A-CAA-CBA
15	bA	806	CLA	C3A-C2A-CAA-CBA
15	bA	806	CLA	CHA-CBD-CGD-O1D
15	bA	806	CLA	CHA-CBD-CGD-O2D
15	bA	806	CLA	CAD-CBD-CGD-O1D
15	bA	807	CLA	C1A-C2A-CAA-CBA
15	bA	809	CLA	C3A-C2A-CAA-CBA
15	bA	809	CLA	CHA-CBD-CGD-O1D
15	bA	809	CLA	CHA-CBD-CGD-O2D
15	bA	810	CLA	CBD-CGD-O2D-CED
15	bA	811	CLA	C1A-C2A-CAA-CBA
15	bA	811	CLA	C3A-C2A-CAA-CBA
15	bA	811	CLA	CHA-CBD-CGD-O1D
15	bA	811	CLA	CHA-CBD-CGD-O2D
15	bA	811	CLA	CBD-CGD-O2D-CED
15	bA	816	CLA	CAD-CBD-CGD-O1D
15	bA	816	CLA	CAD-CBD-CGD-O2D
15	bA	819	CLA	C3A-C2A-CAA-CBA
15	bA	820	CLA	C1A-C2A-CAA-CBA
15	bA	820	CLA	C3A-C2A-CAA-CBA
15	bA	820	CLA	CHA-CBD-CGD-O1D
15	bA	820	CLA	CHA-CBD-CGD-O2D
15	bA	821	CLA	C1A-C2A-CAA-CBA
15	bA	821	CLA	C3A-C2A-CAA-CBA
15	bA	824	CLA	CHA-CBD-CGD-O1D
15	bA	824	CLA	CHA-CBD-CGD-O2D
15	bA	824	CLA	C2-C3-C5-C6
15	bA	824	CLA	C4-C3-C5-C6
15	bA	825	CLA	CHA-CBD-CGD-O1D
15	bA	825	CLA	CHA-CBD-CGD-O2D
15	bA	829	CLA	C1A-C2A-CAA-CBA
15	bA	829	CLA	C3A-C2A-CAA-CBA
15	bA	830	CLA	CHA-CBD-CGD-O1D
15	bA	830	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	831	CLA	CHA-CBD-CGD-O1D
15	bA	831	CLA	CHA-CBD-CGD-O2D
15	bA	839	CLA	CHA-CBD-CGD-O1D
15	bA	839	CLA	CHA-CBD-CGD-O2D
15	bA	839	CLA	CAD-CBD-CGD-O1D
15	bA	839	CLA	CBD-CGD-O2D-CED
15	bA	842	CLA	CHA-CBD-CGD-O2D
15	bA	842	CLA	CBD-CGD-O2D-CED
15	bA	842	CLA	C2-C3-C5-C6
15	bA	842	CLA	C4-C3-C5-C6
15	bA	843	CLA	C1A-C2A-CAA-CBA
15	bA	845	CLA	CHA-CBD-CGD-O1D
15	bA	845	CLA	CHA-CBD-CGD-O2D
15	bA	845	CLA	CAD-CBD-CGD-O1D
15	bB	801	CLA	C4-C3-C5-C6
15	bB	802	CLA	CHA-CBD-CGD-O1D
15	bB	802	CLA	CHA-CBD-CGD-O2D
15	bB	802	CLA	CBD-CGD-O2D-CED
15	bB	803	CLA	C2-C3-C5-C6
15	bB	803	CLA	C4-C3-C5-C6
15	bB	806	CLA	C1A-C2A-CAA-CBA
15	bB	806	CLA	C3A-C2A-CAA-CBA
15	bB	806	CLA	CHA-CBD-CGD-O1D
15	bB	806	CLA	CHA-CBD-CGD-O2D
15	bB	806	CLA	C6-C7-C8-C9
15	bB	810	CLA	C1A-C2A-CAA-CBA
15	bB	810	CLA	C3A-C2A-CAA-CBA
15	bB	812	CLA	CBD-CGD-O2D-CED
15	bB	814	CLA	C1A-C2A-CAA-CBA
15	bB	814	CLA	C3A-C2A-CAA-CBA
15	bB	814	CLA	CHA-CBD-CGD-O1D
15	bB	814	CLA	CHA-CBD-CGD-O2D
15	bB	816	CLA	CHA-CBD-CGD-O1D
15	bB	816	CLA	CHA-CBD-CGD-O2D
15	bB	817	CLA	C1A-C2A-CAA-CBA
15	bB	819	CLA	C1A-C2A-CAA-CBA
15	bB	819	CLA	C3A-C2A-CAA-CBA
15	bB	821	CLA	C1A-C2A-CAA-CBA
15	bB	821	CLA	C3A-C2A-CAA-CBA
15	bB	825	CLA	C2-C3-C5-C6
15	bB	825	CLA	C4-C3-C5-C6
15	bB	826	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	827	CLA	C1A-C2A-CAA-CBA
15	bB	827	CLA	C3A-C2A-CAA-CBA
15	bB	827	CLA	C11-C10-C8-C7
15	bB	828	CLA	CBD-CGD-O2D-CED
15	bB	829	CLA	C1A-C2A-CAA-CBA
15	bB	829	CLA	C3A-C2A-CAA-CBA
15	bB	829	CLA	CHA-CBD-CGD-O1D
15	bB	829	CLA	CHA-CBD-CGD-O2D
15	bB	831	CLA	C1A-C2A-CAA-CBA
15	bB	831	CLA	C3A-C2A-CAA-CBA
15	bB	834	CLA	C1A-C2A-CAA-CBA
15	bB	834	CLA	CBD-CGD-O2D-CED
15	bB	835	CLA	C1A-C2A-CAA-CBA
15	bB	835	CLA	C3A-C2A-CAA-CBA
15	bB	837	CLA	CHA-CBD-CGD-O1D
15	bB	837	CLA	CHA-CBD-CGD-O2D
15	bB	840	CLA	C1A-C2A-CAA-CBA
15	bB	840	CLA	C3A-C2A-CAA-CBA
15	bF	201	CLA	CAD-CBD-CGD-O1D
15	bF	201	CLA	CAD-CBD-CGD-O2D
15	bF	201	CLA	CBD-CGD-O2D-CED
15	bJ	101	CLA	CHA-CBD-CGD-O1D
15	bJ	101	CLA	CAD-CBD-CGD-O1D
15	bJ	101	CLA	CAD-CBD-CGD-O2D
15	bJ	101	CLA	CBD-CGD-O2D-CED
15	bL	202	CLA	C1A-C2A-CAA-CBA
15	bL	202	CLA	C3A-C2A-CAA-CBA
15	bL	203	CLA	C2A-CAA-CBA-CGA
15	b1	408	CLA	C1A-C2A-CAA-CBA
15	b1	408	CLA	CBD-CGD-O2D-CED
15	b1	411	CLA	C1A-C2A-CAA-CBA
15	b1	414	CLA	CBD-CGD-O2D-CED
15	b1	415	CLA	CBD-CGD-O2D-CED
15	b1	416	CLA	C1A-C2A-CAA-CBA
15	b1	416	CLA	C3A-C2A-CAA-CBA
15	b1	416	CLA	C2A-CAA-CBA-CGA
15	b1	416	CLA	CBD-CGD-O2D-CED
15	b2	406	CLA	C1A-C2A-CAA-CBA
15	b2	406	CLA	CBD-CGD-O2D-CED
15	b2	406	CLA	C11-C12-C13-C14
15	b2	409	CLA	C1A-C2A-CAA-CBA
15	b2	409	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	412	CLA	C1A-C2A-CAA-CBA
15	b2	413	CLA	CBD-CGD-O2D-CED
15	b2	415	CLA	CBD-CGD-O2D-CED
15	b2	416	CLA	CBD-CGD-O2D-CED
15	b2	417	CLA	C1A-C2A-CAA-CBA
15	b2	417	CLA	C3A-C2A-CAA-CBA
15	b2	417	CLA	C2A-CAA-CBA-CGA
15	b2	417	CLA	CBD-CGD-O2D-CED
15	b2	422	CLA	C1A-C2A-CAA-CBA
15	b2	422	CLA	CBD-CGD-O2D-CED
15	b3	408	CLA	C1A-C2A-CAA-CBA
15	b3	408	CLA	CBD-CGD-O2D-CED
15	b3	411	CLA	C1A-C2A-CAA-CBA
15	b3	412	CLA	CBD-CGD-O2D-CED
15	b3	414	CLA	CBD-CGD-O2D-CED
15	b3	415	CLA	CBD-CGD-O2D-CED
15	b3	416	CLA	C1A-C2A-CAA-CBA
15	b3	416	CLA	C3A-C2A-CAA-CBA
15	b3	416	CLA	C2A-CAA-CBA-CGA
15	b3	416	CLA	CBD-CGD-O2D-CED
15	b3	417	CLA	CBD-CGD-O2D-CED
15	b3	421	CLA	C1A-C2A-CAA-CBA
15	b3	421	CLA	CBD-CGD-O2D-CED
15	b4	408	CLA	CBD-CGD-O2D-CED
15	b4	411	CLA	C1A-C2A-CAA-CBA
15	b4	414	CLA	CBD-CGD-O2D-CED
15	b4	415	CLA	CBD-CGD-O2D-CED
15	b4	416	CLA	C1A-C2A-CAA-CBA
15	b4	416	CLA	C3A-C2A-CAA-CBA
15	b4	416	CLA	C2A-CAA-CBA-CGA
15	b4	416	CLA	CBD-CGD-O2D-CED
15	b4	417	CLA	CBD-CGD-O2D-CED
15	b4	421	CLA	C1A-C2A-CAA-CBA
15	b4	421	CLA	CBD-CGD-O2D-CED
15	b5	408	CLA	C1A-C2A-CAA-CBA
15	b5	408	CLA	CBD-CGD-O2D-CED
15	b5	411	CLA	C1A-C2A-CAA-CBA
15	b5	414	CLA	CBD-CGD-O2D-CED
15	b5	415	CLA	CBD-CGD-O2D-CED
15	b5	416	CLA	C1A-C2A-CAA-CBA
15	b5	416	CLA	C3A-C2A-CAA-CBA
15	b5	416	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b5	416	CLA	CBD-CGD-O2D-CED
15	b5	417	CLA	CBD-CGD-O2D-CED
15	b5	420	CLA	CBD-CGD-O2D-CED
15	b6	406	CLA	CBD-CGD-O2D-CED
15	b6	409	CLA	C1A-C2A-CAA-CBA
15	b6	409	CLA	CBD-CGD-O2D-CED
15	b6	412	CLA	C1A-C2A-CAA-CBA
15	b6	415	CLA	CBD-CGD-O2D-CED
15	b6	416	CLA	CBD-CGD-O2D-CED
15	b6	417	CLA	C1A-C2A-CAA-CBA
15	b6	417	CLA	C3A-C2A-CAA-CBA
15	b6	417	CLA	C2A-CAA-CBA-CGA
15	b6	417	CLA	CBD-CGD-O2D-CED
15	b6	422	CLA	CBD-CGD-O2D-CED
15	cA	803	CLA	CBA-CGA-O2A-C1
15	cA	803	CLA	O1A-CGA-O2A-C1
15	cA	804	CLA	C1A-C2A-CAA-CBA
15	cA	804	CLA	CHA-CBD-CGD-O1D
15	cA	804	CLA	CHA-CBD-CGD-O2D
15	cA	806	CLA	C1A-C2A-CAA-CBA
15	cA	806	CLA	C3A-C2A-CAA-CBA
15	cA	806	CLA	CHA-CBD-CGD-O1D
15	cA	806	CLA	CHA-CBD-CGD-O2D
15	cA	806	CLA	CAD-CBD-CGD-O1D
15	cA	807	CLA	C1A-C2A-CAA-CBA
15	cA	809	CLA	C3A-C2A-CAA-CBA
15	cA	809	CLA	CHA-CBD-CGD-O1D
15	cA	809	CLA	CHA-CBD-CGD-O2D
15	cA	810	CLA	CBD-CGD-O2D-CED
15	cA	811	CLA	C1A-C2A-CAA-CBA
15	cA	811	CLA	C3A-C2A-CAA-CBA
15	cA	811	CLA	CHA-CBD-CGD-O1D
15	cA	811	CLA	CHA-CBD-CGD-O2D
15	cA	811	CLA	CBD-CGD-O2D-CED
15	cA	816	CLA	CAD-CBD-CGD-O1D
15	cA	816	CLA	CAD-CBD-CGD-O2D
15	cA	819	CLA	C3A-C2A-CAA-CBA
15	cA	820	CLA	C1A-C2A-CAA-CBA
15	cA	820	CLA	C3A-C2A-CAA-CBA
15	cA	820	CLA	CHA-CBD-CGD-O1D
15	cA	820	CLA	CHA-CBD-CGD-O2D
15	cA	821	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	821	CLA	C3A-C2A-CAA-CBA
15	cA	824	CLA	CHA-CBD-CGD-O1D
15	cA	824	CLA	CHA-CBD-CGD-O2D
15	cA	824	CLA	C2-C3-C5-C6
15	cA	824	CLA	C4-C3-C5-C6
15	cA	825	CLA	CHA-CBD-CGD-O1D
15	cA	825	CLA	CHA-CBD-CGD-O2D
15	cA	829	CLA	C1A-C2A-CAA-CBA
15	cA	829	CLA	C3A-C2A-CAA-CBA
15	cA	830	CLA	CHA-CBD-CGD-O1D
15	cA	830	CLA	CHA-CBD-CGD-O2D
15	cA	831	CLA	CHA-CBD-CGD-O1D
15	cA	831	CLA	CHA-CBD-CGD-O2D
15	cA	839	CLA	CHA-CBD-CGD-O1D
15	cA	839	CLA	CHA-CBD-CGD-O2D
15	cA	839	CLA	CAD-CBD-CGD-O1D
15	cA	839	CLA	CBD-CGD-O2D-CED
15	cA	842	CLA	C1A-C2A-CAA-CBA
15	cA	844	CLA	CHA-CBD-CGD-O1D
15	cA	844	CLA	CHA-CBD-CGD-O2D
15	cA	844	CLA	CAD-CBD-CGD-O1D
15	cB	801	CLA	C4-C3-C5-C6
15	cB	802	CLA	CHA-CBD-CGD-O1D
15	cB	802	CLA	CHA-CBD-CGD-O2D
15	cB	802	CLA	CBD-CGD-O2D-CED
15	cB	803	CLA	C2-C3-C5-C6
15	cB	803	CLA	C4-C3-C5-C6
15	cB	806	CLA	C1A-C2A-CAA-CBA
15	cB	806	CLA	C3A-C2A-CAA-CBA
15	cB	806	CLA	CHA-CBD-CGD-O1D
15	cB	806	CLA	CHA-CBD-CGD-O2D
15	cB	806	CLA	C6-C7-C8-C9
15	cB	810	CLA	C1A-C2A-CAA-CBA
15	cB	810	CLA	C3A-C2A-CAA-CBA
15	cB	812	CLA	CBD-CGD-O2D-CED
15	cB	814	CLA	C1A-C2A-CAA-CBA
15	cB	814	CLA	C3A-C2A-CAA-CBA
15	cB	814	CLA	CHA-CBD-CGD-O1D
15	cB	814	CLA	CHA-CBD-CGD-O2D
15	cB	816	CLA	CHA-CBD-CGD-O1D
15	cB	816	CLA	CHA-CBD-CGD-O2D
15	cB	817	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	819	CLA	C1A-C2A-CAA-CBA
15	cB	819	CLA	C3A-C2A-CAA-CBA
15	cB	821	CLA	C1A-C2A-CAA-CBA
15	cB	821	CLA	C3A-C2A-CAA-CBA
15	cB	825	CLA	CHA-CBD-CGD-O2D
15	cB	825	CLA	C2-C3-C5-C6
15	cB	825	CLA	C4-C3-C5-C6
15	cB	826	CLA	C1A-C2A-CAA-CBA
15	cB	827	CLA	C1A-C2A-CAA-CBA
15	cB	827	CLA	C3A-C2A-CAA-CBA
15	cB	827	CLA	C11-C10-C8-C7
15	cB	828	CLA	CBD-CGD-O2D-CED
15	cB	829	CLA	C1A-C2A-CAA-CBA
15	cB	829	CLA	C3A-C2A-CAA-CBA
15	cB	829	CLA	CHA-CBD-CGD-O1D
15	cB	829	CLA	CHA-CBD-CGD-O2D
15	cB	831	CLA	C1A-C2A-CAA-CBA
15	cB	831	CLA	C3A-C2A-CAA-CBA
15	cB	834	CLA	C1A-C2A-CAA-CBA
15	cB	834	CLA	CBD-CGD-O2D-CED
15	cB	835	CLA	C1A-C2A-CAA-CBA
15	cB	835	CLA	C3A-C2A-CAA-CBA
15	cB	837	CLA	CHA-CBD-CGD-O1D
15	cB	837	CLA	CHA-CBD-CGD-O2D
15	cB	840	CLA	C1A-C2A-CAA-CBA
15	cB	840	CLA	C3A-C2A-CAA-CBA
15	cF	201	CLA	CHA-CBD-CGD-O2D
15	cF	201	CLA	CBD-CGD-O2D-CED
15	cF	201	CLA	C2-C3-C5-C6
15	cF	201	CLA	C4-C3-C5-C6
15	cF	203	CLA	CAD-CBD-CGD-O1D
15	cF	203	CLA	CAD-CBD-CGD-O2D
15	cF	203	CLA	CBD-CGD-O2D-CED
15	cJ	101	CLA	CHA-CBD-CGD-O1D
15	cJ	101	CLA	CAD-CBD-CGD-O1D
15	cJ	101	CLA	CAD-CBD-CGD-O2D
15	cJ	101	CLA	CBD-CGD-O2D-CED
15	cL	201	CLA	C1A-C2A-CAA-CBA
15	cL	201	CLA	C3A-C2A-CAA-CBA
15	cL	202	CLA	C2A-CAA-CBA-CGA
15	c1	408	CLA	C1A-C2A-CAA-CBA
15	c1	408	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	411	CLA	C1A-C2A-CAA-CBA
15	c1	414	CLA	CBD-CGD-O2D-CED
15	c1	415	CLA	CBD-CGD-O2D-CED
15	c1	416	CLA	C1A-C2A-CAA-CBA
15	c1	416	CLA	C3A-C2A-CAA-CBA
15	c1	416	CLA	C2A-CAA-CBA-CGA
15	c1	416	CLA	CBD-CGD-O2D-CED
15	c2	406	CLA	C1A-C2A-CAA-CBA
15	c2	406	CLA	CBD-CGD-O2D-CED
15	c2	406	CLA	C11-C12-C13-C14
15	c2	409	CLA	C1A-C2A-CAA-CBA
15	c2	409	CLA	CBD-CGD-O2D-CED
15	c2	412	CLA	C1A-C2A-CAA-CBA
15	c2	415	CLA	CBD-CGD-O2D-CED
15	c2	416	CLA	CBD-CGD-O2D-CED
15	c2	417	CLA	C1A-C2A-CAA-CBA
15	c2	417	CLA	C3A-C2A-CAA-CBA
15	c2	417	CLA	C2A-CAA-CBA-CGA
15	c2	417	CLA	CBD-CGD-O2D-CED
15	c2	422	CLA	C1A-C2A-CAA-CBA
15	c2	422	CLA	CBD-CGD-O2D-CED
15	c3	408	CLA	C1A-C2A-CAA-CBA
15	c3	408	CLA	CBD-CGD-O2D-CED
15	c3	411	CLA	C1A-C2A-CAA-CBA
15	c3	414	CLA	CBD-CGD-O2D-CED
15	c3	415	CLA	CBD-CGD-O2D-CED
15	c3	416	CLA	C1A-C2A-CAA-CBA
15	c3	416	CLA	C3A-C2A-CAA-CBA
15	c3	416	CLA	C2A-CAA-CBA-CGA
15	c3	416	CLA	CBD-CGD-O2D-CED
15	c3	417	CLA	CBD-CGD-O2D-CED
15	c3	421	CLA	C1A-C2A-CAA-CBA
15	c3	421	CLA	CBD-CGD-O2D-CED
15	c4	408	CLA	CBD-CGD-O2D-CED
15	c4	411	CLA	C1A-C2A-CAA-CBA
15	c4	414	CLA	CBD-CGD-O2D-CED
15	c4	415	CLA	CBD-CGD-O2D-CED
15	c4	416	CLA	C1A-C2A-CAA-CBA
15	c4	416	CLA	C3A-C2A-CAA-CBA
15	c4	416	CLA	C2A-CAA-CBA-CGA
15	c4	416	CLA	CBD-CGD-O2D-CED
15	c4	417	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	421	CLA	C1A-C2A-CAA-CBA
15	c4	421	CLA	CBD-CGD-O2D-CED
15	c4	421	CLA	C11-C12-C13-C14
15	c5	408	CLA	C1A-C2A-CAA-CBA
15	c5	408	CLA	CBD-CGD-O2D-CED
15	c5	411	CLA	C1A-C2A-CAA-CBA
15	c5	414	CLA	CBD-CGD-O2D-CED
15	c5	416	CLA	C1A-C2A-CAA-CBA
15	c5	416	CLA	C3A-C2A-CAA-CBA
15	c5	416	CLA	C2A-CAA-CBA-CGA
15	c5	416	CLA	CBD-CGD-O2D-CED
15	c5	417	CLA	CBD-CGD-O2D-CED
15	c5	420	CLA	CBD-CGD-O2D-CED
15	c6	409	CLA	C1A-C2A-CAA-CBA
15	c6	409	CLA	CBD-CGD-O2D-CED
15	c6	412	CLA	C1A-C2A-CAA-CBA
15	c6	415	CLA	CBD-CGD-O2D-CED
15	c6	416	CLA	CBD-CGD-O2D-CED
15	c6	417	CLA	C1A-C2A-CAA-CBA
15	c6	417	CLA	C3A-C2A-CAA-CBA
15	c6	417	CLA	C2A-CAA-CBA-CGA
15	c6	417	CLA	CBD-CGD-O2D-CED
18	aA	848	BCR	C11-C12-C13-C35
18	aA	848	BCR	C20-C21-C22-C23
18	aA	848	BCR	C20-C21-C22-C37
18	aA	848	BCR	C22-C23-C24-C25
18	aA	848	BCR	C23-C24-C25-C30
18	aA	849	BCR	C1-C6-C7-C8
18	aA	849	BCR	C6-C7-C8-C9
18	aA	849	BCR	C7-C8-C9-C10
18	aA	849	BCR	C7-C8-C9-C34
18	aA	849	BCR	C16-C17-C18-C36
18	aA	849	BCR	C37-C22-C23-C24
18	aA	850	BCR	C1-C6-C7-C8
18	aA	850	BCR	C6-C7-C8-C9
18	aA	850	BCR	C7-C8-C9-C34
18	aA	850	BCR	C17-C18-C19-C20
18	aA	850	BCR	C21-C22-C23-C24
18	aA	850	BCR	C22-C23-C24-C25
18	aA	851	BCR	C1-C6-C7-C8
18	aA	851	BCR	C20-C21-C22-C37
18	aA	851	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aA	851	BCR	C37-C22-C23-C24
18	aA	851	BCR	C23-C24-C25-C30
18	aA	852	BCR	C7-C8-C9-C10
18	aA	852	BCR	C11-C10-C9-C8
18	aA	852	BCR	C11-C12-C13-C35
18	aA	852	BCR	C16-C17-C18-C19
18	aA	852	BCR	C18-C19-C20-C21
18	aA	852	BCR	C20-C21-C22-C23
18	aA	852	BCR	C20-C21-C22-C37
18	aA	852	BCR	C21-C22-C23-C24
18	aB	844	BCR	C1-C6-C7-C8
18	aB	844	BCR	C7-C8-C9-C10
18	aB	844	BCR	C37-C22-C23-C24
18	aB	845	BCR	C11-C12-C13-C35
18	aB	845	BCR	C21-C22-C23-C24
18	aB	846	BCR	C1-C6-C7-C8
18	aB	846	BCR	C11-C12-C13-C35
18	aB	846	BCR	C37-C22-C23-C24
18	aB	847	BCR	C16-C17-C18-C36
18	aB	847	BCR	C36-C18-C19-C20
18	aB	847	BCR	C18-C19-C20-C21
18	aB	847	BCR	C20-C21-C22-C23
18	aB	847	BCR	C20-C21-C22-C37
18	aB	848	BCR	C1-C6-C7-C8
18	aB	848	BCR	C7-C8-C9-C10
18	aB	848	BCR	C7-C8-C9-C34
18	aB	848	BCR	C20-C21-C22-C23
18	aB	848	BCR	C37-C22-C23-C24
18	aB	848	BCR	C22-C23-C24-C25
18	aB	848	BCR	C23-C24-C25-C30
18	aB	849	BCR	C1-C6-C7-C8
18	aB	849	BCR	C20-C21-C22-C37
18	aB	849	BCR	C22-C23-C24-C25
18	aF	201	BCR	C7-C8-C9-C34
18	aF	201	BCR	C11-C12-C13-C35
18	aF	201	BCR	C14-C15-C16-C17
18	aF	201	BCR	C21-C22-C23-C24
18	aF	201	BCR	C37-C22-C23-C24
18	aF	202	BCR	C7-C8-C9-C10
18	aF	202	BCR	C12-C13-C14-C15
18	aF	202	BCR	C37-C22-C23-C24
18	aF	203	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aF	203	BCR	C7-C8-C9-C34
18	aF	203	BCR	C23-C24-C25-C30
18	aI	101	BCR	C6-C7-C8-C9
18	aI	101	BCR	C7-C8-C9-C34
18	aI	101	BCR	C20-C21-C22-C23
18	aI	101	BCR	C21-C22-C23-C24
18	aI	101	BCR	C37-C22-C23-C24
18	aI	102	BCR	C7-C8-C9-C10
18	aI	102	BCR	C20-C21-C22-C23
18	aI	102	BCR	C20-C21-C22-C37
18	aI	103	BCR	C1-C6-C7-C8
18	aI	103	BCR	C7-C8-C9-C34
18	aI	103	BCR	C37-C22-C23-C24
18	aI	103	BCR	C23-C24-C25-C26
18	aJ	204	BCR	C11-C12-C13-C14
18	aJ	204	BCR	C12-C13-C14-C15
18	aJ	204	BCR	C16-C17-C18-C36
18	aJ	205	BCR	C1-C6-C7-C8
18	aJ	205	BCR	C6-C7-C8-C9
18	aJ	205	BCR	C7-C8-C9-C34
18	aJ	205	BCR	C11-C10-C9-C8
18	aJ	205	BCR	C37-C22-C23-C24
18	aK	101	BCR	C1-C6-C7-C8
18	aK	101	BCR	C6-C7-C8-C9
18	aK	101	BCR	C7-C8-C9-C10
18	aK	101	BCR	C7-C8-C9-C34
18	aK	101	BCR	C37-C22-C23-C24
18	aL	205	BCR	C1-C6-C7-C8
18	aL	205	BCR	C7-C8-C9-C34
18	aL	205	BCR	C11-C12-C13-C35
18	aL	205	BCR	C37-C22-C23-C24
18	aM	101	BCR	C7-C8-C9-C34
18	aM	101	BCR	C20-C21-C22-C23
18	aM	101	BCR	C20-C21-C22-C37
18	a1	417	BCR	C1-C6-C7-C8
18	a1	417	BCR	C7-C8-C9-C10
18	a1	418	BCR	C7-C8-C9-C34
18	a1	418	BCR	C19-C20-C21-C22
18	a1	418	BCR	C21-C22-C23-C24
18	a1	419	BCR	C1-C6-C7-C8
18	a1	419	BCR	C6-C7-C8-C9
18	a1	419	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a1	419	BCR	C11-C12-C13-C35
18	a1	419	BCR	C22-C23-C24-C25
18	a1	420	BCR	C1-C6-C7-C8
18	a1	420	BCR	C7-C8-C9-C10
18	a1	420	BCR	C21-C22-C23-C24
18	a1	421	BCR	C1-C6-C7-C8
18	a1	421	BCR	C6-C7-C8-C9
18	a1	421	BCR	C7-C8-C9-C10
18	a1	421	BCR	C22-C23-C24-C25
18	a2	401	BCR	C6-C7-C8-C9
18	a2	401	BCR	C7-C8-C9-C10
18	a2	401	BCR	C7-C8-C9-C34
18	a2	401	BCR	C11-C12-C13-C35
18	a2	401	BCR	C22-C23-C24-C25
18	a2	419	BCR	C1-C6-C7-C8
18	a2	419	BCR	C7-C8-C9-C10
18	a2	419	BCR	C23-C24-C25-C30
18	a2	420	BCR	C7-C8-C9-C10
18	a2	420	BCR	C21-C22-C23-C24
18	a2	421	BCR	C1-C6-C7-C8
18	a2	421	BCR	C6-C7-C8-C9
18	a2	421	BCR	C7-C8-C9-C34
18	a2	421	BCR	C20-C21-C22-C37
18	a2	421	BCR	C22-C23-C24-C25
18	a3	401	BCR	C1-C6-C7-C8
18	a3	401	BCR	C6-C7-C8-C9
18	a3	401	BCR	C7-C8-C9-C10
18	a3	401	BCR	C7-C8-C9-C34
18	a3	401	BCR	C10-C11-C12-C13
18	a3	401	BCR	C11-C12-C13-C35
18	a3	401	BCR	C22-C23-C24-C25
18	a3	418	BCR	C1-C6-C7-C8
18	a3	418	BCR	C7-C8-C9-C10
18	a3	418	BCR	C23-C24-C25-C30
18	a3	419	BCR	C1-C6-C7-C8
18	a3	419	BCR	C19-C20-C21-C22
18	a3	419	BCR	C21-C22-C23-C24
18	a3	420	BCR	C1-C6-C7-C8
18	a3	420	BCR	C6-C7-C8-C9
18	a3	420	BCR	C7-C8-C9-C34
18	a3	420	BCR	C11-C12-C13-C35
18	a3	420	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a4	401	BCR	C6-C7-C8-C9
18	a4	401	BCR	C7-C8-C9-C10
18	a4	401	BCR	C7-C8-C9-C34
18	a4	401	BCR	C10-C11-C12-C13
18	a4	401	BCR	C11-C12-C13-C35
18	a4	401	BCR	C22-C23-C24-C25
18	a4	418	BCR	C1-C6-C7-C8
18	a4	418	BCR	C7-C8-C9-C10
18	a4	418	BCR	C23-C24-C25-C30
18	a4	419	BCR	C1-C6-C7-C8
18	a4	419	BCR	C21-C22-C23-C24
18	a4	420	BCR	C1-C6-C7-C8
18	a4	420	BCR	C6-C7-C8-C9
18	a4	420	BCR	C7-C8-C9-C34
18	a4	420	BCR	C11-C12-C13-C35
18	a4	420	BCR	C22-C23-C24-C25
18	a5	401	BCR	C6-C7-C8-C9
18	a5	401	BCR	C7-C8-C9-C10
18	a5	401	BCR	C7-C8-C9-C34
18	a5	401	BCR	C10-C11-C12-C13
18	a5	401	BCR	C11-C12-C13-C35
18	a5	401	BCR	C22-C23-C24-C25
18	a5	418	BCR	C1-C6-C7-C8
18	a5	418	BCR	C7-C8-C9-C10
18	a5	418	BCR	C23-C24-C25-C30
18	a5	419	BCR	C1-C6-C7-C8
18	a5	419	BCR	C6-C7-C8-C9
18	a5	419	BCR	C7-C8-C9-C34
18	a5	419	BCR	C11-C12-C13-C35
18	a5	419	BCR	C22-C23-C24-C25
18	a6	401	BCR	C1-C6-C7-C8
18	a6	401	BCR	C7-C8-C9-C10
18	a6	401	BCR	C19-C20-C21-C22
18	a6	401	BCR	C21-C22-C23-C24
18	a6	402	BCR	C6-C7-C8-C9
18	a6	402	BCR	C7-C8-C9-C10
18	a6	402	BCR	C7-C8-C9-C34
18	a6	402	BCR	C10-C11-C12-C13
18	a6	402	BCR	C22-C23-C24-C25
18	a6	419	BCR	C1-C6-C7-C8
18	a6	419	BCR	C7-C8-C9-C10
18	a6	419	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a6	420	BCR	C1-C6-C7-C8
18	a6	420	BCR	C6-C7-C8-C9
18	a6	420	BCR	C7-C8-C9-C34
18	a6	420	BCR	C11-C12-C13-C35
18	a6	420	BCR	C20-C21-C22-C37
18	a6	420	BCR	C22-C23-C24-C25
18	a6	421	BCR	C1-C6-C7-C8
18	a6	421	BCR	C6-C7-C8-C9
18	a6	421	BCR	C7-C8-C9-C10
18	a6	421	BCR	C7-C8-C9-C34
18	a6	421	BCR	C10-C11-C12-C13
18	a6	421	BCR	C22-C23-C24-C25
18	bA	848	BCR	C1-C6-C7-C8
18	bA	848	BCR	C6-C7-C8-C9
18	bA	848	BCR	C7-C8-C9-C10
18	bA	848	BCR	C7-C8-C9-C34
18	bA	848	BCR	C37-C22-C23-C24
18	bA	849	BCR	C11-C12-C13-C35
18	bA	849	BCR	C20-C21-C22-C23
18	bA	849	BCR	C20-C21-C22-C37
18	bA	849	BCR	C22-C23-C24-C25
18	bA	849	BCR	C23-C24-C25-C30
18	bA	850	BCR	C1-C6-C7-C8
18	bA	850	BCR	C6-C7-C8-C9
18	bA	850	BCR	C7-C8-C9-C10
18	bA	850	BCR	C7-C8-C9-C34
18	bA	850	BCR	C16-C17-C18-C36
18	bA	850	BCR	C37-C22-C23-C24
18	bA	851	BCR	C1-C6-C7-C8
18	bA	851	BCR	C6-C7-C8-C9
18	bA	851	BCR	C7-C8-C9-C34
18	bA	851	BCR	C17-C18-C19-C20
18	bA	851	BCR	C21-C22-C23-C24
18	bA	851	BCR	C22-C23-C24-C25
18	bA	852	BCR	C1-C6-C7-C8
18	bA	852	BCR	C20-C21-C22-C37
18	bA	852	BCR	C21-C22-C23-C24
18	bA	852	BCR	C37-C22-C23-C24
18	bA	852	BCR	C23-C24-C25-C30
18	bA	853	BCR	C7-C8-C9-C10
18	bA	853	BCR	C11-C10-C9-C8
18	bA	853	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bA	853	BCR	C16-C17-C18-C19
18	bA	853	BCR	C18-C19-C20-C21
18	bA	853	BCR	C20-C21-C22-C23
18	bA	853	BCR	C20-C21-C22-C37
18	bA	853	BCR	C21-C22-C23-C24
18	bB	844	BCR	C1-C6-C7-C8
18	bB	844	BCR	C7-C8-C9-C10
18	bB	844	BCR	C37-C22-C23-C24
18	bB	845	BCR	C11-C12-C13-C35
18	bB	845	BCR	C21-C22-C23-C24
18	bB	846	BCR	C1-C6-C7-C8
18	bB	846	BCR	C11-C12-C13-C35
18	bB	846	BCR	C37-C22-C23-C24
18	bB	847	BCR	C16-C17-C18-C36
18	bB	847	BCR	C36-C18-C19-C20
18	bB	847	BCR	C18-C19-C20-C21
18	bB	847	BCR	C20-C21-C22-C23
18	bB	847	BCR	C20-C21-C22-C37
18	bB	848	BCR	C1-C6-C7-C8
18	bB	848	BCR	C7-C8-C9-C10
18	bB	848	BCR	C7-C8-C9-C34
18	bB	848	BCR	C20-C21-C22-C23
18	bB	848	BCR	C37-C22-C23-C24
18	bB	848	BCR	C22-C23-C24-C25
18	bB	848	BCR	C23-C24-C25-C30
18	bB	849	BCR	C7-C8-C9-C34
18	bB	849	BCR	C11-C12-C13-C35
18	bB	849	BCR	C14-C15-C16-C17
18	bB	849	BCR	C21-C22-C23-C24
18	bB	849	BCR	C37-C22-C23-C24
18	bB	850	BCR	C1-C6-C7-C8
18	bB	850	BCR	C20-C21-C22-C37
18	bB	850	BCR	C22-C23-C24-C25
18	bF	202	BCR	C7-C8-C9-C10
18	bF	202	BCR	C12-C13-C14-C15
18	bF	202	BCR	C37-C22-C23-C24
18	bI	101	BCR	C6-C7-C8-C9
18	bI	101	BCR	C7-C8-C9-C34
18	bI	101	BCR	C20-C21-C22-C23
18	bI	101	BCR	C21-C22-C23-C24
18	bI	101	BCR	C37-C22-C23-C24
18	bI	102	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bI	102	BCR	C20-C21-C22-C23
18	bI	102	BCR	C20-C21-C22-C37
18	bJ	103	BCR	C11-C12-C13-C14
18	bJ	103	BCR	C12-C13-C14-C15
18	bJ	103	BCR	C16-C17-C18-C36
18	bJ	104	BCR	C1-C6-C7-C8
18	bJ	104	BCR	C6-C7-C8-C9
18	bJ	104	BCR	C7-C8-C9-C34
18	bJ	104	BCR	C11-C10-C9-C8
18	bJ	104	BCR	C37-C22-C23-C24
18	bJ	105	BCR	C7-C8-C9-C10
18	bJ	105	BCR	C7-C8-C9-C34
18	bJ	105	BCR	C23-C24-C25-C30
18	bL	201	BCR	C1-C6-C7-C8
18	bL	201	BCR	C7-C8-C9-C34
18	bL	201	BCR	C11-C12-C13-C35
18	bL	201	BCR	C37-C22-C23-C24
18	bL	205	BCR	C1-C6-C7-C8
18	bL	205	BCR	C7-C8-C9-C34
18	bL	205	BCR	C37-C22-C23-C24
18	bL	205	BCR	C23-C24-C25-C26
18	bL	206	BCR	C1-C6-C7-C8
18	bL	206	BCR	C7-C8-C9-C34
18	bL	206	BCR	C11-C12-C13-C35
18	bL	206	BCR	C37-C22-C23-C24
18	bM	101	BCR	C7-C8-C9-C34
18	bM	101	BCR	C20-C21-C22-C23
18	bM	101	BCR	C20-C21-C22-C37
18	b1	401	BCR	C1-C6-C7-C8
18	b1	401	BCR	C11-C10-C9-C34
18	b1	401	BCR	C19-C20-C21-C22
18	b1	401	BCR	C21-C22-C23-C24
18	b1	418	BCR	C1-C6-C7-C8
18	b1	418	BCR	C7-C8-C9-C10
18	b1	419	BCR	C7-C8-C9-C34
18	b1	419	BCR	C19-C20-C21-C22
18	b1	419	BCR	C21-C22-C23-C24
18	b1	420	BCR	C1-C6-C7-C8
18	b1	420	BCR	C6-C7-C8-C9
18	b1	420	BCR	C7-C8-C9-C34
18	b1	420	BCR	C11-C12-C13-C35
18	b1	420	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b2	401	BCR	C6-C7-C8-C9
18	b2	401	BCR	C7-C8-C9-C10
18	b2	401	BCR	C7-C8-C9-C34
18	b2	401	BCR	C11-C12-C13-C35
18	b2	401	BCR	C22-C23-C24-C25
18	b2	419	BCR	C1-C6-C7-C8
18	b2	419	BCR	C7-C8-C9-C10
18	b2	419	BCR	C23-C24-C25-C30
18	b2	420	BCR	C1-C6-C7-C8
18	b2	420	BCR	C7-C8-C9-C10
18	b2	420	BCR	C21-C22-C23-C24
18	b2	421	BCR	C1-C6-C7-C8
18	b2	421	BCR	C6-C7-C8-C9
18	b2	421	BCR	C7-C8-C9-C34
18	b2	421	BCR	C20-C21-C22-C37
18	b2	421	BCR	C22-C23-C24-C25
18	b3	401	BCR	C1-C6-C7-C8
18	b3	401	BCR	C6-C7-C8-C9
18	b3	401	BCR	C7-C8-C9-C10
18	b3	401	BCR	C7-C8-C9-C34
18	b3	401	BCR	C10-C11-C12-C13
18	b3	401	BCR	C11-C12-C13-C35
18	b3	401	BCR	C22-C23-C24-C25
18	b3	418	BCR	C1-C6-C7-C8
18	b3	418	BCR	C7-C8-C9-C10
18	b3	418	BCR	C23-C24-C25-C30
18	b3	419	BCR	C1-C6-C7-C8
18	b3	419	BCR	C19-C20-C21-C22
18	b3	419	BCR	C21-C22-C23-C24
18	b3	420	BCR	C1-C6-C7-C8
18	b3	420	BCR	C6-C7-C8-C9
18	b3	420	BCR	C7-C8-C9-C34
18	b3	420	BCR	C11-C12-C13-C35
18	b3	420	BCR	C22-C23-C24-C25
18	b4	401	BCR	C6-C7-C8-C9
18	b4	401	BCR	C7-C8-C9-C10
18	b4	401	BCR	C7-C8-C9-C34
18	b4	401	BCR	C10-C11-C12-C13
18	b4	401	BCR	C11-C12-C13-C35
18	b4	401	BCR	C22-C23-C24-C25
18	b4	418	BCR	C1-C6-C7-C8
18	b4	418	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b4	418	BCR	C23-C24-C25-C30
18	b4	419	BCR	C1-C6-C7-C8
18	b4	419	BCR	C21-C22-C23-C24
18	b4	420	BCR	C1-C6-C7-C8
18	b4	420	BCR	C6-C7-C8-C9
18	b4	420	BCR	C7-C8-C9-C34
18	b4	420	BCR	C11-C12-C13-C35
18	b4	420	BCR	C22-C23-C24-C25
18	b5	401	BCR	C6-C7-C8-C9
18	b5	401	BCR	C7-C8-C9-C10
18	b5	401	BCR	C7-C8-C9-C34
18	b5	401	BCR	C10-C11-C12-C13
18	b5	401	BCR	C11-C12-C13-C35
18	b5	401	BCR	C22-C23-C24-C25
18	b5	418	BCR	C1-C6-C7-C8
18	b5	418	BCR	C7-C8-C9-C10
18	b5	418	BCR	C23-C24-C25-C30
18	b5	419	BCR	C1-C6-C7-C8
18	b5	419	BCR	C6-C7-C8-C9
18	b5	419	BCR	C7-C8-C9-C34
18	b5	419	BCR	C11-C12-C13-C35
18	b5	419	BCR	C20-C21-C22-C37
18	b6	401	BCR	C1-C6-C7-C8
18	b6	401	BCR	C7-C8-C9-C10
18	b6	401	BCR	C19-C20-C21-C22
18	b6	401	BCR	C21-C22-C23-C24
18	b6	402	BCR	C6-C7-C8-C9
18	b6	402	BCR	C7-C8-C9-C10
18	b6	402	BCR	C7-C8-C9-C34
18	b6	402	BCR	C10-C11-C12-C13
18	b6	402	BCR	C22-C23-C24-C25
18	b6	419	BCR	C1-C6-C7-C8
18	b6	419	BCR	C7-C8-C9-C10
18	b6	419	BCR	C23-C24-C25-C30
18	b6	420	BCR	C1-C6-C7-C8
18	b6	420	BCR	C6-C7-C8-C9
18	b6	420	BCR	C7-C8-C9-C34
18	b6	420	BCR	C11-C12-C13-C35
18	b6	420	BCR	C22-C23-C24-C25
18	b6	421	BCR	C1-C6-C7-C8
18	b6	421	BCR	C6-C7-C8-C9
18	b6	421	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b6	421	BCR	C7-C8-C9-C34
18	b6	421	BCR	C10-C11-C12-C13
18	b6	421	BCR	C22-C23-C24-C25
18	cA	847	BCR	C11-C12-C13-C35
18	cA	847	BCR	C20-C21-C22-C23
18	cA	847	BCR	C20-C21-C22-C37
18	cA	847	BCR	C22-C23-C24-C25
18	cA	847	BCR	C23-C24-C25-C30
18	cA	848	BCR	C1-C6-C7-C8
18	cA	848	BCR	C6-C7-C8-C9
18	cA	848	BCR	C7-C8-C9-C10
18	cA	848	BCR	C7-C8-C9-C34
18	cA	848	BCR	C16-C17-C18-C36
18	cA	848	BCR	C37-C22-C23-C24
18	cA	849	BCR	C1-C6-C7-C8
18	cA	849	BCR	C6-C7-C8-C9
18	cA	849	BCR	C7-C8-C9-C34
18	cA	849	BCR	C17-C18-C19-C20
18	cA	849	BCR	C21-C22-C23-C24
18	cA	849	BCR	C22-C23-C24-C25
18	cA	850	BCR	C1-C6-C7-C8
18	cA	850	BCR	C20-C21-C22-C37
18	cA	850	BCR	C21-C22-C23-C24
18	cA	850	BCR	C37-C22-C23-C24
18	cA	850	BCR	C23-C24-C25-C30
18	cA	851	BCR	C7-C8-C9-C10
18	cA	851	BCR	C11-C10-C9-C8
18	cA	851	BCR	C11-C12-C13-C35
18	cA	851	BCR	C16-C17-C18-C19
18	cA	851	BCR	C18-C19-C20-C21
18	cA	851	BCR	C20-C21-C22-C23
18	cA	851	BCR	C20-C21-C22-C37
18	cA	851	BCR	C21-C22-C23-C24
18	cB	844	BCR	C1-C6-C7-C8
18	cB	844	BCR	C7-C8-C9-C10
18	cB	844	BCR	C37-C22-C23-C24
18	cB	845	BCR	C11-C12-C13-C35
18	cB	845	BCR	C21-C22-C23-C24
18	cB	846	BCR	C1-C6-C7-C8
18	cB	846	BCR	C11-C12-C13-C35
18	cB	846	BCR	C37-C22-C23-C24
18	cB	847	BCR	C16-C17-C18-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cB	847	BCR	C36-C18-C19-C20
18	cB	847	BCR	C18-C19-C20-C21
18	cB	847	BCR	C20-C21-C22-C23
18	cB	847	BCR	C20-C21-C22-C37
18	cB	848	BCR	C1-C6-C7-C8
18	cB	848	BCR	C7-C8-C9-C10
18	cB	848	BCR	C7-C8-C9-C34
18	cB	848	BCR	C20-C21-C22-C23
18	cB	848	BCR	C37-C22-C23-C24
18	cB	848	BCR	C22-C23-C24-C25
18	cB	848	BCR	C23-C24-C25-C30
18	cB	849	BCR	C1-C6-C7-C8
18	cB	849	BCR	C20-C21-C22-C37
18	cB	849	BCR	C22-C23-C24-C25
18	cF	202	BCR	C7-C8-C9-C34
18	cF	202	BCR	C11-C12-C13-C35
18	cF	202	BCR	C14-C15-C16-C17
18	cF	202	BCR	C21-C22-C23-C24
18	cF	202	BCR	C37-C22-C23-C24
18	cF	204	BCR	C7-C8-C9-C10
18	cF	204	BCR	C12-C13-C14-C15
18	cF	204	BCR	C37-C22-C23-C24
18	cF	205	BCR	C7-C8-C9-C10
18	cF	205	BCR	C7-C8-C9-C34
18	cF	205	BCR	C23-C24-C25-C30
18	cI	101	BCR	C6-C7-C8-C9
18	cI	101	BCR	C7-C8-C9-C34
18	cI	101	BCR	C20-C21-C22-C23
18	cI	101	BCR	C21-C22-C23-C24
18	cI	101	BCR	C37-C22-C23-C24
18	cI	102	BCR	C7-C8-C9-C10
18	cI	102	BCR	C20-C21-C22-C23
18	cI	102	BCR	C20-C21-C22-C37
18	cJ	103	BCR	C11-C12-C13-C14
18	cJ	103	BCR	C12-C13-C14-C15
18	cJ	103	BCR	C16-C17-C18-C36
18	cJ	104	BCR	C1-C6-C7-C8
18	cJ	104	BCR	C6-C7-C8-C9
18	cJ	104	BCR	C7-C8-C9-C34
18	cJ	104	BCR	C11-C10-C9-C8
18	cJ	104	BCR	C37-C22-C23-C24
18	cK	101	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cK	101	BCR	C6-C7-C8-C9
18	cK	101	BCR	C7-C8-C9-C10
18	cK	101	BCR	C7-C8-C9-C34
18	cK	101	BCR	C37-C22-C23-C24
18	cL	204	BCR	C1-C6-C7-C8
18	cL	204	BCR	C7-C8-C9-C34
18	cL	204	BCR	C37-C22-C23-C24
18	cL	204	BCR	C23-C24-C25-C26
18	cM	101	BCR	C7-C8-C9-C34
18	cM	101	BCR	C20-C21-C22-C23
18	cM	101	BCR	C20-C21-C22-C37
18	c1	401	BCR	C11-C10-C9-C34
18	c1	401	BCR	C21-C22-C23-C24
18	c1	418	BCR	C1-C6-C7-C8
18	c1	418	BCR	C7-C8-C9-C10
18	c1	419	BCR	C19-C20-C21-C22
18	c1	419	BCR	C21-C22-C23-C24
18	c1	420	BCR	C1-C6-C7-C8
18	c1	420	BCR	C6-C7-C8-C9
18	c1	420	BCR	C7-C8-C9-C34
18	c1	420	BCR	C11-C12-C13-C35
18	c1	420	BCR	C22-C23-C24-C25
18	c2	401	BCR	C6-C7-C8-C9
18	c2	401	BCR	C7-C8-C9-C10
18	c2	401	BCR	C7-C8-C9-C34
18	c2	401	BCR	C11-C12-C13-C35
18	c2	401	BCR	C22-C23-C24-C25
18	c2	419	BCR	C1-C6-C7-C8
18	c2	419	BCR	C7-C8-C9-C10
18	c2	419	BCR	C23-C24-C25-C30
18	c2	420	BCR	C7-C8-C9-C10
18	c2	420	BCR	C21-C22-C23-C24
18	c2	421	BCR	C1-C6-C7-C8
18	c2	421	BCR	C6-C7-C8-C9
18	c2	421	BCR	C7-C8-C9-C34
18	c2	421	BCR	C20-C21-C22-C37
18	c2	421	BCR	C22-C23-C24-C25
18	c3	401	BCR	C1-C6-C7-C8
18	c3	401	BCR	C6-C7-C8-C9
18	c3	401	BCR	C7-C8-C9-C10
18	c3	401	BCR	C7-C8-C9-C34
18	c3	401	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c3	401	BCR	C11-C12-C13-C35
18	c3	401	BCR	C22-C23-C24-C25
18	c3	418	BCR	C1-C6-C7-C8
18	c3	418	BCR	C7-C8-C9-C10
18	c3	418	BCR	C23-C24-C25-C30
18	c3	419	BCR	C1-C6-C7-C8
18	c3	419	BCR	C19-C20-C21-C22
18	c3	419	BCR	C21-C22-C23-C24
18	c3	420	BCR	C1-C6-C7-C8
18	c3	420	BCR	C6-C7-C8-C9
18	c3	420	BCR	C7-C8-C9-C34
18	c3	420	BCR	C11-C12-C13-C35
18	c3	420	BCR	C22-C23-C24-C25
18	c4	401	BCR	C6-C7-C8-C9
18	c4	401	BCR	C7-C8-C9-C10
18	c4	401	BCR	C7-C8-C9-C34
18	c4	401	BCR	C10-C11-C12-C13
18	c4	401	BCR	C11-C12-C13-C35
18	c4	401	BCR	C22-C23-C24-C25
18	c4	418	BCR	C1-C6-C7-C8
18	c4	418	BCR	C7-C8-C9-C10
18	c4	418	BCR	C23-C24-C25-C30
18	c4	419	BCR	C1-C6-C7-C8
18	c4	419	BCR	C21-C22-C23-C24
18	c4	420	BCR	C1-C6-C7-C8
18	c4	420	BCR	C6-C7-C8-C9
18	c4	420	BCR	C7-C8-C9-C34
18	c4	420	BCR	C11-C12-C13-C35
18	c4	420	BCR	C22-C23-C24-C25
18	c5	401	BCR	C6-C7-C8-C9
18	c5	401	BCR	C7-C8-C9-C10
18	c5	401	BCR	C7-C8-C9-C34
18	c5	401	BCR	C10-C11-C12-C13
18	c5	401	BCR	C11-C12-C13-C35
18	c5	401	BCR	C22-C23-C24-C25
18	c5	418	BCR	C1-C6-C7-C8
18	c5	418	BCR	C7-C8-C9-C10
18	c5	418	BCR	C23-C24-C25-C30
18	c5	419	BCR	C1-C6-C7-C8
18	c5	419	BCR	C6-C7-C8-C9
18	c5	419	BCR	C7-C8-C9-C34
18	c5	419	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c5	419	BCR	C22-C23-C24-C25
18	c6	401	BCR	C1-C6-C7-C8
18	c6	401	BCR	C7-C8-C9-C10
18	c6	401	BCR	C19-C20-C21-C22
18	c6	401	BCR	C21-C22-C23-C24
18	c6	402	BCR	C6-C7-C8-C9
18	c6	402	BCR	C7-C8-C9-C10
18	c6	402	BCR	C7-C8-C9-C34
18	c6	402	BCR	C10-C11-C12-C13
18	c6	402	BCR	C22-C23-C24-C25
18	c6	419	BCR	C1-C6-C7-C8
18	c6	419	BCR	C7-C8-C9-C10
18	c6	419	BCR	C23-C24-C25-C30
18	c6	420	BCR	C1-C6-C7-C8
18	c6	420	BCR	C6-C7-C8-C9
18	c6	420	BCR	C7-C8-C9-C34
18	c6	420	BCR	C11-C12-C13-C35
18	c6	420	BCR	C22-C23-C24-C25
19	aA	853	LHG	C3-O3-P-O5
19	aA	854	LHG	C1-C2-C3-O3
19	aA	854	LHG	C3-O3-P-O5
19	aA	854	LHG	C4-O6-P-O5
19	aX	101	LHG	O1-C1-C2-C3
19	aX	101	LHG	C3-O3-P-O4
19	aX	101	LHG	C3-O3-P-O5
19	bA	854	LHG	C3-O3-P-O5
19	bA	855	LHG	C1-C2-C3-O3
19	bA	855	LHG	C3-O3-P-O5
19	bX	101	LHG	O1-C1-C2-C3
19	bX	101	LHG	C3-O3-P-O4
19	bX	101	LHG	C3-O3-P-O5
19	cA	852	LHG	C3-O3-P-O5
19	cA	853	LHG	C1-C2-C3-O3
19	cA	853	LHG	C3-O3-P-O5
19	cX	101	LHG	O1-C1-C2-C3
19	cX	101	LHG	C3-O3-P-O4
19	cX	101	LHG	C3-O3-P-O5
15	aA	845	CLA	C4C-C3C-CAC-CBC
15	a1	409	CLA	C4C-C3C-CAC-CBC
15	a2	411	CLA	C4C-C3C-CAC-CBC
15	a3	410	CLA	C4C-C3C-CAC-CBC
15	a4	410	CLA	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	410	CLA	C4C-C3C-CAC-CBC
15	a6	411	CLA	C4C-C3C-CAC-CBC
15	bA	845	CLA	C4C-C3C-CAC-CBC
15	b1	410	CLA	C4C-C3C-CAC-CBC
15	b2	411	CLA	C4C-C3C-CAC-CBC
15	b3	410	CLA	C4C-C3C-CAC-CBC
15	b4	410	CLA	C4C-C3C-CAC-CBC
15	b5	410	CLA	C4C-C3C-CAC-CBC
15	b6	411	CLA	C4C-C3C-CAC-CBC
15	cA	844	CLA	C4C-C3C-CAC-CBC
15	c1	410	CLA	C4C-C3C-CAC-CBC
15	c2	411	CLA	C4C-C3C-CAC-CBC
15	c4	410	CLA	C4C-C3C-CAC-CBC
15	c5	410	CLA	C4C-C3C-CAC-CBC
15	c6	411	CLA	C4C-C3C-CAC-CBC
15	aX	102	CLA	O1D-CGD-O2D-CED
15	a1	405	CLA	O1D-CGD-O2D-CED
15	a2	407	CLA	O1D-CGD-O2D-CED
15	a2	422	CLA	O1D-CGD-O2D-CED
15	a3	406	CLA	O1D-CGD-O2D-CED
15	a4	406	CLA	O1D-CGD-O2D-CED
15	a4	421	CLA	O1D-CGD-O2D-CED
15	a5	406	CLA	O1D-CGD-O2D-CED
15	a6	407	CLA	O1D-CGD-O2D-CED
15	a6	422	CLA	O1D-CGD-O2D-CED
15	bX	102	CLA	O1D-CGD-O2D-CED
15	b1	406	CLA	O1D-CGD-O2D-CED
15	b2	407	CLA	O1D-CGD-O2D-CED
15	b2	422	CLA	O1D-CGD-O2D-CED
15	b3	406	CLA	O1D-CGD-O2D-CED
15	b4	406	CLA	O1D-CGD-O2D-CED
15	b4	421	CLA	O1D-CGD-O2D-CED
15	b5	406	CLA	O1D-CGD-O2D-CED
15	b6	407	CLA	O1D-CGD-O2D-CED
15	cX	102	CLA	O1D-CGD-O2D-CED
15	c1	406	CLA	O1D-CGD-O2D-CED
15	c2	407	CLA	O1D-CGD-O2D-CED
15	c2	422	CLA	O1D-CGD-O2D-CED
15	c3	406	CLA	O1D-CGD-O2D-CED
15	c4	406	CLA	O1D-CGD-O2D-CED
15	c4	421	CLA	O1D-CGD-O2D-CED
15	c5	406	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c6	407	CLA	O1D-CGD-O2D-CED
15	aA	845	CLA	C2C-C3C-CAC-CBC
15	a1	409	CLA	C2C-C3C-CAC-CBC
15	a2	411	CLA	C2C-C3C-CAC-CBC
15	a3	410	CLA	C2C-C3C-CAC-CBC
15	a4	410	CLA	C2C-C3C-CAC-CBC
15	a5	410	CLA	C2C-C3C-CAC-CBC
15	a6	411	CLA	C2C-C3C-CAC-CBC
15	bA	845	CLA	C2C-C3C-CAC-CBC
15	b1	410	CLA	C2C-C3C-CAC-CBC
15	b2	411	CLA	C2C-C3C-CAC-CBC
15	b3	410	CLA	C2C-C3C-CAC-CBC
15	b4	410	CLA	C2C-C3C-CAC-CBC
15	b5	410	CLA	C2C-C3C-CAC-CBC
15	b6	411	CLA	C2C-C3C-CAC-CBC
15	cA	844	CLA	C2C-C3C-CAC-CBC
15	c1	410	CLA	C2C-C3C-CAC-CBC
15	c2	411	CLA	C2C-C3C-CAC-CBC
15	c3	410	CLA	C4C-C3C-CAC-CBC
15	c4	410	CLA	C2C-C3C-CAC-CBC
15	c5	410	CLA	C2C-C3C-CAC-CBC
15	c6	411	CLA	C2C-C3C-CAC-CBC
15	aA	811	CLA	O1D-CGD-O2D-CED
15	aA	839	CLA	O1D-CGD-O2D-CED
15	a1	415	CLA	O1D-CGD-O2D-CED
15	a1	422	CLA	O1D-CGD-O2D-CED
15	a2	406	CLA	O1D-CGD-O2D-CED
15	a2	417	CLA	O1D-CGD-O2D-CED
15	a3	416	CLA	O1D-CGD-O2D-CED
15	a4	416	CLA	O1D-CGD-O2D-CED
15	a5	416	CLA	O1D-CGD-O2D-CED
15	a6	417	CLA	O1D-CGD-O2D-CED
15	bA	811	CLA	O1D-CGD-O2D-CED
15	bA	839	CLA	O1D-CGD-O2D-CED
15	b1	416	CLA	O1D-CGD-O2D-CED
15	b2	406	CLA	O1D-CGD-O2D-CED
15	b2	417	CLA	O1D-CGD-O2D-CED
15	b3	416	CLA	O1D-CGD-O2D-CED
15	b4	416	CLA	O1D-CGD-O2D-CED
15	b5	416	CLA	O1D-CGD-O2D-CED
15	b6	417	CLA	O1D-CGD-O2D-CED
15	b6	422	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	811	CLA	O1D-CGD-O2D-CED
15	cA	839	CLA	O1D-CGD-O2D-CED
15	cB	835	CLA	O1D-CGD-O2D-CED
15	c1	416	CLA	O1D-CGD-O2D-CED
15	c2	406	CLA	O1D-CGD-O2D-CED
15	c2	417	CLA	O1D-CGD-O2D-CED
15	c3	416	CLA	O1D-CGD-O2D-CED
15	c4	416	CLA	O1D-CGD-O2D-CED
15	c5	416	CLA	O1D-CGD-O2D-CED
15	c6	417	CLA	O1D-CGD-O2D-CED
15	aA	802	CLA	CBD-CGD-O2D-CED
15	aA	812	CLA	CBD-CGD-O2D-CED
15	aA	829	CLA	CBD-CGD-O2D-CED
15	aA	838	CLA	CBD-CGD-O2D-CED
15	aA	840	CLA	CBD-CGD-O2D-CED
15	aA	841	CLA	CBD-CGD-O2D-CED
15	aA	845	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	CBD-CGD-O2D-CED
15	aB	804	CLA	CBD-CGD-O2D-CED
15	aB	815	CLA	CBD-CGD-O2D-CED
15	aB	816	CLA	CBD-CGD-O2D-CED
15	aB	821	CLA	CBD-CGD-O2D-CED
15	aB	825	CLA	CBD-CGD-O2D-CED
15	aB	835	CLA	CBD-CGD-O2D-CED
15	aB	836	CLA	CBD-CGD-O2D-CED
15	aB	840	CLA	CBD-CGD-O2D-CED
15	aX	102	CLA	CBD-CGD-O2D-CED
15	a1	402	CLA	CBD-CGD-O2D-CED
15	a1	403	CLA	CBD-CGD-O2D-CED
15	a1	404	CLA	CBD-CGD-O2D-CED
15	a1	405	CLA	CBD-CGD-O2D-CED
15	a1	411	CLA	CBD-CGD-O2D-CED
15	a1	416	CLA	CBD-CGD-O2D-CED
15	a2	403	CLA	CBD-CGD-O2D-CED
15	a2	404	CLA	CBD-CGD-O2D-CED
15	a2	405	CLA	CBD-CGD-O2D-CED
15	a2	407	CLA	CBD-CGD-O2D-CED
15	a2	418	CLA	CBD-CGD-O2D-CED
15	a3	403	CLA	CBD-CGD-O2D-CED
15	a3	404	CLA	CBD-CGD-O2D-CED
15	a3	405	CLA	CBD-CGD-O2D-CED
15	a3	406	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a4	403	CLA	CBD-CGD-O2D-CED
15	a4	404	CLA	CBD-CGD-O2D-CED
15	a4	405	CLA	CBD-CGD-O2D-CED
15	a4	406	CLA	CBD-CGD-O2D-CED
15	a4	412	CLA	CBD-CGD-O2D-CED
15	a5	403	CLA	CBD-CGD-O2D-CED
15	a5	404	CLA	CBD-CGD-O2D-CED
15	a5	405	CLA	CBD-CGD-O2D-CED
15	a5	406	CLA	CBD-CGD-O2D-CED
15	a5	412	CLA	CBD-CGD-O2D-CED
15	a6	404	CLA	CBD-CGD-O2D-CED
15	a6	405	CLA	CBD-CGD-O2D-CED
15	a6	407	CLA	CBD-CGD-O2D-CED
15	a6	413	CLA	CBD-CGD-O2D-CED
15	a6	418	CLA	CBD-CGD-O2D-CED
15	bA	802	CLA	CBD-CGD-O2D-CED
15	bA	812	CLA	CBD-CGD-O2D-CED
15	bA	829	CLA	CBD-CGD-O2D-CED
15	bA	838	CLA	CBD-CGD-O2D-CED
15	bA	840	CLA	CBD-CGD-O2D-CED
15	bA	841	CLA	CBD-CGD-O2D-CED
15	bA	845	CLA	CBD-CGD-O2D-CED
15	bB	803	CLA	CBD-CGD-O2D-CED
15	bB	804	CLA	CBD-CGD-O2D-CED
15	bB	815	CLA	CBD-CGD-O2D-CED
15	bB	816	CLA	CBD-CGD-O2D-CED
15	bB	821	CLA	CBD-CGD-O2D-CED
15	bB	825	CLA	CBD-CGD-O2D-CED
15	bB	835	CLA	CBD-CGD-O2D-CED
15	bB	836	CLA	CBD-CGD-O2D-CED
15	bB	840	CLA	CBD-CGD-O2D-CED
15	bX	102	CLA	CBD-CGD-O2D-CED
15	b1	403	CLA	CBD-CGD-O2D-CED
15	b1	404	CLA	CBD-CGD-O2D-CED
15	b1	405	CLA	CBD-CGD-O2D-CED
15	b1	406	CLA	CBD-CGD-O2D-CED
15	b1	412	CLA	CBD-CGD-O2D-CED
15	b1	417	CLA	CBD-CGD-O2D-CED
15	b2	403	CLA	CBD-CGD-O2D-CED
15	b2	404	CLA	CBD-CGD-O2D-CED
15	b2	405	CLA	CBD-CGD-O2D-CED
15	b2	407	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	418	CLA	CBD-CGD-O2D-CED
15	b3	403	CLA	CBD-CGD-O2D-CED
15	b3	404	CLA	CBD-CGD-O2D-CED
15	b3	405	CLA	CBD-CGD-O2D-CED
15	b3	406	CLA	CBD-CGD-O2D-CED
15	b4	403	CLA	CBD-CGD-O2D-CED
15	b4	404	CLA	CBD-CGD-O2D-CED
15	b4	405	CLA	CBD-CGD-O2D-CED
15	b4	406	CLA	CBD-CGD-O2D-CED
15	b4	412	CLA	CBD-CGD-O2D-CED
15	b5	403	CLA	CBD-CGD-O2D-CED
15	b5	404	CLA	CBD-CGD-O2D-CED
15	b5	405	CLA	CBD-CGD-O2D-CED
15	b5	406	CLA	CBD-CGD-O2D-CED
15	b5	412	CLA	CBD-CGD-O2D-CED
15	b6	404	CLA	CBD-CGD-O2D-CED
15	b6	405	CLA	CBD-CGD-O2D-CED
15	b6	407	CLA	CBD-CGD-O2D-CED
15	b6	413	CLA	CBD-CGD-O2D-CED
15	b6	418	CLA	CBD-CGD-O2D-CED
15	cA	802	CLA	CBD-CGD-O2D-CED
15	cA	812	CLA	CBD-CGD-O2D-CED
15	cA	829	CLA	CBD-CGD-O2D-CED
15	cA	838	CLA	CBD-CGD-O2D-CED
15	cA	840	CLA	CBD-CGD-O2D-CED
15	cA	841	CLA	CBD-CGD-O2D-CED
15	cA	844	CLA	CBD-CGD-O2D-CED
15	cB	803	CLA	CBD-CGD-O2D-CED
15	cB	804	CLA	CBD-CGD-O2D-CED
15	cB	815	CLA	CBD-CGD-O2D-CED
15	cB	816	CLA	CBD-CGD-O2D-CED
15	cB	821	CLA	CBD-CGD-O2D-CED
15	cB	825	CLA	CBD-CGD-O2D-CED
15	cB	835	CLA	CBD-CGD-O2D-CED
15	cB	836	CLA	CBD-CGD-O2D-CED
15	cB	840	CLA	CBD-CGD-O2D-CED
15	cX	102	CLA	CBD-CGD-O2D-CED
15	c1	403	CLA	CBD-CGD-O2D-CED
15	c1	404	CLA	CBD-CGD-O2D-CED
15	c1	405	CLA	CBD-CGD-O2D-CED
15	c1	406	CLA	CBD-CGD-O2D-CED
15	c1	412	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	417	CLA	CBD-CGD-O2D-CED
15	c2	403	CLA	CBD-CGD-O2D-CED
15	c2	404	CLA	CBD-CGD-O2D-CED
15	c2	405	CLA	CBD-CGD-O2D-CED
15	c2	407	CLA	CBD-CGD-O2D-CED
15	c2	413	CLA	CBD-CGD-O2D-CED
15	c2	418	CLA	CBD-CGD-O2D-CED
15	c3	403	CLA	CBD-CGD-O2D-CED
15	c3	404	CLA	CBD-CGD-O2D-CED
15	c3	405	CLA	CBD-CGD-O2D-CED
15	c3	406	CLA	CBD-CGD-O2D-CED
15	c3	412	CLA	CBD-CGD-O2D-CED
15	c4	403	CLA	CBD-CGD-O2D-CED
15	c4	404	CLA	CBD-CGD-O2D-CED
15	c4	405	CLA	CBD-CGD-O2D-CED
15	c4	406	CLA	CBD-CGD-O2D-CED
15	c4	412	CLA	CBD-CGD-O2D-CED
15	c5	403	CLA	CBD-CGD-O2D-CED
15	c5	404	CLA	CBD-CGD-O2D-CED
15	c5	405	CLA	CBD-CGD-O2D-CED
15	c5	406	CLA	CBD-CGD-O2D-CED
15	c5	412	CLA	CBD-CGD-O2D-CED
15	c5	415	CLA	CBD-CGD-O2D-CED
15	c6	404	CLA	CBD-CGD-O2D-CED
15	c6	405	CLA	CBD-CGD-O2D-CED
15	c6	406	CLA	CBD-CGD-O2D-CED
15	c6	407	CLA	CBD-CGD-O2D-CED
15	c6	413	CLA	CBD-CGD-O2D-CED
15	c6	418	CLA	CBD-CGD-O2D-CED
15	c3	410	CLA	C2C-C3C-CAC-CBC
15	aA	842	CLA	O1D-CGD-O2D-CED
15	aB	804	CLA	O1D-CGD-O2D-CED
15	aB	835	CLA	O1D-CGD-O2D-CED
15	aJ	201	CLA	O1D-CGD-O2D-CED
15	a1	411	CLA	O1D-CGD-O2D-CED
15	a2	415	CLA	O1D-CGD-O2D-CED
15	a3	408	CLA	O1D-CGD-O2D-CED
15	a3	414	CLA	O1D-CGD-O2D-CED
15	a3	421	CLA	O1D-CGD-O2D-CED
15	a4	414	CLA	O1D-CGD-O2D-CED
15	a5	414	CLA	O1D-CGD-O2D-CED
15	a5	420	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	413	CLA	O1D-CGD-O2D-CED
15	a6	415	CLA	O1D-CGD-O2D-CED
15	bA	842	CLA	O1D-CGD-O2D-CED
15	bB	804	CLA	O1D-CGD-O2D-CED
15	bB	835	CLA	O1D-CGD-O2D-CED
15	bF	201	CLA	O1D-CGD-O2D-CED
15	b1	412	CLA	O1D-CGD-O2D-CED
15	b3	414	CLA	O1D-CGD-O2D-CED
15	b3	421	CLA	O1D-CGD-O2D-CED
15	b4	414	CLA	O1D-CGD-O2D-CED
15	b5	420	CLA	O1D-CGD-O2D-CED
15	b6	413	CLA	O1D-CGD-O2D-CED
15	b6	415	CLA	O1D-CGD-O2D-CED
15	cB	804	CLA	O1D-CGD-O2D-CED
15	cF	201	CLA	O1D-CGD-O2D-CED
15	cF	203	CLA	O1D-CGD-O2D-CED
15	c1	412	CLA	O1D-CGD-O2D-CED
15	c2	415	CLA	O1D-CGD-O2D-CED
15	c3	414	CLA	O1D-CGD-O2D-CED
15	c3	421	CLA	O1D-CGD-O2D-CED
15	c4	414	CLA	O1D-CGD-O2D-CED
15	c5	414	CLA	O1D-CGD-O2D-CED
15	c5	420	CLA	O1D-CGD-O2D-CED
15	c6	413	CLA	O1D-CGD-O2D-CED
15	c6	415	CLA	O1D-CGD-O2D-CED
15	aA	810	CLA	O1D-CGD-O2D-CED
15	aB	802	CLA	O1D-CGD-O2D-CED
15	aB	815	CLA	O1D-CGD-O2D-CED
15	aB	825	CLA	O1D-CGD-O2D-CED
15	aB	834	CLA	O1D-CGD-O2D-CED
15	aJ	202	CLA	O1D-CGD-O2D-CED
15	a1	407	CLA	O1D-CGD-O2D-CED
15	a1	413	CLA	O1D-CGD-O2D-CED
15	a1	416	CLA	O1D-CGD-O2D-CED
15	a2	413	CLA	O1D-CGD-O2D-CED
15	a2	418	CLA	O1D-CGD-O2D-CED
15	a3	412	CLA	O1D-CGD-O2D-CED
15	a3	417	CLA	O1D-CGD-O2D-CED
15	a4	412	CLA	O1D-CGD-O2D-CED
15	a4	415	CLA	O1D-CGD-O2D-CED
15	a4	417	CLA	O1D-CGD-O2D-CED
15	a5	408	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	412	CLA	O1D-CGD-O2D-CED
15	a5	415	CLA	O1D-CGD-O2D-CED
15	a5	417	CLA	O1D-CGD-O2D-CED
15	a6	409	CLA	O1D-CGD-O2D-CED
15	a6	418	CLA	O1D-CGD-O2D-CED
15	bA	810	CLA	O1D-CGD-O2D-CED
15	bB	802	CLA	O1D-CGD-O2D-CED
15	bB	815	CLA	O1D-CGD-O2D-CED
15	bB	825	CLA	O1D-CGD-O2D-CED
15	bB	834	CLA	O1D-CGD-O2D-CED
15	bJ	101	CLA	O1D-CGD-O2D-CED
15	b1	414	CLA	O1D-CGD-O2D-CED
15	b1	417	CLA	O1D-CGD-O2D-CED
15	b2	413	CLA	O1D-CGD-O2D-CED
15	b2	415	CLA	O1D-CGD-O2D-CED
15	b2	416	CLA	O1D-CGD-O2D-CED
15	b2	418	CLA	O1D-CGD-O2D-CED
15	b3	408	CLA	O1D-CGD-O2D-CED
15	b3	412	CLA	O1D-CGD-O2D-CED
15	b3	417	CLA	O1D-CGD-O2D-CED
15	b4	412	CLA	O1D-CGD-O2D-CED
15	b4	415	CLA	O1D-CGD-O2D-CED
15	b4	417	CLA	O1D-CGD-O2D-CED
15	b5	408	CLA	O1D-CGD-O2D-CED
15	b5	412	CLA	O1D-CGD-O2D-CED
15	b5	414	CLA	O1D-CGD-O2D-CED
15	b5	415	CLA	O1D-CGD-O2D-CED
15	b5	417	CLA	O1D-CGD-O2D-CED
15	b6	409	CLA	O1D-CGD-O2D-CED
15	b6	418	CLA	O1D-CGD-O2D-CED
15	cA	810	CLA	O1D-CGD-O2D-CED
15	cB	802	CLA	O1D-CGD-O2D-CED
15	cB	815	CLA	O1D-CGD-O2D-CED
15	cB	825	CLA	O1D-CGD-O2D-CED
15	cB	834	CLA	O1D-CGD-O2D-CED
15	cJ	101	CLA	O1D-CGD-O2D-CED
15	c1	408	CLA	O1D-CGD-O2D-CED
15	c1	414	CLA	O1D-CGD-O2D-CED
15	c1	417	CLA	O1D-CGD-O2D-CED
15	c2	413	CLA	O1D-CGD-O2D-CED
15	c2	416	CLA	O1D-CGD-O2D-CED
15	c2	418	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	408	CLA	O1D-CGD-O2D-CED
15	c3	412	CLA	O1D-CGD-O2D-CED
15	c3	417	CLA	O1D-CGD-O2D-CED
15	c4	412	CLA	O1D-CGD-O2D-CED
15	c4	415	CLA	O1D-CGD-O2D-CED
15	c4	417	CLA	O1D-CGD-O2D-CED
15	c5	408	CLA	O1D-CGD-O2D-CED
15	c5	412	CLA	O1D-CGD-O2D-CED
15	c5	415	CLA	O1D-CGD-O2D-CED
15	c5	417	CLA	O1D-CGD-O2D-CED
15	c6	409	CLA	O1D-CGD-O2D-CED
15	c6	418	CLA	O1D-CGD-O2D-CED
15	aA	819	CLA	CBD-CGD-O2D-CED
15	aA	820	CLA	CBD-CGD-O2D-CED
15	aA	835	CLA	CBD-CGD-O2D-CED
15	aB	809	CLA	CBD-CGD-O2D-CED
15	aB	832	CLA	CBD-CGD-O2D-CED
15	aB	839	CLA	CBD-CGD-O2D-CED
15	a1	401	CLA	CBD-CGD-O2D-CED
15	a1	406	CLA	CBD-CGD-O2D-CED
15	a2	402	CLA	CBD-CGD-O2D-CED
15	a2	408	CLA	CBD-CGD-O2D-CED
15	a3	402	CLA	CBD-CGD-O2D-CED
15	a3	407	CLA	CBD-CGD-O2D-CED
15	a4	402	CLA	CBD-CGD-O2D-CED
15	a4	407	CLA	CBD-CGD-O2D-CED
15	a5	402	CLA	CBD-CGD-O2D-CED
15	a5	407	CLA	CBD-CGD-O2D-CED
15	a6	403	CLA	CBD-CGD-O2D-CED
15	a6	408	CLA	CBD-CGD-O2D-CED
15	bA	819	CLA	CBD-CGD-O2D-CED
15	bA	820	CLA	CBD-CGD-O2D-CED
15	bA	835	CLA	CBD-CGD-O2D-CED
15	bB	809	CLA	CBD-CGD-O2D-CED
15	bB	832	CLA	CBD-CGD-O2D-CED
15	bB	839	CLA	CBD-CGD-O2D-CED
15	b1	402	CLA	CBD-CGD-O2D-CED
15	b1	407	CLA	CBD-CGD-O2D-CED
15	b2	402	CLA	CBD-CGD-O2D-CED
15	b2	408	CLA	CBD-CGD-O2D-CED
15	b3	402	CLA	CBD-CGD-O2D-CED
15	b3	407	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b4	402	CLA	CBD-CGD-O2D-CED
15	b4	407	CLA	CBD-CGD-O2D-CED
15	b5	402	CLA	CBD-CGD-O2D-CED
15	b5	407	CLA	CBD-CGD-O2D-CED
15	b6	403	CLA	CBD-CGD-O2D-CED
15	b6	408	CLA	CBD-CGD-O2D-CED
15	cA	819	CLA	CBD-CGD-O2D-CED
15	cA	820	CLA	CBD-CGD-O2D-CED
15	cA	835	CLA	CBD-CGD-O2D-CED
15	cB	809	CLA	CBD-CGD-O2D-CED
15	cB	832	CLA	CBD-CGD-O2D-CED
15	cB	839	CLA	CBD-CGD-O2D-CED
15	c1	402	CLA	CBD-CGD-O2D-CED
15	c1	407	CLA	CBD-CGD-O2D-CED
15	c2	402	CLA	CBD-CGD-O2D-CED
15	c2	408	CLA	CBD-CGD-O2D-CED
15	c3	402	CLA	CBD-CGD-O2D-CED
15	c3	407	CLA	CBD-CGD-O2D-CED
15	c4	402	CLA	CBD-CGD-O2D-CED
15	c4	407	CLA	CBD-CGD-O2D-CED
15	c5	402	CLA	CBD-CGD-O2D-CED
15	c5	407	CLA	CBD-CGD-O2D-CED
15	c6	403	CLA	CBD-CGD-O2D-CED
15	c6	408	CLA	CBD-CGD-O2D-CED
15	aA	806	CLA	O1A-CGA-O2A-C1
15	aB	817	CLA	O1A-CGA-O2A-C1
15	a3	416	CLA	O1A-CGA-O2A-C1
15	a4	416	CLA	O1A-CGA-O2A-C1
15	a5	416	CLA	O1A-CGA-O2A-C1
15	a6	417	CLA	O1A-CGA-O2A-C1
15	bA	806	CLA	O1A-CGA-O2A-C1
15	bB	817	CLA	O1A-CGA-O2A-C1
15	b1	416	CLA	O1A-CGA-O2A-C1
15	b2	417	CLA	O1A-CGA-O2A-C1
15	b3	416	CLA	O1A-CGA-O2A-C1
15	b4	416	CLA	O1A-CGA-O2A-C1
15	b5	416	CLA	O1A-CGA-O2A-C1
15	b6	417	CLA	O1A-CGA-O2A-C1
15	cA	806	CLA	O1A-CGA-O2A-C1
15	cB	817	CLA	O1A-CGA-O2A-C1
15	c1	416	CLA	O1A-CGA-O2A-C1
15	c2	417	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	416	CLA	O1A-CGA-O2A-C1
15	c4	416	CLA	O1A-CGA-O2A-C1
15	c5	416	CLA	O1A-CGA-O2A-C1
15	c6	417	CLA	O1A-CGA-O2A-C1
15	a2	409	CLA	O1D-CGD-O2D-CED
15	a2	416	CLA	O1D-CGD-O2D-CED
15	a4	408	CLA	O1D-CGD-O2D-CED
15	b1	408	CLA	O1D-CGD-O2D-CED
15	b2	409	CLA	O1D-CGD-O2D-CED
15	b4	408	CLA	O1D-CGD-O2D-CED
15	c1	415	CLA	O1D-CGD-O2D-CED
15	c2	409	CLA	O1D-CGD-O2D-CED
15	c4	408	CLA	O1D-CGD-O2D-CED
15	aB	812	CLA	O1D-CGD-O2D-CED
15	a1	414	CLA	O1D-CGD-O2D-CED
15	a3	415	CLA	O1D-CGD-O2D-CED
15	bB	812	CLA	O1D-CGD-O2D-CED
15	b1	415	CLA	O1D-CGD-O2D-CED
15	b3	415	CLA	O1D-CGD-O2D-CED
15	cB	812	CLA	O1D-CGD-O2D-CED
15	c3	415	CLA	O1D-CGD-O2D-CED
15	aB	828	CLA	O1D-CGD-O2D-CED
15	a6	406	CLA	O1D-CGD-O2D-CED
15	a6	416	CLA	O1D-CGD-O2D-CED
15	bB	828	CLA	O1D-CGD-O2D-CED
15	b6	406	CLA	O1D-CGD-O2D-CED
15	b6	416	CLA	O1D-CGD-O2D-CED
15	cB	828	CLA	O1D-CGD-O2D-CED
15	c6	406	CLA	O1D-CGD-O2D-CED
15	c6	416	CLA	O1D-CGD-O2D-CED
15	a1	415	CLA	O1A-CGA-O2A-C1
15	a2	417	CLA	O1A-CGA-O2A-C1
15	aA	841	CLA	O1D-CGD-O2D-CED
15	bA	841	CLA	O1D-CGD-O2D-CED
15	cA	841	CLA	O1D-CGD-O2D-CED
15	aA	803	CLA	C3-C5-C6-C7
15	aA	806	CLA	C3-C5-C6-C7
15	aA	809	CLA	C3-C5-C6-C7
15	aA	810	CLA	C3-C5-C6-C7
15	aB	807	CLA	C3-C5-C6-C7
15	aB	810	CLA	C3-C5-C6-C7
15	aB	811	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	828	CLA	C3-C5-C6-C7
15	aB	839	CLA	C3-C5-C6-C7
15	a1	409	CLA	C3-C5-C6-C7
15	a2	411	CLA	C3-C5-C6-C7
15	a3	410	CLA	C3-C5-C6-C7
15	a5	410	CLA	C3-C5-C6-C7
15	a6	411	CLA	C3-C5-C6-C7
15	bA	803	CLA	C3-C5-C6-C7
15	bA	806	CLA	C3-C5-C6-C7
15	bA	809	CLA	C3-C5-C6-C7
15	bA	810	CLA	C3-C5-C6-C7
15	bA	827	CLA	C3-C5-C6-C7
15	bB	807	CLA	C3-C5-C6-C7
15	bB	810	CLA	C3-C5-C6-C7
15	bB	811	CLA	C3-C5-C6-C7
15	bB	828	CLA	C3-C5-C6-C7
15	bB	839	CLA	C3-C5-C6-C7
15	b1	410	CLA	C3-C5-C6-C7
15	b2	411	CLA	C3-C5-C6-C7
15	b3	410	CLA	C3-C5-C6-C7
15	b5	410	CLA	C3-C5-C6-C7
15	b6	411	CLA	C3-C5-C6-C7
15	cA	803	CLA	C3-C5-C6-C7
15	cA	806	CLA	C3-C5-C6-C7
15	cA	809	CLA	C3-C5-C6-C7
15	cA	810	CLA	C3-C5-C6-C7
15	cA	827	CLA	C3-C5-C6-C7
15	cB	807	CLA	C3-C5-C6-C7
15	cB	810	CLA	C3-C5-C6-C7
15	cB	811	CLA	C3-C5-C6-C7
15	cB	828	CLA	C3-C5-C6-C7
15	cB	839	CLA	C3-C5-C6-C7
15	c2	411	CLA	C3-C5-C6-C7
15	c3	410	CLA	C3-C5-C6-C7
15	c5	410	CLA	C3-C5-C6-C7
15	c6	411	CLA	C3-C5-C6-C7
15	aA	806	CLA	CBA-CGA-O2A-C1
15	aA	840	CLA	CBA-CGA-O2A-C1
15	aB	817	CLA	CBA-CGA-O2A-C1
15	bA	806	CLA	CBA-CGA-O2A-C1
15	bA	840	CLA	CBA-CGA-O2A-C1
15	bB	817	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	806	CLA	CBA-CGA-O2A-C1
15	cA	840	CLA	CBA-CGA-O2A-C1
15	cB	817	CLA	CBA-CGA-O2A-C1
15	a2	405	CLA	O1D-CGD-O2D-CED
15	a4	404	CLA	O1D-CGD-O2D-CED
15	b2	405	CLA	O1D-CGD-O2D-CED
15	c2	405	CLA	O1D-CGD-O2D-CED
15	c4	405	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	CBD-CGD-O2D-CED
15	bA	825	CLA	CBD-CGD-O2D-CED
15	cA	825	CLA	CBD-CGD-O2D-CED
15	cB	837	CLA	CBD-CGD-O2D-CED
15	b5	405	CLA	O1D-CGD-O2D-CED
15	aA	843	CLA	C4-C3-C5-C6
15	a1	416	CLA	C4-C3-C5-C6
15	a5	417	CLA	C4-C3-C5-C6
15	bA	843	CLA	C4-C3-C5-C6
15	b1	417	CLA	C4-C3-C5-C6
15	b5	417	CLA	C4-C3-C5-C6
15	cA	842	CLA	C4-C3-C5-C6
15	c1	417	CLA	C4-C3-C5-C6
15	aB	801	CLA	C2-C3-C5-C6
15	bB	801	CLA	C2-C3-C5-C6
15	cB	801	CLA	C2-C3-C5-C6
15	aB	820	CLA	CBD-CGD-O2D-CED
15	aB	837	CLA	CBD-CGD-O2D-CED
15	bB	820	CLA	CBD-CGD-O2D-CED
15	bB	837	CLA	CBD-CGD-O2D-CED
15	cB	820	CLA	CBD-CGD-O2D-CED
15	aA	802	CLA	C2A-CAA-CBA-CGA
15	aA	830	CLA	C2A-CAA-CBA-CGA
15	aA	832	CLA	C2A-CAA-CBA-CGA
15	aA	845	CLA	C2A-CAA-CBA-CGA
15	aB	801	CLA	C2A-CAA-CBA-CGA
15	aB	803	CLA	C2A-CAA-CBA-CGA
15	aB	825	CLA	C2A-CAA-CBA-CGA
15	aB	828	CLA	C2A-CAA-CBA-CGA
15	aB	839	CLA	C2A-CAA-CBA-CGA
15	a1	401	CLA	C2A-CAA-CBA-CGA
15	a1	422	CLA	C2A-CAA-CBA-CGA
15	a2	402	CLA	C2A-CAA-CBA-CGA
15	a3	402	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a4	402	CLA	C2A-CAA-CBA-CGA
15	a5	402	CLA	C2A-CAA-CBA-CGA
15	a6	403	CLA	C2A-CAA-CBA-CGA
15	bA	802	CLA	C2A-CAA-CBA-CGA
15	bA	830	CLA	C2A-CAA-CBA-CGA
15	bA	832	CLA	C2A-CAA-CBA-CGA
15	bA	845	CLA	C2A-CAA-CBA-CGA
15	bB	801	CLA	C2A-CAA-CBA-CGA
15	bB	803	CLA	C2A-CAA-CBA-CGA
15	bB	825	CLA	C2A-CAA-CBA-CGA
15	bB	828	CLA	C2A-CAA-CBA-CGA
15	bB	839	CLA	C2A-CAA-CBA-CGA
15	b1	402	CLA	C2A-CAA-CBA-CGA
15	b2	402	CLA	C2A-CAA-CBA-CGA
15	b3	402	CLA	C2A-CAA-CBA-CGA
15	b4	402	CLA	C2A-CAA-CBA-CGA
15	b5	402	CLA	C2A-CAA-CBA-CGA
15	b6	403	CLA	C2A-CAA-CBA-CGA
15	b6	422	CLA	C2A-CAA-CBA-CGA
15	cA	802	CLA	C2A-CAA-CBA-CGA
15	cA	830	CLA	C2A-CAA-CBA-CGA
15	cA	832	CLA	C2A-CAA-CBA-CGA
15	cA	844	CLA	C2A-CAA-CBA-CGA
15	cB	801	CLA	C2A-CAA-CBA-CGA
15	cB	803	CLA	C2A-CAA-CBA-CGA
15	cB	825	CLA	C2A-CAA-CBA-CGA
15	cB	828	CLA	C2A-CAA-CBA-CGA
15	cB	839	CLA	C2A-CAA-CBA-CGA
15	c1	402	CLA	C2A-CAA-CBA-CGA
15	c2	402	CLA	C2A-CAA-CBA-CGA
15	c3	402	CLA	C2A-CAA-CBA-CGA
15	c4	402	CLA	C2A-CAA-CBA-CGA
15	c5	402	CLA	C2A-CAA-CBA-CGA
15	c6	403	CLA	C2A-CAA-CBA-CGA
15	aA	820	CLA	O1A-CGA-O2A-C1
15	bA	820	CLA	O1A-CGA-O2A-C1
15	cA	820	CLA	O1A-CGA-O2A-C1
15	a5	405	CLA	O1D-CGD-O2D-CED
15	b4	405	CLA	O1D-CGD-O2D-CED
15	c5	405	CLA	O1D-CGD-O2D-CED
15	aA	813	CLA	C3-C5-C6-C7
15	aA	827	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	809	CLA	C3-C5-C6-C7
15	aB	817	CLA	C3-C5-C6-C7
15	a4	410	CLA	C3-C5-C6-C7
15	bA	813	CLA	C3-C5-C6-C7
15	bB	809	CLA	C3-C5-C6-C7
15	bB	817	CLA	C3-C5-C6-C7
15	b4	410	CLA	C3-C5-C6-C7
15	cA	813	CLA	C3-C5-C6-C7
15	cB	809	CLA	C3-C5-C6-C7
15	cB	817	CLA	C3-C5-C6-C7
15	c1	410	CLA	C3-C5-C6-C7
15	c4	410	CLA	C3-C5-C6-C7
15	aA	809	CLA	CBA-CGA-O2A-C1
15	aA	820	CLA	CBA-CGA-O2A-C1
15	aA	836	CLA	CBA-CGA-O2A-C1
15	aB	819	CLA	CBA-CGA-O2A-C1
15	aB	821	CLA	CBA-CGA-O2A-C1
15	aL	201	CLA	CBA-CGA-O2A-C1
15	a1	415	CLA	CBA-CGA-O2A-C1
15	a2	417	CLA	CBA-CGA-O2A-C1
15	a3	416	CLA	CBA-CGA-O2A-C1
15	a4	416	CLA	CBA-CGA-O2A-C1
15	a5	416	CLA	CBA-CGA-O2A-C1
15	a6	417	CLA	CBA-CGA-O2A-C1
15	bA	809	CLA	CBA-CGA-O2A-C1
15	bA	820	CLA	CBA-CGA-O2A-C1
15	bA	836	CLA	CBA-CGA-O2A-C1
15	bB	819	CLA	CBA-CGA-O2A-C1
15	bB	821	CLA	CBA-CGA-O2A-C1
15	bL	202	CLA	CBA-CGA-O2A-C1
15	b1	416	CLA	CBA-CGA-O2A-C1
15	b2	417	CLA	CBA-CGA-O2A-C1
15	b3	416	CLA	CBA-CGA-O2A-C1
15	b4	416	CLA	CBA-CGA-O2A-C1
15	b5	416	CLA	CBA-CGA-O2A-C1
15	b6	417	CLA	CBA-CGA-O2A-C1
15	cA	809	CLA	CBA-CGA-O2A-C1
15	cA	820	CLA	CBA-CGA-O2A-C1
15	cA	836	CLA	CBA-CGA-O2A-C1
15	cB	819	CLA	CBA-CGA-O2A-C1
15	cB	821	CLA	CBA-CGA-O2A-C1
15	cL	201	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	416	CLA	CBA-CGA-O2A-C1
15	c2	417	CLA	CBA-CGA-O2A-C1
15	c3	416	CLA	CBA-CGA-O2A-C1
15	c4	416	CLA	CBA-CGA-O2A-C1
15	c5	416	CLA	CBA-CGA-O2A-C1
15	c6	417	CLA	CBA-CGA-O2A-C1
15	aA	829	CLA	O1D-CGD-O2D-CED
15	a4	405	CLA	O1D-CGD-O2D-CED
15	bA	829	CLA	O1D-CGD-O2D-CED
15	b4	404	CLA	O1D-CGD-O2D-CED
15	b6	405	CLA	O1D-CGD-O2D-CED
15	c4	404	CLA	O1D-CGD-O2D-CED
15	aA	840	CLA	O1D-CGD-O2D-CED
15	aB	840	CLA	O1D-CGD-O2D-CED
15	a1	402	CLA	O1D-CGD-O2D-CED
15	a1	403	CLA	O1D-CGD-O2D-CED
15	a4	403	CLA	O1D-CGD-O2D-CED
15	a5	404	CLA	O1D-CGD-O2D-CED
15	a6	405	CLA	O1D-CGD-O2D-CED
15	bA	840	CLA	O1D-CGD-O2D-CED
15	bB	840	CLA	O1D-CGD-O2D-CED
15	b1	404	CLA	O1D-CGD-O2D-CED
15	b1	405	CLA	O1D-CGD-O2D-CED
15	b3	404	CLA	O1D-CGD-O2D-CED
15	b3	405	CLA	O1D-CGD-O2D-CED
15	cA	829	CLA	O1D-CGD-O2D-CED
15	cA	840	CLA	O1D-CGD-O2D-CED
15	cB	840	CLA	O1D-CGD-O2D-CED
15	c1	404	CLA	O1D-CGD-O2D-CED
15	c1	405	CLA	O1D-CGD-O2D-CED
15	c3	404	CLA	O1D-CGD-O2D-CED
15	c3	405	CLA	O1D-CGD-O2D-CED
15	c5	404	CLA	O1D-CGD-O2D-CED
15	c6	405	CLA	O1D-CGD-O2D-CED
15	aA	813	CLA	O1A-CGA-O2A-C1
15	aA	838	CLA	O1A-CGA-O2A-C1
15	aB	819	CLA	O1A-CGA-O2A-C1
15	aL	201	CLA	O1A-CGA-O2A-C1
15	bA	813	CLA	O1A-CGA-O2A-C1
15	bA	838	CLA	O1A-CGA-O2A-C1
15	bB	819	CLA	O1A-CGA-O2A-C1
15	bL	202	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	813	CLA	O1A-CGA-O2A-C1
15	cA	838	CLA	O1A-CGA-O2A-C1
15	cB	819	CLA	O1A-CGA-O2A-C1
15	cL	201	CLA	O1A-CGA-O2A-C1
15	a1	404	CLA	O1D-CGD-O2D-CED
15	a2	404	CLA	O1D-CGD-O2D-CED
15	a3	404	CLA	O1D-CGD-O2D-CED
15	a3	405	CLA	O1D-CGD-O2D-CED
15	b2	404	CLA	O1D-CGD-O2D-CED
15	b5	403	CLA	O1D-CGD-O2D-CED
15	b5	404	CLA	O1D-CGD-O2D-CED
15	c2	404	CLA	O1D-CGD-O2D-CED
18	aJ	204	BCR	C9-C10-C11-C12
18	a1	420	BCR	C19-C20-C21-C22
18	a1	421	BCR	C9-C10-C11-C12
18	a2	401	BCR	C9-C10-C11-C12
18	a2	420	BCR	C19-C20-C21-C22
18	a3	401	BCR	C9-C10-C11-C12
18	a4	419	BCR	C19-C20-C21-C22
18	a6	402	BCR	C9-C10-C11-C12
18	bJ	103	BCR	C9-C10-C11-C12
18	b2	401	BCR	C9-C10-C11-C12
18	b2	420	BCR	C19-C20-C21-C22
18	b3	401	BCR	C9-C10-C11-C12
18	b4	419	BCR	C19-C20-C21-C22
18	b6	402	BCR	C9-C10-C11-C12
18	cJ	103	BCR	C9-C10-C11-C12
18	c1	401	BCR	C19-C20-C21-C22
18	c2	401	BCR	C9-C10-C11-C12
18	c2	420	BCR	C19-C20-C21-C22
18	c3	401	BCR	C9-C10-C11-C12
18	c4	419	BCR	C19-C20-C21-C22
18	c6	402	BCR	C9-C10-C11-C12
15	aA	805	CLA	CBD-CGD-O2D-CED
15	aA	830	CLA	CBD-CGD-O2D-CED
15	aB	814	CLA	CBD-CGD-O2D-CED
15	a1	408	CLA	CBD-CGD-O2D-CED
15	a2	410	CLA	CBD-CGD-O2D-CED
15	a6	410	CLA	CBD-CGD-O2D-CED
15	bA	805	CLA	CBD-CGD-O2D-CED
15	bA	830	CLA	CBD-CGD-O2D-CED
15	bB	814	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b1	409	CLA	CBD-CGD-O2D-CED
15	b2	410	CLA	CBD-CGD-O2D-CED
15	b6	410	CLA	CBD-CGD-O2D-CED
15	cA	805	CLA	CBD-CGD-O2D-CED
15	cA	830	CLA	CBD-CGD-O2D-CED
15	cB	814	CLA	CBD-CGD-O2D-CED
15	c1	409	CLA	CBD-CGD-O2D-CED
15	c2	410	CLA	CBD-CGD-O2D-CED
15	c4	409	CLA	CBD-CGD-O2D-CED
15	aA	838	CLA	O1D-CGD-O2D-CED
15	aB	816	CLA	O1D-CGD-O2D-CED
15	aB	821	CLA	O1D-CGD-O2D-CED
15	a5	403	CLA	O1D-CGD-O2D-CED
15	a6	404	CLA	O1D-CGD-O2D-CED
15	bA	838	CLA	O1D-CGD-O2D-CED
15	bB	816	CLA	O1D-CGD-O2D-CED
15	bB	821	CLA	O1D-CGD-O2D-CED
15	b1	403	CLA	O1D-CGD-O2D-CED
15	b4	403	CLA	O1D-CGD-O2D-CED
15	b6	404	CLA	O1D-CGD-O2D-CED
15	cA	838	CLA	O1D-CGD-O2D-CED
15	cB	816	CLA	O1D-CGD-O2D-CED
15	cB	821	CLA	O1D-CGD-O2D-CED
15	c1	403	CLA	O1D-CGD-O2D-CED
15	c4	403	CLA	O1D-CGD-O2D-CED
15	c5	403	CLA	O1D-CGD-O2D-CED
15	c6	404	CLA	O1D-CGD-O2D-CED
19	aA	854	LHG	O2-C2-C3-O3
19	bA	855	LHG	O2-C2-C3-O3
19	cA	853	LHG	O2-C2-C3-O3
15	aA	802	CLA	C3-C5-C6-C7
15	bA	802	CLA	C3-C5-C6-C7
15	bA	836	CLA	C3-C5-C6-C7
15	cA	802	CLA	C3-C5-C6-C7
15	aA	813	CLA	CBA-CGA-O2A-C1
15	aA	838	CLA	CBA-CGA-O2A-C1
15	bA	813	CLA	CBA-CGA-O2A-C1
15	bA	838	CLA	CBA-CGA-O2A-C1
15	cA	813	CLA	CBA-CGA-O2A-C1
15	cA	838	CLA	CBA-CGA-O2A-C1
15	aA	836	CLA	O1A-CGA-O2A-C1
15	aA	840	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	821	CLA	O1A-CGA-O2A-C1
15	bA	836	CLA	O1A-CGA-O2A-C1
15	bA	840	CLA	O1A-CGA-O2A-C1
15	cA	836	CLA	O1A-CGA-O2A-C1
15	cA	840	CLA	O1A-CGA-O2A-C1
15	aA	845	CLA	O1D-CGD-O2D-CED
15	a3	403	CLA	O1D-CGD-O2D-CED
15	bA	845	CLA	O1D-CGD-O2D-CED
15	cA	844	CLA	O1D-CGD-O2D-CED
15	c2	403	CLA	O1D-CGD-O2D-CED
15	aL	203	CLA	CBD-CGD-O2D-CED
15	a4	409	CLA	CBD-CGD-O2D-CED
15	bL	204	CLA	CBD-CGD-O2D-CED
15	b4	409	CLA	CBD-CGD-O2D-CED
15	b5	409	CLA	CBD-CGD-O2D-CED
15	cL	203	CLA	CBD-CGD-O2D-CED
15	c6	410	CLA	CBD-CGD-O2D-CED
15	b3	403	CLA	O1D-CGD-O2D-CED
15	c3	403	CLA	O1D-CGD-O2D-CED
15	bB	821	CLA	O1A-CGA-O2A-C1
15	cB	821	CLA	O1A-CGA-O2A-C1
15	aA	802	CLA	O1D-CGD-O2D-CED
15	aA	812	CLA	O1D-CGD-O2D-CED
15	aA	835	CLA	O1D-CGD-O2D-CED
15	a2	403	CLA	O1D-CGD-O2D-CED
15	bA	802	CLA	O1D-CGD-O2D-CED
15	bA	812	CLA	O1D-CGD-O2D-CED
15	cA	802	CLA	O1D-CGD-O2D-CED
15	cA	812	CLA	O1D-CGD-O2D-CED
15	cA	835	CLA	O1D-CGD-O2D-CED
15	aB	807	CLA	CBD-CGD-O2D-CED
15	bB	807	CLA	CBD-CGD-O2D-CED
15	cB	807	CLA	CBD-CGD-O2D-CED
15	aA	826	CLA	C3-C5-C6-C7
15	aA	836	CLA	C3-C5-C6-C7
15	aB	833	CLA	C3-C5-C6-C7
15	bA	826	CLA	C3-C5-C6-C7
15	bB	833	CLA	C3-C5-C6-C7
15	cA	826	CLA	C3-C5-C6-C7
15	cA	836	CLA	C3-C5-C6-C7
15	cB	833	CLA	C3-C5-C6-C7
15	bA	835	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	814	CLA	C2C-C3C-CAC-CBC
15	cB	814	CLA	C2C-C3C-CAC-CBC
15	aA	809	CLA	O1A-CGA-O2A-C1
15	bB	814	CLA	C2C-C3C-CAC-CBC
20	aB	850	LMG	O6-C5-C6-O5
20	bB	851	LMG	O6-C5-C6-O5
20	cB	850	LMG	O6-C5-C6-O5
15	aA	818	CLA	C4-C3-C5-C6
15	aB	819	CLA	C4-C3-C5-C6
15	bA	818	CLA	C4-C3-C5-C6
15	bB	819	CLA	C4-C3-C5-C6
15	b4	417	CLA	C4-C3-C5-C6
15	cA	818	CLA	C4-C3-C5-C6
15	cB	819	CLA	C4-C3-C5-C6
15	c5	417	CLA	C4-C3-C5-C6
15	aA	818	CLA	C2-C3-C5-C6
15	aB	819	CLA	C2-C3-C5-C6
15	bA	818	CLA	C2-C3-C5-C6
15	bB	819	CLA	C2-C3-C5-C6
15	cA	818	CLA	C2-C3-C5-C6
15	cB	819	CLA	C2-C3-C5-C6
15	aA	844	CLA	C2A-CAA-CBA-CGA
15	aB	832	CLA	C2A-CAA-CBA-CGA
15	bA	844	CLA	C2A-CAA-CBA-CGA
15	bB	832	CLA	C2A-CAA-CBA-CGA
15	cA	843	CLA	C2A-CAA-CBA-CGA
15	cB	832	CLA	C2A-CAA-CBA-CGA
15	aB	809	CLA	O1D-CGD-O2D-CED
15	bB	809	CLA	O1D-CGD-O2D-CED
15	b2	403	CLA	O1D-CGD-O2D-CED
15	cB	809	CLA	O1D-CGD-O2D-CED
15	bA	809	CLA	O1A-CGA-O2A-C1
15	cA	809	CLA	O1A-CGA-O2A-C1
20	aB	850	LMG	O6-C1-O1-C7
20	bB	851	LMG	O6-C1-O1-C7
20	cB	850	LMG	O6-C1-O1-C7
15	aB	801	CLA	CBA-CGA-O2A-C1
15	a3	417	CLA	CBA-CGA-O2A-C1
15	bB	801	CLA	CBA-CGA-O2A-C1
15	b3	417	CLA	CBA-CGA-O2A-C1
15	cB	801	CLA	CBA-CGA-O2A-C1
15	aA	809	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	834	CLA	CBD-CGD-O2D-CED
15	bA	809	CLA	CBD-CGD-O2D-CED
15	b2	411	CLA	CBD-CGD-O2D-CED
15	cA	809	CLA	CBD-CGD-O2D-CED
15	cA	834	CLA	CBD-CGD-O2D-CED
15	c5	409	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	O1D-CGD-O2D-CED
15	bB	803	CLA	O1D-CGD-O2D-CED
15	cB	803	CLA	O1D-CGD-O2D-CED
15	aB	836	CLA	O1D-CGD-O2D-CED
15	a4	402	CLA	O1D-CGD-O2D-CED
15	a6	403	CLA	O1D-CGD-O2D-CED
15	bB	836	CLA	O1D-CGD-O2D-CED
15	b4	402	CLA	O1D-CGD-O2D-CED
15	b6	403	CLA	O1D-CGD-O2D-CED
15	cB	836	CLA	O1D-CGD-O2D-CED
15	c2	402	CLA	O1D-CGD-O2D-CED
15	c4	402	CLA	O1D-CGD-O2D-CED
15	c6	403	CLA	O1D-CGD-O2D-CED
15	aA	822	CLA	CBD-CGD-O2D-CED
15	a2	411	CLA	CBD-CGD-O2D-CED
15	a5	409	CLA	CBD-CGD-O2D-CED
15	bA	822	CLA	CBD-CGD-O2D-CED
15	bA	834	CLA	CBD-CGD-O2D-CED
15	cA	822	CLA	CBD-CGD-O2D-CED
15	b2	402	CLA	O1D-CGD-O2D-CED
15	b5	402	CLA	O1D-CGD-O2D-CED
15	c5	402	CLA	O1D-CGD-O2D-CED
19	aX	101	LHG	C1-C2-C3-O3
19	bX	101	LHG	C1-C2-C3-O3
19	cX	101	LHG	C1-C2-C3-O3
15	aB	801	CLA	O1A-CGA-O2A-C1
15	a3	417	CLA	O1A-CGA-O2A-C1
15	bB	801	CLA	O1A-CGA-O2A-C1
15	b3	417	CLA	O1A-CGA-O2A-C1
15	cB	801	CLA	O1A-CGA-O2A-C1
15	a5	402	CLA	O1D-CGD-O2D-CED
15	a5	407	CLA	O1D-CGD-O2D-CED
15	b5	407	CLA	O1D-CGD-O2D-CED
15	c5	407	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	CBA-CGA-O2A-C1
15	aA	833	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	832	CLA	CBA-CGA-O2A-C1
15	a1	416	CLA	CBA-CGA-O2A-C1
15	a2	418	CLA	CBA-CGA-O2A-C1
15	a4	417	CLA	CBA-CGA-O2A-C1
15	a5	417	CLA	CBA-CGA-O2A-C1
15	a6	418	CLA	CBA-CGA-O2A-C1
15	bA	825	CLA	CBA-CGA-O2A-C1
15	bA	833	CLA	CBA-CGA-O2A-C1
15	bB	832	CLA	CBA-CGA-O2A-C1
15	b1	417	CLA	CBA-CGA-O2A-C1
15	b2	418	CLA	CBA-CGA-O2A-C1
15	b4	417	CLA	CBA-CGA-O2A-C1
15	b5	417	CLA	CBA-CGA-O2A-C1
15	b6	418	CLA	CBA-CGA-O2A-C1
15	cA	825	CLA	CBA-CGA-O2A-C1
15	cA	833	CLA	CBA-CGA-O2A-C1
15	cB	832	CLA	CBA-CGA-O2A-C1
15	c1	417	CLA	CBA-CGA-O2A-C1
15	c2	418	CLA	CBA-CGA-O2A-C1
15	c3	417	CLA	CBA-CGA-O2A-C1
15	c4	417	CLA	CBA-CGA-O2A-C1
15	c5	417	CLA	CBA-CGA-O2A-C1
15	c6	418	CLA	CBA-CGA-O2A-C1
18	a6	421	BCR	C9-C10-C11-C12
18	b6	421	BCR	C9-C10-C11-C12
15	aB	807	CLA	C8-C10-C11-C12
15	bB	807	CLA	C8-C10-C11-C12
20	aB	850	LMG	C4-C5-C6-O5
20	bB	851	LMG	C4-C5-C6-O5
20	cB	850	LMG	C4-C5-C6-O5
15	aA	802	CLA	C10-C11-C12-C13
15	aA	821	CLA	C5-C6-C7-C8
15	aB	814	CLA	C8-C10-C11-C12
15	bA	802	CLA	C10-C11-C12-C13
15	bA	821	CLA	C5-C6-C7-C8
15	bB	814	CLA	C8-C10-C11-C12
15	cA	802	CLA	C10-C11-C12-C13
15	cA	821	CLA	C5-C6-C7-C8
15	cB	807	CLA	C8-C10-C11-C12
15	cB	814	CLA	C8-C10-C11-C12
15	aA	845	CLA	C3-C5-C6-C7
15	bA	845	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	844	CLA	C3-C5-C6-C7
15	aA	833	CLA	O1A-CGA-O2A-C1
15	a2	418	CLA	O1A-CGA-O2A-C1
15	a6	418	CLA	O1A-CGA-O2A-C1
15	bA	833	CLA	O1A-CGA-O2A-C1
15	b2	418	CLA	O1A-CGA-O2A-C1
15	b6	418	CLA	O1A-CGA-O2A-C1
15	cA	833	CLA	O1A-CGA-O2A-C1
15	c2	418	CLA	O1A-CGA-O2A-C1
15	c3	417	CLA	O1A-CGA-O2A-C1
15	c6	418	CLA	O1A-CGA-O2A-C1
15	aB	827	CLA	C4-C3-C5-C6
15	a3	417	CLA	C4-C3-C5-C6
15	a4	417	CLA	C4-C3-C5-C6
15	a6	418	CLA	C4-C3-C5-C6
15	bB	827	CLA	C4-C3-C5-C6
15	b2	418	CLA	C4-C3-C5-C6
15	b6	418	CLA	C4-C3-C5-C6
15	cB	827	CLA	C4-C3-C5-C6
15	c2	418	CLA	C4-C3-C5-C6
15	c3	417	CLA	C4-C3-C5-C6
15	c4	417	CLA	C4-C3-C5-C6
15	c6	418	CLA	C4-C3-C5-C6
15	aA	843	CLA	C2-C3-C5-C6
15	bA	843	CLA	C2-C3-C5-C6
15	b1	417	CLA	C2-C3-C5-C6
15	cA	842	CLA	C2-C3-C5-C6
15	aA	804	CLA	C11-C12-C13-C14
15	aA	806	CLA	C6-C7-C8-C9
15	aA	807	CLA	C6-C7-C8-C9
15	aA	812	CLA	C14-C13-C15-C16
15	aA	821	CLA	C11-C12-C13-C14
15	aA	828	CLA	C6-C7-C8-C9
15	aA	834	CLA	C6-C7-C8-C9
15	aA	843	CLA	C11-C10-C8-C9
15	aB	807	CLA	C14-C13-C15-C16
15	aB	819	CLA	C6-C7-C8-C9
15	a1	402	CLA	C6-C7-C8-C9
15	a2	403	CLA	C6-C7-C8-C9
15	a2	422	CLA	C11-C12-C13-C14
15	a3	403	CLA	C6-C7-C8-C9
15	a3	421	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a4	403	CLA	C6-C7-C8-C9
15	a4	421	CLA	C11-C12-C13-C14
15	a5	403	CLA	C6-C7-C8-C9
15	a5	420	CLA	C11-C12-C13-C14
15	a6	404	CLA	C6-C7-C8-C9
15	a6	422	CLA	C11-C12-C13-C14
15	bA	804	CLA	C11-C12-C13-C14
15	bA	806	CLA	C6-C7-C8-C9
15	bA	807	CLA	C6-C7-C8-C9
15	bA	812	CLA	C14-C13-C15-C16
15	bA	821	CLA	C11-C12-C13-C14
15	bA	828	CLA	C6-C7-C8-C9
15	bA	834	CLA	C6-C7-C8-C9
15	bA	843	CLA	C11-C10-C8-C9
15	bB	807	CLA	C14-C13-C15-C16
15	bB	819	CLA	C6-C7-C8-C9
15	b1	403	CLA	C6-C7-C8-C9
15	b2	403	CLA	C6-C7-C8-C9
15	b2	422	CLA	C11-C12-C13-C14
15	b3	403	CLA	C6-C7-C8-C9
15	b3	421	CLA	C11-C12-C13-C14
15	b4	403	CLA	C6-C7-C8-C9
15	b4	421	CLA	C11-C12-C13-C14
15	b5	403	CLA	C6-C7-C8-C9
15	b5	420	CLA	C11-C12-C13-C14
15	b6	404	CLA	C6-C7-C8-C9
15	b6	422	CLA	C11-C12-C13-C14
15	cA	804	CLA	C11-C12-C13-C14
15	cA	806	CLA	C6-C7-C8-C9
15	cA	807	CLA	C6-C7-C8-C9
15	cA	812	CLA	C14-C13-C15-C16
15	cA	821	CLA	C11-C12-C13-C14
15	cA	828	CLA	C6-C7-C8-C9
15	cA	834	CLA	C6-C7-C8-C9
15	cA	842	CLA	C11-C10-C8-C9
15	cB	807	CLA	C14-C13-C15-C16
15	cB	819	CLA	C6-C7-C8-C9
15	c1	403	CLA	C6-C7-C8-C9
15	c2	403	CLA	C6-C7-C8-C9
15	c2	422	CLA	C11-C12-C13-C14
15	c3	403	CLA	C6-C7-C8-C9
15	c3	421	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	403	CLA	C6-C7-C8-C9
15	c5	403	CLA	C6-C7-C8-C9
15	c5	420	CLA	C11-C12-C13-C14
15	c6	404	CLA	C6-C7-C8-C9
15	aB	832	CLA	O1D-CGD-O2D-CED
15	aB	839	CLA	O1D-CGD-O2D-CED
15	a2	402	CLA	O1D-CGD-O2D-CED
15	a3	402	CLA	O1D-CGD-O2D-CED
15	a6	408	CLA	O1D-CGD-O2D-CED
15	bB	832	CLA	O1D-CGD-O2D-CED
15	bB	839	CLA	O1D-CGD-O2D-CED
15	b1	402	CLA	O1D-CGD-O2D-CED
15	b3	402	CLA	O1D-CGD-O2D-CED
15	b3	407	CLA	O1D-CGD-O2D-CED
15	b6	408	CLA	O1D-CGD-O2D-CED
15	cB	832	CLA	O1D-CGD-O2D-CED
15	cB	839	CLA	O1D-CGD-O2D-CED
15	c3	402	CLA	O1D-CGD-O2D-CED
15	c3	407	CLA	O1D-CGD-O2D-CED
15	c6	408	CLA	O1D-CGD-O2D-CED
15	aA	814	CLA	CBD-CGD-O2D-CED
15	b3	409	CLA	CBD-CGD-O2D-CED
15	cA	814	CLA	CBD-CGD-O2D-CED
18	aA	852	BCR	C7-C8-C9-C34
18	aA	852	BCR	C37-C22-C23-C24
18	aB	844	BCR	C7-C8-C9-C34
18	aI	102	BCR	C7-C8-C9-C34
18	aI	102	BCR	C11-C12-C13-C35
18	a1	417	BCR	C7-C8-C9-C34
18	a1	421	BCR	C7-C8-C9-C34
18	a2	419	BCR	C7-C8-C9-C34
18	a2	420	BCR	C7-C8-C9-C34
18	a2	421	BCR	C11-C12-C13-C35
18	a3	418	BCR	C7-C8-C9-C34
18	a3	419	BCR	C7-C8-C9-C34
18	a4	418	BCR	C7-C8-C9-C34
18	a4	419	BCR	C7-C8-C9-C34
18	a5	418	BCR	C7-C8-C9-C34
18	a6	402	BCR	C11-C12-C13-C35
18	a6	419	BCR	C7-C8-C9-C34
18	bA	853	BCR	C7-C8-C9-C34
18	bA	853	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bB	844	BCR	C7-C8-C9-C34
18	bI	102	BCR	C7-C8-C9-C34
18	bI	102	BCR	C11-C12-C13-C35
18	b1	418	BCR	C7-C8-C9-C34
18	b2	419	BCR	C7-C8-C9-C34
18	b2	420	BCR	C7-C8-C9-C34
18	b2	421	BCR	C11-C12-C13-C35
18	b3	418	BCR	C7-C8-C9-C34
18	b3	419	BCR	C7-C8-C9-C34
18	b4	418	BCR	C7-C8-C9-C34
18	b4	419	BCR	C7-C8-C9-C34
18	b5	418	BCR	C7-C8-C9-C34
18	b6	419	BCR	C7-C8-C9-C34
18	cA	851	BCR	C7-C8-C9-C34
18	cA	851	BCR	C37-C22-C23-C24
18	cB	844	BCR	C7-C8-C9-C34
18	cI	102	BCR	C7-C8-C9-C34
18	cI	102	BCR	C11-C12-C13-C35
18	c1	418	BCR	C7-C8-C9-C34
18	c1	419	BCR	C7-C8-C9-C34
18	c2	419	BCR	C7-C8-C9-C34
18	c2	420	BCR	C7-C8-C9-C34
18	c2	421	BCR	C11-C12-C13-C35
18	c3	418	BCR	C7-C8-C9-C34
18	c3	419	BCR	C7-C8-C9-C34
18	c4	418	BCR	C7-C8-C9-C34
18	c4	419	BCR	C7-C8-C9-C34
18	c5	418	BCR	C7-C8-C9-C34
18	c6	402	BCR	C11-C12-C13-C35
18	c6	419	BCR	C7-C8-C9-C34
18	aB	844	BCR	C21-C22-C23-C24
18	aI	103	BCR	C7-C8-C9-C10
18	aI	103	BCR	C21-C22-C23-C24
18	aL	205	BCR	C7-C8-C9-C10
18	a1	418	BCR	C7-C8-C9-C10
18	a3	419	BCR	C7-C8-C9-C10
18	a4	419	BCR	C7-C8-C9-C10
18	bB	844	BCR	C21-C22-C23-C24
18	bL	201	BCR	C7-C8-C9-C10
18	bL	205	BCR	C7-C8-C9-C10
18	bL	205	BCR	C21-C22-C23-C24
18	bL	206	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b1	401	BCR	C7-C8-C9-C10
18	b1	419	BCR	C7-C8-C9-C10
18	b3	419	BCR	C7-C8-C9-C10
18	b4	419	BCR	C7-C8-C9-C10
18	cB	844	BCR	C21-C22-C23-C24
18	cL	204	BCR	C7-C8-C9-C10
18	cL	204	BCR	C21-C22-C23-C24
18	c1	401	BCR	C7-C8-C9-C10
18	c1	419	BCR	C7-C8-C9-C10
18	c3	419	BCR	C7-C8-C9-C10
18	c4	419	BCR	C7-C8-C9-C10
15	bA	819	CLA	O1D-CGD-O2D-CED
15	c1	402	CLA	O1D-CGD-O2D-CED
15	a4	417	CLA	O1A-CGA-O2A-C1
15	a5	417	CLA	O1A-CGA-O2A-C1
15	b4	417	CLA	O1A-CGA-O2A-C1
15	b5	417	CLA	O1A-CGA-O2A-C1
15	c4	417	CLA	O1A-CGA-O2A-C1
15	c5	417	CLA	O1A-CGA-O2A-C1
15	aA	828	CLA	C10-C11-C12-C13
15	aA	843	CLA	C10-C11-C12-C13
15	bA	828	CLA	C10-C11-C12-C13
15	bA	843	CLA	C10-C11-C12-C13
15	cA	828	CLA	C10-C11-C12-C13
15	cA	842	CLA	C10-C11-C12-C13
15	aA	819	CLA	O1D-CGD-O2D-CED
15	cA	819	CLA	O1D-CGD-O2D-CED
15	c4	407	CLA	O1D-CGD-O2D-CED
15	a3	409	CLA	CBD-CGD-O2D-CED
15	bA	814	CLA	CBD-CGD-O2D-CED
15	bB	826	CLA	CBD-CGD-O2D-CED
15	cB	826	CLA	CBD-CGD-O2D-CED
15	c2	411	CLA	CBD-CGD-O2D-CED
15	a4	407	CLA	O1D-CGD-O2D-CED
15	b4	407	CLA	O1D-CGD-O2D-CED
15	aA	828	CLA	C3-C5-C6-C7
15	aA	839	CLA	C3-C5-C6-C7
15	bA	828	CLA	C3-C5-C6-C7
15	bA	839	CLA	C3-C5-C6-C7
15	cA	828	CLA	C3-C5-C6-C7
15	cA	839	CLA	C3-C5-C6-C7
14	aA	801	CL0	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	bA	801	CL0	C8-C10-C11-C12
14	cA	801	CL0	C8-C10-C11-C12
15	aB	804	CLA	C10-C11-C12-C13
15	aB	814	CLA	C10-C11-C12-C13
15	aB	836	CLA	C8-C10-C11-C12
15	bB	804	CLA	C10-C11-C12-C13
15	bB	814	CLA	C10-C11-C12-C13
15	bB	819	CLA	C5-C6-C7-C8
15	bB	836	CLA	C8-C10-C11-C12
15	cA	829	CLA	C15-C16-C17-C18
15	cB	804	CLA	C10-C11-C12-C13
15	cB	814	CLA	C10-C11-C12-C13
15	cB	819	CLA	C5-C6-C7-C8
15	a1	401	CLA	O1D-CGD-O2D-CED
15	a3	407	CLA	O1D-CGD-O2D-CED
15	b1	407	CLA	O1D-CGD-O2D-CED
15	aB	826	CLA	CBD-CGD-O2D-CED
15	c2	408	CLA	O1D-CGD-O2D-CED
15	aA	804	CLA	C10-C11-C12-C13
15	aA	809	CLA	C15-C16-C17-C18
15	aA	810	CLA	C5-C6-C7-C8
15	aA	829	CLA	C15-C16-C17-C18
15	aA	839	CLA	C8-C10-C11-C12
15	aA	843	CLA	C8-C10-C11-C12
15	aA	843	CLA	C13-C15-C16-C17
15	aB	807	CLA	C13-C15-C16-C17
15	aB	815	CLA	C5-C6-C7-C8
15	aB	819	CLA	C5-C6-C7-C8
15	aB	829	CLA	C5-C6-C7-C8
15	bA	804	CLA	C10-C11-C12-C13
15	bA	809	CLA	C15-C16-C17-C18
15	bA	810	CLA	C5-C6-C7-C8
15	bA	839	CLA	C8-C10-C11-C12
15	bA	843	CLA	C8-C10-C11-C12
15	bA	843	CLA	C13-C15-C16-C17
15	bB	807	CLA	C13-C15-C16-C17
15	bB	815	CLA	C5-C6-C7-C8
15	bB	829	CLA	C5-C6-C7-C8
15	cA	804	CLA	C10-C11-C12-C13
15	cA	809	CLA	C15-C16-C17-C18
15	cA	810	CLA	C5-C6-C7-C8
15	cA	839	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	842	CLA	C8-C10-C11-C12
15	cA	842	CLA	C13-C15-C16-C17
15	cB	807	CLA	C13-C15-C16-C17
15	cB	815	CLA	C5-C6-C7-C8
15	cB	829	CLA	C5-C6-C7-C8
15	cB	836	CLA	C8-C10-C11-C12
15	aA	820	CLA	O1D-CGD-O2D-CED
15	cA	820	CLA	O1D-CGD-O2D-CED
15	a1	416	CLA	O1A-CGA-O2A-C1
15	c1	417	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	CBD-CGD-O2D-CED
15	bA	804	CLA	CBD-CGD-O2D-CED
15	b6	411	CLA	CBD-CGD-O2D-CED
15	cA	804	CLA	CBD-CGD-O2D-CED
15	a2	408	CLA	O1D-CGD-O2D-CED
15	bA	820	CLA	O1D-CGD-O2D-CED
15	b2	408	CLA	O1D-CGD-O2D-CED
15	aB	810	CLA	C5-C6-C7-C8
15	a3	402	CLA	C15-C16-C17-C18
15	a5	402	CLA	C15-C16-C17-C18
15	bA	829	CLA	C15-C16-C17-C18
15	bB	810	CLA	C5-C6-C7-C8
15	b3	402	CLA	C15-C16-C17-C18
15	b5	402	CLA	C15-C16-C17-C18
15	cB	810	CLA	C5-C6-C7-C8
15	c3	402	CLA	C15-C16-C17-C18
15	c5	402	CLA	C15-C16-C17-C18
16	aA	846	PQN	C23-C25-C26-C27
16	bA	846	PQN	C23-C25-C26-C27
16	cA	845	PQN	C23-C25-C26-C27
15	a1	406	CLA	O1D-CGD-O2D-CED
15	c1	407	CLA	O1D-CGD-O2D-CED
15	aL	203	CLA	C10-C11-C12-C13
15	a4	402	CLA	C15-C16-C17-C18
15	bL	204	CLA	C10-C11-C12-C13
15	b4	402	CLA	C15-C16-C17-C18
15	cL	203	CLA	C10-C11-C12-C13
15	c1	402	CLA	C15-C16-C17-C18
15	c4	402	CLA	C15-C16-C17-C18
19	aA	854	LHG	C7-C8-C9-C10
19	bA	855	LHG	C7-C8-C9-C10
19	cA	853	LHG	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	833	CLA	CBD-CGD-O2D-CED
15	a6	411	CLA	CBD-CGD-O2D-CED
15	bB	833	CLA	CBD-CGD-O2D-CED
15	cB	833	CLA	CBD-CGD-O2D-CED
15	c3	410	CLA	CBD-CGD-O2D-CED
15	c6	411	CLA	CBD-CGD-O2D-CED
15	aB	809	CLA	C13-C15-C16-C17
15	bA	812	CLA	C15-C16-C17-C18
15	bB	809	CLA	C13-C15-C16-C17
15	b1	402	CLA	C15-C16-C17-C18
15	cA	812	CLA	C15-C16-C17-C18
15	cB	809	CLA	C13-C15-C16-C17
15	aA	810	CLA	C11-C10-C8-C7
15	aA	831	CLA	C11-C10-C8-C7
15	aA	843	CLA	C11-C10-C8-C7
15	aB	833	CLA	C11-C12-C13-C15
15	aB	840	CLA	C12-C13-C15-C16
15	a4	403	CLA	C6-C7-C8-C10
15	bA	810	CLA	C11-C10-C8-C7
15	bA	831	CLA	C11-C10-C8-C7
15	bA	843	CLA	C11-C10-C8-C7
15	bB	833	CLA	C11-C12-C13-C15
15	bB	840	CLA	C12-C13-C15-C16
15	b4	403	CLA	C6-C7-C8-C10
15	cA	810	CLA	C11-C10-C8-C7
15	cA	831	CLA	C11-C10-C8-C7
15	cA	842	CLA	C11-C10-C8-C7
15	cB	833	CLA	C11-C12-C13-C15
15	cB	840	CLA	C12-C13-C15-C16
15	c4	403	CLA	C6-C7-C8-C10
16	aB	843	PQN	C17-C18-C20-C21
16	bB	843	PQN	C17-C18-C20-C21
16	cB	843	PQN	C17-C18-C20-C21
15	aB	832	CLA	O1A-CGA-O2A-C1
15	bB	832	CLA	O1A-CGA-O2A-C1
15	b1	417	CLA	O1A-CGA-O2A-C1
15	cB	832	CLA	O1A-CGA-O2A-C1
18	aA	852	BCR	C13-C14-C15-C16
18	aA	852	BCR	C15-C16-C17-C18
18	a1	417	BCR	C19-C20-C21-C22
18	a2	419	BCR	C19-C20-C21-C22
18	a3	418	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a4	418	BCR	C19-C20-C21-C22
18	a5	401	BCR	C9-C10-C11-C12
18	a5	418	BCR	C19-C20-C21-C22
18	bA	853	BCR	C13-C14-C15-C16
18	bA	853	BCR	C15-C16-C17-C18
18	b1	418	BCR	C19-C20-C21-C22
18	b3	418	BCR	C19-C20-C21-C22
18	b4	418	BCR	C19-C20-C21-C22
18	b5	401	BCR	C9-C10-C11-C12
18	b5	418	BCR	C19-C20-C21-C22
18	cA	851	BCR	C13-C14-C15-C16
18	cA	851	BCR	C15-C16-C17-C18
18	c1	418	BCR	C19-C20-C21-C22
18	c2	419	BCR	C19-C20-C21-C22
18	c3	418	BCR	C19-C20-C21-C22
18	c4	418	BCR	C19-C20-C21-C22
18	c5	401	BCR	C9-C10-C11-C12
18	c5	418	BCR	C19-C20-C21-C22
15	aA	810	CLA	C2A-CAA-CBA-CGA
15	aA	825	CLA	C2A-CAA-CBA-CGA
15	aB	805	CLA	C2A-CAA-CBA-CGA
15	aB	840	CLA	C2A-CAA-CBA-CGA
15	a1	403	CLA	C2A-CAA-CBA-CGA
15	a2	404	CLA	C2A-CAA-CBA-CGA
15	a3	404	CLA	C2A-CAA-CBA-CGA
15	a4	404	CLA	C2A-CAA-CBA-CGA
15	a5	404	CLA	C2A-CAA-CBA-CGA
15	a6	405	CLA	C2A-CAA-CBA-CGA
15	bA	810	CLA	C2A-CAA-CBA-CGA
15	bA	825	CLA	C2A-CAA-CBA-CGA
15	bB	805	CLA	C2A-CAA-CBA-CGA
15	bB	840	CLA	C2A-CAA-CBA-CGA
15	b1	404	CLA	C2A-CAA-CBA-CGA
15	b2	404	CLA	C2A-CAA-CBA-CGA
15	b3	404	CLA	C2A-CAA-CBA-CGA
15	b4	404	CLA	C2A-CAA-CBA-CGA
15	b5	404	CLA	C2A-CAA-CBA-CGA
15	b6	405	CLA	C2A-CAA-CBA-CGA
15	cA	810	CLA	C2A-CAA-CBA-CGA
15	cA	825	CLA	C2A-CAA-CBA-CGA
15	cB	805	CLA	C2A-CAA-CBA-CGA
15	cB	840	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	404	CLA	C2A-CAA-CBA-CGA
15	c2	404	CLA	C2A-CAA-CBA-CGA
15	c3	404	CLA	C2A-CAA-CBA-CGA
15	c4	404	CLA	C2A-CAA-CBA-CGA
15	c5	404	CLA	C2A-CAA-CBA-CGA
15	c6	405	CLA	C2A-CAA-CBA-CGA
15	aA	812	CLA	C15-C16-C17-C18
15	aA	827	CLA	C8-C10-C11-C12
15	aA	828	CLA	C13-C15-C16-C17
15	aB	804	CLA	C15-C16-C17-C18
15	aB	811	CLA	C15-C16-C17-C18
15	aB	839	CLA	C8-C10-C11-C12
15	a1	401	CLA	C15-C16-C17-C18
15	a2	402	CLA	C15-C16-C17-C18
15	a6	403	CLA	C15-C16-C17-C18
15	bA	827	CLA	C8-C10-C11-C12
15	bA	828	CLA	C13-C15-C16-C17
15	bB	804	CLA	C15-C16-C17-C18
15	bB	811	CLA	C15-C16-C17-C18
15	bB	839	CLA	C8-C10-C11-C12
15	b2	402	CLA	C15-C16-C17-C18
15	b6	403	CLA	C15-C16-C17-C18
15	cA	827	CLA	C8-C10-C11-C12
15	cA	828	CLA	C13-C15-C16-C17
15	cB	804	CLA	C15-C16-C17-C18
15	cB	811	CLA	C15-C16-C17-C18
15	cB	839	CLA	C8-C10-C11-C12
15	c2	402	CLA	C15-C16-C17-C18
15	aB	814	CLA	C4C-C3C-CAC-CBC
15	bB	814	CLA	C4C-C3C-CAC-CBC
15	cB	814	CLA	C4C-C3C-CAC-CBC
18	b5	419	BCR	C22-C23-C24-C25
15	aA	825	CLA	O1A-CGA-O2A-C1
15	bA	825	CLA	O1A-CGA-O2A-C1
15	cA	825	CLA	O1A-CGA-O2A-C1
15	aA	832	CLA	CBD-CGD-O2D-CED
15	aB	801	CLA	CBD-CGD-O2D-CED
15	bA	832	CLA	CBD-CGD-O2D-CED
15	bB	801	CLA	CBD-CGD-O2D-CED
15	b3	410	CLA	CBD-CGD-O2D-CED
15	cA	832	CLA	CBD-CGD-O2D-CED
15	cB	801	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	409	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	C13-C15-C16-C17
15	a1	422	CLA	C10-C11-C12-C13
15	bB	803	CLA	C13-C15-C16-C17
15	cB	803	CLA	C13-C15-C16-C17
18	aA	850	BCR	C18-C19-C20-C21
18	aB	844	BCR	C18-C19-C20-C21
18	aF	203	BCR	C18-C19-C20-C21
18	aJ	204	BCR	C18-C19-C20-C21
18	a1	418	BCR	C10-C11-C12-C13
18	a1	419	BCR	C10-C11-C12-C13
18	a1	420	BCR	C10-C11-C12-C13
18	a1	420	BCR	C18-C19-C20-C21
18	a1	421	BCR	C10-C11-C12-C13
18	a1	421	BCR	C18-C19-C20-C21
18	a2	401	BCR	C10-C11-C12-C13
18	a2	401	BCR	C18-C19-C20-C21
18	a2	420	BCR	C10-C11-C12-C13
18	a2	421	BCR	C10-C11-C12-C13
18	a3	401	BCR	C18-C19-C20-C21
18	a3	419	BCR	C10-C11-C12-C13
18	a3	420	BCR	C10-C11-C12-C13
18	a4	401	BCR	C18-C19-C20-C21
18	a4	419	BCR	C18-C19-C20-C21
18	a4	420	BCR	C10-C11-C12-C13
18	a5	401	BCR	C18-C19-C20-C21
18	a5	419	BCR	C10-C11-C12-C13
18	a6	401	BCR	C10-C11-C12-C13
18	a6	402	BCR	C18-C19-C20-C21
18	a6	420	BCR	C10-C11-C12-C13
18	a6	421	BCR	C18-C19-C20-C21
18	bA	851	BCR	C18-C19-C20-C21
18	bB	844	BCR	C18-C19-C20-C21
18	bJ	103	BCR	C18-C19-C20-C21
18	bJ	105	BCR	C18-C19-C20-C21
18	b1	401	BCR	C10-C11-C12-C13
18	b1	401	BCR	C18-C19-C20-C21
18	b1	419	BCR	C10-C11-C12-C13
18	b1	420	BCR	C10-C11-C12-C13
18	b2	401	BCR	C18-C19-C20-C21
18	b2	420	BCR	C10-C11-C12-C13
18	b2	421	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b3	401	BCR	C18-C19-C20-C21
18	b3	419	BCR	C10-C11-C12-C13
18	b3	420	BCR	C10-C11-C12-C13
18	b4	401	BCR	C18-C19-C20-C21
18	b4	419	BCR	C18-C19-C20-C21
18	b4	420	BCR	C10-C11-C12-C13
18	b5	401	BCR	C18-C19-C20-C21
18	b5	419	BCR	C10-C11-C12-C13
18	b6	401	BCR	C10-C11-C12-C13
18	b6	402	BCR	C18-C19-C20-C21
18	b6	420	BCR	C10-C11-C12-C13
18	b6	421	BCR	C18-C19-C20-C21
18	cA	849	BCR	C18-C19-C20-C21
18	cB	844	BCR	C18-C19-C20-C21
18	cJ	103	BCR	C18-C19-C20-C21
18	c1	401	BCR	C10-C11-C12-C13
18	c1	401	BCR	C18-C19-C20-C21
18	c1	419	BCR	C10-C11-C12-C13
18	c1	420	BCR	C10-C11-C12-C13
18	c2	401	BCR	C18-C19-C20-C21
18	c2	420	BCR	C10-C11-C12-C13
18	c2	421	BCR	C10-C11-C12-C13
18	c3	401	BCR	C18-C19-C20-C21
18	c3	419	BCR	C10-C11-C12-C13
18	c3	420	BCR	C10-C11-C12-C13
18	c4	401	BCR	C18-C19-C20-C21
18	c4	419	BCR	C18-C19-C20-C21
18	c4	420	BCR	C10-C11-C12-C13
18	c5	401	BCR	C18-C19-C20-C21
18	c5	419	BCR	C10-C11-C12-C13
18	c6	401	BCR	C10-C11-C12-C13
18	c6	402	BCR	C18-C19-C20-C21
18	c6	420	BCR	C10-C11-C12-C13
19	aX	101	LHG	O2-C2-C3-O3
19	bX	101	LHG	O2-C2-C3-O3
19	cX	101	LHG	O2-C2-C3-O3
15	aA	803	CLA	C15-C16-C17-C18
15	aA	807	CLA	C15-C16-C17-C18
15	aB	834	CLA	C5-C6-C7-C8
15	a3	402	CLA	C8-C10-C11-C12
15	a6	403	CLA	C8-C10-C11-C12
15	bA	803	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	807	CLA	C15-C16-C17-C18
15	bB	834	CLA	C5-C6-C7-C8
15	b1	402	CLA	C8-C10-C11-C12
15	b6	403	CLA	C8-C10-C11-C12
15	cA	803	CLA	C15-C16-C17-C18
15	cA	807	CLA	C15-C16-C17-C18
15	cB	834	CLA	C5-C6-C7-C8
15	c1	402	CLA	C8-C10-C11-C12
15	c4	402	CLA	C8-C10-C11-C12
15	c6	403	CLA	C8-C10-C11-C12
15	c6	403	CLA	C15-C16-C17-C18
15	a3	410	CLA	CBD-CGD-O2D-CED
15	aB	826	CLA	CBA-CGA-O2A-C1
15	bB	826	CLA	CBA-CGA-O2A-C1
15	cB	826	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	C8-C10-C11-C12
15	aA	825	CLA	C8-C10-C11-C12
15	aB	837	CLA	C13-C15-C16-C17
15	a2	422	CLA	C10-C11-C12-C13
15	a6	422	CLA	C10-C11-C12-C13
15	bA	803	CLA	C8-C10-C11-C12
15	bA	825	CLA	C8-C10-C11-C12
15	bB	837	CLA	C13-C15-C16-C17
15	b2	422	CLA	C10-C11-C12-C13
15	b6	422	CLA	C10-C11-C12-C13
15	cA	803	CLA	C8-C10-C11-C12
15	cA	825	CLA	C8-C10-C11-C12
15	cB	837	CLA	C13-C15-C16-C17
15	c2	422	CLA	C10-C11-C12-C13
15	bA	826	CLA	CBD-CGD-O2D-CED
15	aA	829	CLA	C5-C6-C7-C8
15	aB	802	CLA	C8-C10-C11-C12
15	aB	806	CLA	C15-C16-C17-C18
15	aB	815	CLA	C15-C16-C17-C18
15	aB	833	CLA	C10-C11-C12-C13
15	a2	406	CLA	C10-C11-C12-C13
15	a3	421	CLA	C10-C11-C12-C13
15	a4	402	CLA	C8-C10-C11-C12
15	a4	421	CLA	C10-C11-C12-C13
15	a5	402	CLA	C8-C10-C11-C12
15	a5	420	CLA	C10-C11-C12-C13
15	bB	802	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	806	CLA	C15-C16-C17-C18
15	bB	815	CLA	C15-C16-C17-C18
15	bB	833	CLA	C10-C11-C12-C13
15	b3	402	CLA	C8-C10-C11-C12
15	b4	402	CLA	C8-C10-C11-C12
15	b4	421	CLA	C10-C11-C12-C13
15	b5	402	CLA	C8-C10-C11-C12
15	cB	802	CLA	C8-C10-C11-C12
15	cB	806	CLA	C15-C16-C17-C18
15	cB	815	CLA	C15-C16-C17-C18
15	cB	833	CLA	C10-C11-C12-C13
15	c3	402	CLA	C8-C10-C11-C12
15	c3	421	CLA	C10-C11-C12-C13
15	c4	421	CLA	C10-C11-C12-C13
15	c5	402	CLA	C8-C10-C11-C12
19	aA	854	LHG	C3-O3-P-O6
19	aA	854	LHG	C4-O6-P-O3
19	aX	101	LHG	C3-O3-P-O6
19	bA	855	LHG	C3-O3-P-O6
19	bA	855	LHG	C4-O6-P-O3
19	bX	101	LHG	C3-O3-P-O6
19	cA	853	LHG	C3-O3-P-O6
19	cX	101	LHG	C3-O3-P-O6
15	aB	814	CLA	C3-C5-C6-C7
15	bB	814	CLA	C3-C5-C6-C7
15	cB	814	CLA	C3-C5-C6-C7
15	aB	837	CLA	O1D-CGD-O2D-CED
15	bB	837	CLA	O1D-CGD-O2D-CED
15	cB	837	CLA	O1D-CGD-O2D-CED
15	aA	826	CLA	CBD-CGD-O2D-CED
15	cA	826	CLA	CBD-CGD-O2D-CED
15	aB	828	CLA	C10-C11-C12-C13
15	bA	829	CLA	C5-C6-C7-C8
15	bB	828	CLA	C10-C11-C12-C13
15	b2	406	CLA	C10-C11-C12-C13
15	b3	421	CLA	C10-C11-C12-C13
15	b5	420	CLA	C10-C11-C12-C13
15	cA	829	CLA	C5-C6-C7-C8
15	cB	828	CLA	C10-C11-C12-C13
15	c2	406	CLA	C10-C11-C12-C13
15	c5	420	CLA	C10-C11-C12-C13
15	a2	418	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b3	417	CLA	C4-C3-C5-C6
15	a1	416	CLA	C2-C3-C5-C6
15	c1	417	CLA	C2-C3-C5-C6
15	aA	829	CLA	C13-C15-C16-C17
15	a1	401	CLA	C8-C10-C11-C12
15	bA	829	CLA	C13-C15-C16-C17
15	cA	829	CLA	C13-C15-C16-C17
16	aB	843	PQN	C25-C26-C27-C28
16	bB	843	PQN	C25-C26-C27-C28
16	cB	843	PQN	C25-C26-C27-C28
15	aA	813	CLA	C2A-CAA-CBA-CGA
15	aA	816	CLA	C2A-CAA-CBA-CGA
15	aA	823	CLA	C2A-CAA-CBA-CGA
15	bA	813	CLA	C2A-CAA-CBA-CGA
15	bA	816	CLA	C2A-CAA-CBA-CGA
15	bA	823	CLA	C2A-CAA-CBA-CGA
15	cA	813	CLA	C2A-CAA-CBA-CGA
15	cA	816	CLA	C2A-CAA-CBA-CGA
15	cA	823	CLA	C2A-CAA-CBA-CGA
15	aB	801	CLA	C3-C5-C6-C7
15	aB	819	CLA	C3-C5-C6-C7
15	bB	801	CLA	C3-C5-C6-C7
15	bB	819	CLA	C3-C5-C6-C7
15	cB	801	CLA	C3-C5-C6-C7
15	cB	819	CLA	C3-C5-C6-C7
15	aA	821	CLA	CBA-CGA-O2A-C1
15	aB	818	CLA	CBA-CGA-O2A-C1
15	a1	401	CLA	CBA-CGA-O2A-C1
15	a3	402	CLA	CBA-CGA-O2A-C1
15	bA	821	CLA	CBA-CGA-O2A-C1
15	bB	818	CLA	CBA-CGA-O2A-C1
15	cA	821	CLA	CBA-CGA-O2A-C1
15	cB	818	CLA	CBA-CGA-O2A-C1
15	c2	402	CLA	CBA-CGA-O2A-C1
15	c5	410	CLA	CBA-CGA-O2A-C1
15	aB	803	CLA	C8-C10-C11-C12
15	aB	814	CLA	C13-C15-C16-C17
15	bB	803	CLA	C8-C10-C11-C12
15	bB	814	CLA	C13-C15-C16-C17
15	b2	402	CLA	C8-C10-C11-C12
15	cB	803	CLA	C8-C10-C11-C12
15	cB	814	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	810	CLA	C13-C15-C16-C17
15	aA	826	CLA	C5-C6-C7-C8
15	aB	815	CLA	C8-C10-C11-C12
15	a2	402	CLA	C8-C10-C11-C12
15	bA	810	CLA	C13-C15-C16-C17
15	bA	826	CLA	C5-C6-C7-C8
15	bB	815	CLA	C8-C10-C11-C12
15	cA	810	CLA	C13-C15-C16-C17
15	cA	826	CLA	C5-C6-C7-C8
15	cA	841	CLA	C5-C6-C7-C8
15	c2	402	CLA	C8-C10-C11-C12
18	a4	401	BCR	C9-C10-C11-C12
18	a6	419	BCR	C19-C20-C21-C22
18	b2	419	BCR	C19-C20-C21-C22
18	b4	401	BCR	C9-C10-C11-C12
18	b6	419	BCR	C19-C20-C21-C22
18	c4	401	BCR	C9-C10-C11-C12
18	c6	419	BCR	C19-C20-C21-C22
15	aA	841	CLA	C5-C6-C7-C8
15	bA	841	CLA	C5-C6-C7-C8
15	cB	815	CLA	C8-C10-C11-C12
18	aA	848	BCR	C16-C17-C18-C36
18	aA	849	BCR	C20-C21-C22-C37
18	aA	850	BCR	C20-C21-C22-C37
18	aA	852	BCR	C16-C17-C18-C36
18	aB	845	BCR	C16-C17-C18-C36
18	aB	845	BCR	C20-C21-C22-C37
18	aF	201	BCR	C16-C17-C18-C36
18	aF	201	BCR	C20-C21-C22-C37
18	aF	202	BCR	C35-C13-C14-C15
18	aF	202	BCR	C16-C17-C18-C36
18	aF	203	BCR	C16-C17-C18-C36
18	aI	101	BCR	C16-C17-C18-C36
18	aI	102	BCR	C16-C17-C18-C36
18	aI	103	BCR	C20-C21-C22-C37
18	aJ	204	BCR	C35-C13-C14-C15
18	aJ	204	BCR	C20-C21-C22-C37
18	a1	417	BCR	C16-C17-C18-C36
18	a1	418	BCR	C20-C21-C22-C37
18	a1	419	BCR	C20-C21-C22-C37
18	a1	420	BCR	C11-C10-C9-C34
18	a1	420	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a2	419	BCR	C20-C21-C22-C37
18	a2	420	BCR	C20-C21-C22-C37
18	a3	419	BCR	C20-C21-C22-C37
18	a3	420	BCR	C20-C21-C22-C37
18	a4	419	BCR	C20-C21-C22-C37
18	a4	420	BCR	C20-C21-C22-C37
18	a5	419	BCR	C20-C21-C22-C37
18	a6	401	BCR	C11-C10-C9-C34
18	a6	401	BCR	C20-C21-C22-C37
18	a6	419	BCR	C16-C17-C18-C36
18	bA	849	BCR	C16-C17-C18-C36
18	bA	850	BCR	C20-C21-C22-C37
18	bA	851	BCR	C20-C21-C22-C37
18	bA	853	BCR	C16-C17-C18-C36
18	bB	845	BCR	C16-C17-C18-C36
18	bB	845	BCR	C20-C21-C22-C37
18	bB	849	BCR	C16-C17-C18-C36
18	bB	849	BCR	C20-C21-C22-C37
18	bF	202	BCR	C35-C13-C14-C15
18	bF	202	BCR	C16-C17-C18-C36
18	bI	101	BCR	C16-C17-C18-C36
18	bI	102	BCR	C16-C17-C18-C36
18	bJ	103	BCR	C35-C13-C14-C15
18	bJ	103	BCR	C20-C21-C22-C37
18	bJ	105	BCR	C16-C17-C18-C36
18	bL	205	BCR	C20-C21-C22-C37
18	b1	401	BCR	C20-C21-C22-C37
18	b1	418	BCR	C16-C17-C18-C36
18	b1	419	BCR	C20-C21-C22-C37
18	b1	420	BCR	C20-C21-C22-C37
18	b2	419	BCR	C20-C21-C22-C37
18	b2	420	BCR	C20-C21-C22-C37
18	b3	419	BCR	C20-C21-C22-C37
18	b3	420	BCR	C20-C21-C22-C37
18	b4	419	BCR	C20-C21-C22-C37
18	b4	420	BCR	C20-C21-C22-C37
18	b6	401	BCR	C11-C10-C9-C34
18	b6	401	BCR	C20-C21-C22-C37
18	b6	419	BCR	C16-C17-C18-C36
18	b6	420	BCR	C20-C21-C22-C37
18	cA	847	BCR	C16-C17-C18-C36
18	cA	848	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cA	849	BCR	C20-C21-C22-C37
18	cA	851	BCR	C16-C17-C18-C36
18	cB	845	BCR	C16-C17-C18-C36
18	cB	845	BCR	C20-C21-C22-C37
18	cF	202	BCR	C16-C17-C18-C36
18	cF	202	BCR	C20-C21-C22-C37
18	cF	204	BCR	C35-C13-C14-C15
18	cF	204	BCR	C16-C17-C18-C36
18	cF	205	BCR	C16-C17-C18-C36
18	cI	101	BCR	C16-C17-C18-C36
18	cI	102	BCR	C16-C17-C18-C36
18	cJ	103	BCR	C35-C13-C14-C15
18	cJ	103	BCR	C20-C21-C22-C37
18	cL	204	BCR	C20-C21-C22-C37
18	c1	401	BCR	C20-C21-C22-C37
18	c1	418	BCR	C16-C17-C18-C36
18	c1	419	BCR	C20-C21-C22-C37
18	c1	420	BCR	C20-C21-C22-C37
18	c2	420	BCR	C20-C21-C22-C37
18	c3	419	BCR	C20-C21-C22-C37
18	c3	420	BCR	C20-C21-C22-C37
18	c4	418	BCR	C20-C21-C22-C37
18	c4	419	BCR	C20-C21-C22-C37
18	c4	420	BCR	C20-C21-C22-C37
18	c5	419	BCR	C20-C21-C22-C37
18	c6	401	BCR	C11-C10-C9-C34
18	c6	401	BCR	C20-C21-C22-C37
18	c6	419	BCR	C16-C17-C18-C36
18	c6	420	BCR	C20-C21-C22-C37
19	aA	854	LHG	C9-C10-C11-C12
19	bA	854	LHG	C26-C27-C28-C29
19	bA	855	LHG	C9-C10-C11-C12
19	cA	852	LHG	C26-C27-C28-C29
19	cA	853	LHG	C9-C10-C11-C12
15	aA	825	CLA	O1D-CGD-O2D-CED
15	aB	814	CLA	O1D-CGD-O2D-CED
15	bA	825	CLA	O1D-CGD-O2D-CED
15	bB	814	CLA	O1D-CGD-O2D-CED
15	cA	825	CLA	O1D-CGD-O2D-CED
15	cB	814	CLA	O1D-CGD-O2D-CED
15	aB	802	CLA	C16-C17-C18-C19
15	bB	802	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	802	CLA	C16-C17-C18-C19
16	aB	843	PQN	C26-C27-C28-C29
16	bB	843	PQN	C26-C27-C28-C29
16	cB	843	PQN	C26-C27-C28-C29
15	aB	814	CLA	CBA-CGA-O2A-C1
15	a1	409	CLA	CBA-CGA-O2A-C1
15	a2	402	CLA	CBA-CGA-O2A-C1
15	a4	402	CLA	CBA-CGA-O2A-C1
15	a5	410	CLA	CBA-CGA-O2A-C1
15	bB	814	CLA	CBA-CGA-O2A-C1
15	b2	402	CLA	CBA-CGA-O2A-C1
15	b3	402	CLA	CBA-CGA-O2A-C1
15	b3	410	CLA	CBA-CGA-O2A-C1
15	b4	402	CLA	CBA-CGA-O2A-C1
15	b5	410	CLA	CBA-CGA-O2A-C1
15	cB	814	CLA	CBA-CGA-O2A-C1
15	c1	402	CLA	CBA-CGA-O2A-C1
15	c3	402	CLA	CBA-CGA-O2A-C1
15	c4	402	CLA	CBA-CGA-O2A-C1
19	aA	853	LHG	C26-C27-C28-C29
15	cB	820	CLA	O1D-CGD-O2D-CED
19	aA	853	LHG	O9-C7-O7-C5
19	bA	854	LHG	O9-C7-O7-C5
19	cA	852	LHG	O9-C7-O7-C5
15	cB	836	CLA	C5-C6-C7-C8
15	aB	820	CLA	O1D-CGD-O2D-CED
15	bB	820	CLA	O1D-CGD-O2D-CED
15	aB	809	CLA	C8-C10-C11-C12
15	bB	809	CLA	C8-C10-C11-C12
15	bB	836	CLA	C5-C6-C7-C8
15	cB	809	CLA	C8-C10-C11-C12
15	aA	843	CLA	C3-C5-C6-C7
15	bA	843	CLA	C3-C5-C6-C7
15	cA	842	CLA	C3-C5-C6-C7
18	aA	849	BCR	C11-C10-C9-C8
18	aA	849	BCR	C16-C17-C18-C19
18	aA	850	BCR	C11-C10-C9-C8
18	aA	851	BCR	C20-C21-C22-C23
18	aA	852	BCR	C12-C13-C14-C15
18	aB	846	BCR	C20-C21-C22-C23
18	aB	848	BCR	C12-C13-C14-C15
18	aB	849	BCR	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aF	201	BCR	C20-C21-C22-C23
18	aI	101	BCR	C16-C17-C18-C19
18	aJ	204	BCR	C16-C17-C18-C19
18	aJ	204	BCR	C20-C21-C22-C23
18	aJ	205	BCR	C16-C17-C18-C19
18	aL	205	BCR	C12-C13-C14-C15
18	aM	101	BCR	C11-C10-C9-C8
18	aM	101	BCR	C16-C17-C18-C19
18	a1	419	BCR	C20-C21-C22-C23
18	a3	420	BCR	C20-C21-C22-C23
18	a4	420	BCR	C20-C21-C22-C23
18	a5	419	BCR	C20-C21-C22-C23
18	bA	850	BCR	C11-C10-C9-C8
18	bA	850	BCR	C16-C17-C18-C19
18	bA	851	BCR	C11-C10-C9-C8
18	bA	852	BCR	C20-C21-C22-C23
18	bA	853	BCR	C12-C13-C14-C15
18	bB	846	BCR	C20-C21-C22-C23
18	bB	848	BCR	C12-C13-C14-C15
18	bB	849	BCR	C20-C21-C22-C23
18	bB	850	BCR	C20-C21-C22-C23
18	bI	101	BCR	C16-C17-C18-C19
18	bJ	103	BCR	C16-C17-C18-C19
18	bJ	103	BCR	C20-C21-C22-C23
18	bJ	104	BCR	C16-C17-C18-C19
18	bL	201	BCR	C12-C13-C14-C15
18	bL	206	BCR	C12-C13-C14-C15
18	bM	101	BCR	C11-C10-C9-C8
18	bM	101	BCR	C16-C17-C18-C19
18	b1	420	BCR	C20-C21-C22-C23
18	b2	421	BCR	C20-C21-C22-C23
18	b5	419	BCR	C20-C21-C22-C23
18	b6	420	BCR	C20-C21-C22-C23
18	cA	848	BCR	C11-C10-C9-C8
18	cA	848	BCR	C16-C17-C18-C19
18	cA	849	BCR	C11-C10-C9-C8
18	cA	850	BCR	C20-C21-C22-C23
18	cA	851	BCR	C12-C13-C14-C15
18	cB	846	BCR	C20-C21-C22-C23
18	cB	848	BCR	C12-C13-C14-C15
18	cB	849	BCR	C20-C21-C22-C23
18	cF	202	BCR	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cI	101	BCR	C16-C17-C18-C19
18	cJ	103	BCR	C16-C17-C18-C19
18	cJ	103	BCR	C20-C21-C22-C23
18	cJ	104	BCR	C16-C17-C18-C19
18	cM	101	BCR	C11-C10-C9-C8
18	cM	101	BCR	C16-C17-C18-C19
18	c1	420	BCR	C20-C21-C22-C23
18	c2	421	BCR	C20-C21-C22-C23
18	c3	420	BCR	C20-C21-C22-C23
18	c5	419	BCR	C20-C21-C22-C23
20	aB	850	LMG	C2-C1-O1-C7
20	bB	851	LMG	C2-C1-O1-C7
20	cB	850	LMG	C2-C1-O1-C7
15	a3	410	CLA	CBA-CGA-O2A-C1
15	b1	402	CLA	CBA-CGA-O2A-C1
15	b1	410	CLA	CBA-CGA-O2A-C1
15	c1	410	CLA	CBA-CGA-O2A-C1
15	c3	410	CLA	CBA-CGA-O2A-C1
19	aA	853	LHG	C18-C19-C20-C21
19	aA	853	LHG	C28-C29-C30-C31
19	bA	854	LHG	C28-C29-C30-C31
19	cA	852	LHG	C28-C29-C30-C31
15	aA	814	CLA	C10-C11-C12-C13
15	aB	836	CLA	C5-C6-C7-C8
15	bA	814	CLA	C10-C11-C12-C13
15	cA	814	CLA	C10-C11-C12-C13
15	aL	203	CLA	C16-C17-C18-C20
15	bL	204	CLA	C16-C17-C18-C20
15	cL	203	CLA	C16-C17-C18-C20
15	a1	408	CLA	O1D-CGD-O2D-CED
15	b1	409	CLA	O1D-CGD-O2D-CED
15	c1	409	CLA	O1D-CGD-O2D-CED
15	aB	808	CLA	C4-C3-C5-C6
15	a2	404	CLA	C4-C3-C5-C6
15	a5	404	CLA	C4-C3-C5-C6
15	a6	405	CLA	C4-C3-C5-C6
15	bB	808	CLA	C4-C3-C5-C6
15	b1	404	CLA	C4-C3-C5-C6
15	b2	404	CLA	C4-C3-C5-C6
15	b3	404	CLA	C4-C3-C5-C6
15	cB	808	CLA	C4-C3-C5-C6
15	c3	404	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c5	404	CLA	C4-C3-C5-C6
15	bB	804	CLA	C2C-C3C-CAC-CBC
15	cB	804	CLA	C2C-C3C-CAC-CBC
19	bA	854	LHG	C18-C19-C20-C21
19	cA	852	LHG	C18-C19-C20-C21
15	a5	417	CLA	C2-C3-C5-C6
15	b5	417	CLA	C2-C3-C5-C6
15	c5	417	CLA	C2-C3-C5-C6
15	aA	821	CLA	C6-C7-C8-C9
15	aA	822	CLA	C14-C13-C15-C16
15	aA	829	CLA	C11-C10-C8-C9
15	aB	814	CLA	C14-C13-C15-C16
15	aB	827	CLA	C6-C7-C8-C9
15	aB	833	CLA	C14-C13-C15-C16
15	a3	402	CLA	C14-C13-C15-C16
15	a4	402	CLA	C14-C13-C15-C16
15	a5	402	CLA	C14-C13-C15-C16
15	bA	821	CLA	C6-C7-C8-C9
15	bA	822	CLA	C14-C13-C15-C16
15	bA	829	CLA	C11-C10-C8-C9
15	bB	814	CLA	C14-C13-C15-C16
15	bB	827	CLA	C6-C7-C8-C9
15	bB	833	CLA	C14-C13-C15-C16
15	b3	402	CLA	C14-C13-C15-C16
15	b4	402	CLA	C14-C13-C15-C16
15	b5	402	CLA	C14-C13-C15-C16
15	cA	821	CLA	C6-C7-C8-C9
15	cA	822	CLA	C14-C13-C15-C16
15	cA	829	CLA	C11-C10-C8-C9
15	cB	814	CLA	C14-C13-C15-C16
15	cB	827	CLA	C6-C7-C8-C9
15	cB	833	CLA	C14-C13-C15-C16
15	c1	402	CLA	C14-C13-C15-C16
15	c3	402	CLA	C14-C13-C15-C16
15	c4	402	CLA	C14-C13-C15-C16
15	c5	402	CLA	C14-C13-C15-C16
15	cB	810	CLA	CBD-CGD-O2D-CED
15	aA	813	CLA	C5-C6-C7-C8
15	bA	813	CLA	C5-C6-C7-C8
15	cA	813	CLA	C5-C6-C7-C8
15	aB	804	CLA	C2A-CAA-CBA-CGA
15	a6	422	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aF	202	BCR	C7-C8-C9-C34
18	a1	420	BCR	C7-C8-C9-C34
18	a6	401	BCR	C7-C8-C9-C34
18	bF	202	BCR	C7-C8-C9-C34
18	b6	401	BCR	C7-C8-C9-C34
18	cF	204	BCR	C7-C8-C9-C34
18	c6	401	BCR	C7-C8-C9-C34
15	aB	804	CLA	C2C-C3C-CAC-CBC
20	aB	850	LMG	C17-C18-C19-C20
20	bB	851	LMG	C17-C18-C19-C20
18	aM	101	BCR	C7-C8-C9-C10
18	a1	419	BCR	C7-C8-C9-C10
18	a2	421	BCR	C7-C8-C9-C10
18	a3	420	BCR	C7-C8-C9-C10
18	a4	420	BCR	C7-C8-C9-C10
18	a5	419	BCR	C7-C8-C9-C10
18	a6	420	BCR	C7-C8-C9-C10
18	bM	101	BCR	C7-C8-C9-C10
18	b1	420	BCR	C7-C8-C9-C10
18	b2	421	BCR	C7-C8-C9-C10
18	b3	420	BCR	C7-C8-C9-C10
18	b4	420	BCR	C7-C8-C9-C10
18	b5	419	BCR	C7-C8-C9-C10
18	b6	420	BCR	C7-C8-C9-C10
18	cM	101	BCR	C7-C8-C9-C10
18	c1	420	BCR	C7-C8-C9-C10
18	c2	421	BCR	C7-C8-C9-C10
18	c3	420	BCR	C7-C8-C9-C10
18	c4	420	BCR	C7-C8-C9-C10
18	c5	419	BCR	C7-C8-C9-C10
18	c6	420	BCR	C7-C8-C9-C10
15	aB	830	CLA	C13-C15-C16-C17
15	bB	830	CLA	C13-C15-C16-C17
15	cB	830	CLA	C13-C15-C16-C17
20	cB	850	LMG	C17-C18-C19-C20
15	aB	810	CLA	CBD-CGD-O2D-CED
15	bB	810	CLA	CBD-CGD-O2D-CED
19	aA	853	LHG	C23-C24-C25-C26
19	bA	854	LHG	C23-C24-C25-C26
19	cA	852	LHG	C23-C24-C25-C26
15	aB	828	CLA	C16-C17-C18-C19
15	aL	203	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	828	CLA	C16-C17-C18-C19
15	bL	204	CLA	C16-C17-C18-C19
15	cB	828	CLA	C16-C17-C18-C19
15	cL	203	CLA	C16-C17-C18-C19
15	aA	841	CLA	C8-C10-C11-C12
15	bA	841	CLA	C8-C10-C11-C12
15	cA	841	CLA	C8-C10-C11-C12
20	aB	850	LMG	C40-C41-C42-C43
20	bB	851	LMG	C40-C41-C42-C43
20	cB	850	LMG	C40-C41-C42-C43
15	aB	829	CLA	CBD-CGD-O2D-CED
15	bB	829	CLA	CBD-CGD-O2D-CED
15	cB	829	CLA	CBD-CGD-O2D-CED
15	c4	411	CLA	CBD-CGD-O2D-CED
15	c4	409	CLA	O1D-CGD-O2D-CED
19	bA	854	LHG	C32-C33-C34-C35
19	cA	852	LHG	C32-C33-C34-C35
15	aA	821	CLA	O1A-CGA-O2A-C1
15	bA	821	CLA	O1A-CGA-O2A-C1
15	cA	821	CLA	O1A-CGA-O2A-C1
19	aA	853	LHG	C32-C33-C34-C35
15	aA	824	CLA	CBA-CGA-O2A-C1
15	a2	411	CLA	CBA-CGA-O2A-C1
15	a4	410	CLA	CBA-CGA-O2A-C1
15	a6	403	CLA	CBA-CGA-O2A-C1
15	a6	411	CLA	CBA-CGA-O2A-C1
15	bA	824	CLA	CBA-CGA-O2A-C1
15	b2	411	CLA	CBA-CGA-O2A-C1
15	b4	410	CLA	CBA-CGA-O2A-C1
15	b6	403	CLA	CBA-CGA-O2A-C1
15	b6	411	CLA	CBA-CGA-O2A-C1
15	cA	824	CLA	CBA-CGA-O2A-C1
15	c2	411	CLA	CBA-CGA-O2A-C1
15	c4	410	CLA	CBA-CGA-O2A-C1
15	c6	411	CLA	CBA-CGA-O2A-C1
20	aB	850	LMG	C34-C35-C36-C37
20	bB	851	LMG	C34-C35-C36-C37
20	cB	850	LMG	C34-C35-C36-C37
15	a2	410	CLA	O1D-CGD-O2D-CED
15	bA	830	CLA	O1D-CGD-O2D-CED
15	b2	410	CLA	O1D-CGD-O2D-CED
15	b6	410	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	830	CLA	O1D-CGD-O2D-CED
15	aA	804	CLA	C3A-C2A-CAA-CBA
15	aA	805	CLA	C3A-C2A-CAA-CBA
15	aA	842	CLA	C3A-C2A-CAA-CBA
15	a1	410	CLA	C3A-C2A-CAA-CBA
15	a1	411	CLA	C3A-C2A-CAA-CBA
15	a2	412	CLA	C3A-C2A-CAA-CBA
15	a3	411	CLA	C3A-C2A-CAA-CBA
15	a4	411	CLA	C3A-C2A-CAA-CBA
15	a5	411	CLA	C3A-C2A-CAA-CBA
15	a6	412	CLA	C3A-C2A-CAA-CBA
15	a6	413	CLA	C3A-C2A-CAA-CBA
15	bA	804	CLA	C3A-C2A-CAA-CBA
15	bA	805	CLA	C3A-C2A-CAA-CBA
15	bA	842	CLA	C3A-C2A-CAA-CBA
15	b1	411	CLA	C3A-C2A-CAA-CBA
15	b2	412	CLA	C3A-C2A-CAA-CBA
15	b3	411	CLA	C3A-C2A-CAA-CBA
15	b4	411	CLA	C3A-C2A-CAA-CBA
15	b5	411	CLA	C3A-C2A-CAA-CBA
15	b6	412	CLA	C3A-C2A-CAA-CBA
15	b6	413	CLA	C3A-C2A-CAA-CBA
15	cA	804	CLA	C3A-C2A-CAA-CBA
15	cA	805	CLA	C3A-C2A-CAA-CBA
15	cF	201	CLA	C3A-C2A-CAA-CBA
15	c1	411	CLA	C3A-C2A-CAA-CBA
15	c2	412	CLA	C3A-C2A-CAA-CBA
15	c3	411	CLA	C3A-C2A-CAA-CBA
15	c4	411	CLA	C3A-C2A-CAA-CBA
15	c5	411	CLA	C3A-C2A-CAA-CBA
15	c6	412	CLA	C3A-C2A-CAA-CBA
15	aL	202	CLA	C10-C11-C12-C13
15	bL	203	CLA	C10-C11-C12-C13
15	cL	202	CLA	C10-C11-C12-C13
18	aA	850	BCR	C19-C20-C21-C22
18	bA	851	BCR	C19-C20-C21-C22
18	cA	849	BCR	C19-C20-C21-C22
15	aA	830	CLA	O1D-CGD-O2D-CED
15	a4	409	CLA	O1D-CGD-O2D-CED
15	a6	410	CLA	O1D-CGD-O2D-CED
15	b4	409	CLA	O1D-CGD-O2D-CED
15	c2	410	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	401	CLA	O1A-CGA-O2A-C1
15	a2	402	CLA	O1A-CGA-O2A-C1
15	a3	402	CLA	O1A-CGA-O2A-C1
15	c1	402	CLA	O1A-CGA-O2A-C1
15	c2	402	CLA	O1A-CGA-O2A-C1
15	aA	814	CLA	C11-C12-C13-C14
15	aA	814	CLA	C11-C12-C13-C15
15	aB	806	CLA	C16-C17-C18-C19
15	bA	814	CLA	C11-C12-C13-C14
15	bA	814	CLA	C11-C12-C13-C15
15	bB	806	CLA	C16-C17-C18-C19
15	cA	814	CLA	C11-C12-C13-C14
15	cA	814	CLA	C11-C12-C13-C15
15	cB	806	CLA	C16-C17-C18-C19
16	aB	843	PQN	C26-C27-C28-C30
16	bB	843	PQN	C26-C27-C28-C30
16	cB	843	PQN	C26-C27-C28-C30
15	b5	409	CLA	O1D-CGD-O2D-CED
15	aB	818	CLA	CBD-CGD-O2D-CED
15	a5	410	CLA	CBD-CGD-O2D-CED
15	bB	818	CLA	CBD-CGD-O2D-CED
15	b5	410	CLA	CBD-CGD-O2D-CED
15	cB	818	CLA	CBD-CGD-O2D-CED
15	c3	411	CLA	CBD-CGD-O2D-CED
15	c5	410	CLA	CBD-CGD-O2D-CED
20	aB	850	LMG	C19-C20-C21-C22
20	bB	851	LMG	C19-C20-C21-C22
20	cB	850	LMG	C19-C20-C21-C22
18	aA	852	BCR	C14-C15-C16-C17
18	bA	853	BCR	C14-C15-C16-C17
18	cA	851	BCR	C14-C15-C16-C17
15	aA	814	CLA	O1D-CGD-O2D-CED
15	bA	814	CLA	O1D-CGD-O2D-CED
15	c1	410	CLA	O1A-CGA-O2A-C1
15	c3	402	CLA	O1A-CGA-O2A-C1
15	a1	403	CLA	C4-C3-C5-C6
15	a3	404	CLA	C4-C3-C5-C6
15	a4	404	CLA	C4-C3-C5-C6
15	b4	404	CLA	C4-C3-C5-C6
15	b5	404	CLA	C4-C3-C5-C6
15	b6	405	CLA	C4-C3-C5-C6
15	c1	404	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c2	404	CLA	C4-C3-C5-C6
15	c4	404	CLA	C4-C3-C5-C6
15	c6	405	CLA	C4-C3-C5-C6
15	aB	815	CLA	CBA-CGA-O2A-C1
15	bB	815	CLA	CBA-CGA-O2A-C1
15	cB	815	CLA	CBA-CGA-O2A-C1
15	c6	403	CLA	CBA-CGA-O2A-C1
15	aB	808	CLA	C2-C3-C5-C6
15	aB	827	CLA	C2-C3-C5-C6
15	a1	403	CLA	C2-C3-C5-C6
15	a3	404	CLA	C2-C3-C5-C6
15	a4	404	CLA	C2-C3-C5-C6
15	bB	808	CLA	C2-C3-C5-C6
15	bB	827	CLA	C2-C3-C5-C6
15	b4	417	CLA	C2-C3-C5-C6
15	cB	808	CLA	C2-C3-C5-C6
15	cB	827	CLA	C2-C3-C5-C6
15	c1	404	CLA	C2-C3-C5-C6
15	c2	404	CLA	C2-C3-C5-C6
15	c4	404	CLA	C2-C3-C5-C6
15	c6	405	CLA	C2-C3-C5-C6
15	cA	814	CLA	O1D-CGD-O2D-CED
15	c1	410	CLA	CBD-CGD-O2D-CED
15	c6	410	CLA	O1D-CGD-O2D-CED
15	bB	804	CLA	C2A-CAA-CBA-CGA
15	cB	804	CLA	C2A-CAA-CBA-CGA
19	aX	101	LHG	O1-C1-C2-O2
19	bX	101	LHG	O1-C1-C2-O2
19	cX	101	LHG	O1-C1-C2-O2
15	aB	809	CLA	C5-C6-C7-C8
15	bB	809	CLA	C5-C6-C7-C8
15	a3	410	CLA	O1A-CGA-O2A-C1
15	a4	402	CLA	O1A-CGA-O2A-C1
15	b1	410	CLA	O1A-CGA-O2A-C1
15	b2	402	CLA	O1A-CGA-O2A-C1
15	b3	402	CLA	O1A-CGA-O2A-C1
15	b4	402	CLA	O1A-CGA-O2A-C1
15	aB	802	CLA	C16-C17-C18-C20
15	bB	802	CLA	C16-C17-C18-C20
15	cB	802	CLA	C16-C17-C18-C20
15	cB	809	CLA	C5-C6-C7-C8
15	aL	202	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	408	CLA	C3-C5-C6-C7
15	a3	409	CLA	C3-C5-C6-C7
15	bL	203	CLA	C3-C5-C6-C7
15	b1	409	CLA	C3-C5-C6-C7
15	b6	410	CLA	C3-C5-C6-C7
15	cL	202	CLA	C3-C5-C6-C7
15	c1	409	CLA	C3-C5-C6-C7
15	a1	409	CLA	O1A-CGA-O2A-C1
15	a5	410	CLA	O1A-CGA-O2A-C1
15	b1	402	CLA	O1A-CGA-O2A-C1
15	b3	410	CLA	O1A-CGA-O2A-C1
15	b5	410	CLA	O1A-CGA-O2A-C1
15	c3	410	CLA	O1A-CGA-O2A-C1
15	c4	402	CLA	O1A-CGA-O2A-C1
15	c5	410	CLA	O1A-CGA-O2A-C1
15	aA	806	CLA	C2-C1-O2A-CGA
15	aA	843	CLA	C2-C1-O2A-CGA
15	bA	806	CLA	C2-C1-O2A-CGA
15	bA	843	CLA	C2-C1-O2A-CGA
15	cA	806	CLA	C2-C1-O2A-CGA
15	cA	842	CLA	C2-C1-O2A-CGA
15	aB	829	CLA	C13-C15-C16-C17
15	bB	829	CLA	C13-C15-C16-C17
15	cB	829	CLA	C13-C15-C16-C17
15	a2	411	CLA	O1A-CGA-O2A-C1
15	a6	403	CLA	O1A-CGA-O2A-C1
15	b6	403	CLA	O1A-CGA-O2A-C1
15	c4	410	CLA	O1A-CGA-O2A-C1
15	c6	403	CLA	O1A-CGA-O2A-C1
15	b1	410	CLA	CBD-CGD-O2D-CED
15	a5	409	CLA	C3-C5-C6-C7
15	a6	410	CLA	C3-C5-C6-C7
15	b3	409	CLA	C3-C5-C6-C7
15	c3	409	CLA	C3-C5-C6-C7
15	c5	409	CLA	C3-C5-C6-C7
18	aA	848	BCR	C1-C6-C7-C8
18	aA	848	BCR	C5-C6-C7-C8
18	aA	848	BCR	C23-C24-C25-C26
18	aA	849	BCR	C5-C6-C7-C8
18	aA	850	BCR	C5-C6-C7-C8
18	aA	850	BCR	C23-C24-C25-C26
18	aA	850	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aA	851	BCR	C5-C6-C7-C8
18	aA	851	BCR	C23-C24-C25-C26
18	aB	844	BCR	C5-C6-C7-C8
18	aB	844	BCR	C23-C24-C25-C26
18	aB	844	BCR	C23-C24-C25-C30
18	aB	845	BCR	C5-C6-C7-C8
18	aB	846	BCR	C5-C6-C7-C8
18	aB	848	BCR	C5-C6-C7-C8
18	aB	848	BCR	C23-C24-C25-C26
18	aB	849	BCR	C5-C6-C7-C8
18	aF	202	BCR	C1-C6-C7-C8
18	aF	202	BCR	C5-C6-C7-C8
18	aF	203	BCR	C23-C24-C25-C26
18	aI	103	BCR	C5-C6-C7-C8
18	aI	103	BCR	C23-C24-C25-C30
18	aJ	204	BCR	C1-C6-C7-C8
18	aJ	204	BCR	C5-C6-C7-C8
18	aJ	205	BCR	C5-C6-C7-C8
18	aJ	205	BCR	C23-C24-C25-C26
18	aJ	205	BCR	C23-C24-C25-C30
18	aK	101	BCR	C5-C6-C7-C8
18	aL	205	BCR	C5-C6-C7-C8
18	aM	101	BCR	C1-C6-C7-C8
18	aM	101	BCR	C5-C6-C7-C8
18	a1	417	BCR	C5-C6-C7-C8
18	a1	417	BCR	C23-C24-C25-C26
18	a1	417	BCR	C23-C24-C25-C30
18	a1	418	BCR	C1-C6-C7-C8
18	a1	418	BCR	C5-C6-C7-C8
18	a1	419	BCR	C5-C6-C7-C8
18	a1	419	BCR	C23-C24-C25-C26
18	a1	419	BCR	C23-C24-C25-C30
18	a1	420	BCR	C5-C6-C7-C8
18	a1	421	BCR	C5-C6-C7-C8
18	a2	419	BCR	C5-C6-C7-C8
18	a2	419	BCR	C23-C24-C25-C26
18	a2	420	BCR	C1-C6-C7-C8
18	a2	420	BCR	C5-C6-C7-C8
18	a2	421	BCR	C5-C6-C7-C8
18	a2	421	BCR	C23-C24-C25-C26
18	a2	421	BCR	C23-C24-C25-C30
18	a3	401	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a3	418	BCR	C5-C6-C7-C8
18	a3	418	BCR	C23-C24-C25-C26
18	a3	419	BCR	C5-C6-C7-C8
18	a3	420	BCR	C5-C6-C7-C8
18	a3	420	BCR	C23-C24-C25-C26
18	a3	420	BCR	C23-C24-C25-C30
18	a4	418	BCR	C5-C6-C7-C8
18	a4	418	BCR	C23-C24-C25-C26
18	a4	419	BCR	C5-C6-C7-C8
18	a4	420	BCR	C5-C6-C7-C8
18	a4	420	BCR	C23-C24-C25-C26
18	a4	420	BCR	C23-C24-C25-C30
18	a5	418	BCR	C5-C6-C7-C8
18	a5	418	BCR	C23-C24-C25-C26
18	a5	419	BCR	C5-C6-C7-C8
18	a5	419	BCR	C23-C24-C25-C26
18	a5	419	BCR	C23-C24-C25-C30
18	a6	401	BCR	C5-C6-C7-C8
18	a6	419	BCR	C5-C6-C7-C8
18	a6	419	BCR	C23-C24-C25-C26
18	a6	420	BCR	C5-C6-C7-C8
18	a6	420	BCR	C23-C24-C25-C26
18	a6	420	BCR	C23-C24-C25-C30
18	a6	421	BCR	C5-C6-C7-C8
18	bA	848	BCR	C5-C6-C7-C8
18	bA	849	BCR	C1-C6-C7-C8
18	bA	849	BCR	C5-C6-C7-C8
18	bA	849	BCR	C23-C24-C25-C26
18	bA	850	BCR	C5-C6-C7-C8
18	bA	851	BCR	C5-C6-C7-C8
18	bA	851	BCR	C23-C24-C25-C26
18	bA	851	BCR	C23-C24-C25-C30
18	bA	852	BCR	C5-C6-C7-C8
18	bA	852	BCR	C23-C24-C25-C26
18	bB	844	BCR	C5-C6-C7-C8
18	bB	844	BCR	C23-C24-C25-C26
18	bB	844	BCR	C23-C24-C25-C30
18	bB	845	BCR	C5-C6-C7-C8
18	bB	846	BCR	C5-C6-C7-C8
18	bB	848	BCR	C5-C6-C7-C8
18	bB	848	BCR	C23-C24-C25-C26
18	bB	850	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bF	202	BCR	C1-C6-C7-C8
18	bF	202	BCR	C5-C6-C7-C8
18	bJ	103	BCR	C1-C6-C7-C8
18	bJ	103	BCR	C5-C6-C7-C8
18	bJ	104	BCR	C5-C6-C7-C8
18	bJ	104	BCR	C23-C24-C25-C26
18	bJ	104	BCR	C23-C24-C25-C30
18	bJ	105	BCR	C23-C24-C25-C26
18	bL	201	BCR	C5-C6-C7-C8
18	bL	205	BCR	C5-C6-C7-C8
18	bL	205	BCR	C23-C24-C25-C30
18	bL	206	BCR	C5-C6-C7-C8
18	bM	101	BCR	C1-C6-C7-C8
18	bM	101	BCR	C5-C6-C7-C8
18	b1	401	BCR	C5-C6-C7-C8
18	b1	418	BCR	C5-C6-C7-C8
18	b1	418	BCR	C23-C24-C25-C26
18	b1	418	BCR	C23-C24-C25-C30
18	b1	419	BCR	C1-C6-C7-C8
18	b1	419	BCR	C5-C6-C7-C8
18	b1	420	BCR	C23-C24-C25-C26
18	b1	420	BCR	C23-C24-C25-C30
18	b2	419	BCR	C5-C6-C7-C8
18	b2	419	BCR	C23-C24-C25-C26
18	b2	420	BCR	C5-C6-C7-C8
18	b2	421	BCR	C5-C6-C7-C8
18	b2	421	BCR	C23-C24-C25-C26
18	b2	421	BCR	C23-C24-C25-C30
18	b3	401	BCR	C5-C6-C7-C8
18	b3	418	BCR	C5-C6-C7-C8
18	b3	418	BCR	C23-C24-C25-C26
18	b3	419	BCR	C5-C6-C7-C8
18	b3	420	BCR	C5-C6-C7-C8
18	b3	420	BCR	C23-C24-C25-C26
18	b3	420	BCR	C23-C24-C25-C30
18	b4	418	BCR	C5-C6-C7-C8
18	b4	418	BCR	C23-C24-C25-C26
18	b4	419	BCR	C5-C6-C7-C8
18	b4	420	BCR	C5-C6-C7-C8
18	b4	420	BCR	C23-C24-C25-C26
18	b4	420	BCR	C23-C24-C25-C30
18	b5	418	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b5	418	BCR	C23-C24-C25-C26
18	b5	419	BCR	C5-C6-C7-C8
18	b5	419	BCR	C23-C24-C25-C26
18	b5	419	BCR	C23-C24-C25-C30
18	b6	401	BCR	C5-C6-C7-C8
18	b6	419	BCR	C5-C6-C7-C8
18	b6	419	BCR	C23-C24-C25-C26
18	b6	420	BCR	C5-C6-C7-C8
18	b6	420	BCR	C23-C24-C25-C26
18	b6	420	BCR	C23-C24-C25-C30
18	b6	421	BCR	C5-C6-C7-C8
18	cA	847	BCR	C1-C6-C7-C8
18	cA	847	BCR	C5-C6-C7-C8
18	cA	847	BCR	C23-C24-C25-C26
18	cA	848	BCR	C5-C6-C7-C8
18	cA	849	BCR	C5-C6-C7-C8
18	cA	849	BCR	C23-C24-C25-C26
18	cA	849	BCR	C23-C24-C25-C30
18	cA	850	BCR	C5-C6-C7-C8
18	cA	850	BCR	C23-C24-C25-C26
18	cB	844	BCR	C5-C6-C7-C8
18	cB	844	BCR	C23-C24-C25-C26
18	cB	844	BCR	C23-C24-C25-C30
18	cB	845	BCR	C5-C6-C7-C8
18	cB	846	BCR	C5-C6-C7-C8
18	cB	848	BCR	C5-C6-C7-C8
18	cB	848	BCR	C23-C24-C25-C26
18	cB	849	BCR	C5-C6-C7-C8
18	cF	204	BCR	C1-C6-C7-C8
18	cF	204	BCR	C5-C6-C7-C8
18	cF	205	BCR	C23-C24-C25-C26
18	cJ	103	BCR	C1-C6-C7-C8
18	cJ	103	BCR	C5-C6-C7-C8
18	cJ	104	BCR	C5-C6-C7-C8
18	cJ	104	BCR	C23-C24-C25-C26
18	cJ	104	BCR	C23-C24-C25-C30
18	cK	101	BCR	C5-C6-C7-C8
18	cL	204	BCR	C5-C6-C7-C8
18	cL	204	BCR	C23-C24-C25-C30
18	cM	101	BCR	C1-C6-C7-C8
18	cM	101	BCR	C5-C6-C7-C8
18	c1	401	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c1	418	BCR	C5-C6-C7-C8
18	c1	418	BCR	C23-C24-C25-C26
18	c1	418	BCR	C23-C24-C25-C30
18	c1	419	BCR	C1-C6-C7-C8
18	c1	419	BCR	C5-C6-C7-C8
18	c1	420	BCR	C5-C6-C7-C8
18	c1	420	BCR	C23-C24-C25-C26
18	c1	420	BCR	C23-C24-C25-C30
18	c2	419	BCR	C5-C6-C7-C8
18	c2	419	BCR	C23-C24-C25-C26
18	c2	420	BCR	C1-C6-C7-C8
18	c2	420	BCR	C5-C6-C7-C8
18	c2	421	BCR	C5-C6-C7-C8
18	c2	421	BCR	C23-C24-C25-C26
18	c2	421	BCR	C23-C24-C25-C30
18	c3	401	BCR	C5-C6-C7-C8
18	c3	418	BCR	C5-C6-C7-C8
18	c3	418	BCR	C23-C24-C25-C26
18	c3	419	BCR	C5-C6-C7-C8
18	c3	420	BCR	C5-C6-C7-C8
18	c3	420	BCR	C23-C24-C25-C26
18	c3	420	BCR	C23-C24-C25-C30
18	c4	418	BCR	C5-C6-C7-C8
18	c4	418	BCR	C23-C24-C25-C26
18	c4	419	BCR	C5-C6-C7-C8
18	c4	420	BCR	C5-C6-C7-C8
18	c4	420	BCR	C23-C24-C25-C26
18	c4	420	BCR	C23-C24-C25-C30
18	c5	418	BCR	C5-C6-C7-C8
18	c5	418	BCR	C23-C24-C25-C26
18	c5	419	BCR	C5-C6-C7-C8
18	c5	419	BCR	C23-C24-C25-C26
18	c5	419	BCR	C23-C24-C25-C30
18	c6	401	BCR	C5-C6-C7-C8
18	c6	402	BCR	C23-C24-C25-C26
18	c6	419	BCR	C5-C6-C7-C8
18	c6	419	BCR	C23-C24-C25-C26
18	c6	420	BCR	C5-C6-C7-C8
18	c6	420	BCR	C23-C24-C25-C26
18	c6	420	BCR	C23-C24-C25-C30
15	b5	402	CLA	CBA-CGA-O2A-C1
15	c5	402	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	806	CLA	C8-C10-C11-C12
15	aA	822	CLA	C8-C10-C11-C12
15	aB	837	CLA	C15-C16-C17-C18
15	a2	403	CLA	C13-C15-C16-C17
15	a4	402	CLA	C13-C15-C16-C17
15	bA	806	CLA	C8-C10-C11-C12
15	bA	822	CLA	C8-C10-C11-C12
15	bB	837	CLA	C15-C16-C17-C18
15	b2	403	CLA	C13-C15-C16-C17
15	cA	806	CLA	C8-C10-C11-C12
15	cA	822	CLA	C8-C10-C11-C12
15	cB	837	CLA	C15-C16-C17-C18
15	c2	403	CLA	C13-C15-C16-C17
15	aA	825	CLA	C11-C12-C13-C14
15	bA	825	CLA	C11-C12-C13-C14
15	cA	825	CLA	C11-C12-C13-C14
15	cA	805	CLA	O1D-CGD-O2D-CED
15	aA	824	CLA	O1A-CGA-O2A-C1
15	aB	818	CLA	O1A-CGA-O2A-C1
15	a4	410	CLA	O1A-CGA-O2A-C1
15	a6	411	CLA	O1A-CGA-O2A-C1
15	bA	824	CLA	O1A-CGA-O2A-C1
15	bB	818	CLA	O1A-CGA-O2A-C1
15	b2	411	CLA	O1A-CGA-O2A-C1
15	b4	410	CLA	O1A-CGA-O2A-C1
15	b6	411	CLA	O1A-CGA-O2A-C1
15	cA	824	CLA	O1A-CGA-O2A-C1
15	cB	818	CLA	O1A-CGA-O2A-C1
15	c2	411	CLA	O1A-CGA-O2A-C1
15	aA	835	CLA	C5-C6-C7-C8
15	a5	402	CLA	C13-C15-C16-C17
15	bA	835	CLA	C5-C6-C7-C8
15	b4	402	CLA	C13-C15-C16-C17
15	cA	835	CLA	C5-C6-C7-C8
15	c3	403	CLA	C13-C15-C16-C17
15	c4	402	CLA	C13-C15-C16-C17
15	c5	402	CLA	C13-C15-C16-C17
15	aA	805	CLA	O1D-CGD-O2D-CED
15	bA	805	CLA	O1D-CGD-O2D-CED
15	aA	821	CLA	C4-C3-C5-C6
15	aB	836	CLA	C4-C3-C5-C6
15	bA	821	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	836	CLA	C4-C3-C5-C6
15	cA	821	CLA	C4-C3-C5-C6
15	cB	836	CLA	C4-C3-C5-C6
15	aA	802	CLA	C11-C10-C8-C7
15	aA	803	CLA	C6-C7-C8-C10
15	aA	804	CLA	C11-C12-C13-C15
15	aA	806	CLA	C6-C7-C8-C10
15	aA	809	CLA	C6-C7-C8-C10
15	aA	822	CLA	C12-C13-C15-C16
15	aB	807	CLA	C12-C13-C15-C16
15	aB	814	CLA	C12-C13-C15-C16
15	aB	819	CLA	C6-C7-C8-C10
15	aB	827	CLA	C6-C7-C8-C10
15	aB	828	CLA	C11-C12-C13-C15
15	aB	834	CLA	C6-C7-C8-C10
15	aB	836	CLA	C2-C3-C5-C6
15	aB	840	CLA	C11-C12-C13-C15
15	a1	402	CLA	C6-C7-C8-C10
15	a2	403	CLA	C6-C7-C8-C10
15	a2	404	CLA	C2-C3-C5-C6
15	a3	402	CLA	C12-C13-C15-C16
15	a3	403	CLA	C6-C7-C8-C10
15	a4	402	CLA	C12-C13-C15-C16
15	a4	417	CLA	C2-C3-C5-C6
15	a5	402	CLA	C12-C13-C15-C16
15	a5	403	CLA	C6-C7-C8-C10
15	a5	404	CLA	C2-C3-C5-C6
15	a6	404	CLA	C6-C7-C8-C10
15	a6	405	CLA	C2-C3-C5-C6
15	bA	802	CLA	C11-C10-C8-C7
15	bA	803	CLA	C6-C7-C8-C10
15	bA	804	CLA	C11-C12-C13-C15
15	bA	806	CLA	C6-C7-C8-C10
15	bA	809	CLA	C6-C7-C8-C10
15	bA	822	CLA	C12-C13-C15-C16
15	bB	807	CLA	C12-C13-C15-C16
15	bB	814	CLA	C11-C10-C8-C7
15	bB	814	CLA	C12-C13-C15-C16
15	bB	819	CLA	C6-C7-C8-C10
15	bB	827	CLA	C6-C7-C8-C10
15	bB	828	CLA	C11-C12-C13-C15
15	bB	834	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	836	CLA	C2-C3-C5-C6
15	bB	840	CLA	C11-C12-C13-C15
15	b1	403	CLA	C6-C7-C8-C10
15	b1	404	CLA	C2-C3-C5-C6
15	b2	403	CLA	C6-C7-C8-C10
15	b2	404	CLA	C2-C3-C5-C6
15	b3	402	CLA	C12-C13-C15-C16
15	b3	403	CLA	C6-C7-C8-C10
15	b3	404	CLA	C2-C3-C5-C6
15	b4	402	CLA	C12-C13-C15-C16
15	b4	404	CLA	C2-C3-C5-C6
15	b5	402	CLA	C12-C13-C15-C16
15	b5	403	CLA	C6-C7-C8-C10
15	b5	404	CLA	C2-C3-C5-C6
15	b6	404	CLA	C6-C7-C8-C10
15	b6	405	CLA	C2-C3-C5-C6
15	cA	802	CLA	C11-C10-C8-C7
15	cA	803	CLA	C6-C7-C8-C10
15	cA	804	CLA	C11-C12-C13-C15
15	cA	806	CLA	C6-C7-C8-C10
15	cA	809	CLA	C6-C7-C8-C10
15	cA	822	CLA	C12-C13-C15-C16
15	cB	807	CLA	C12-C13-C15-C16
15	cB	814	CLA	C11-C10-C8-C7
15	cB	814	CLA	C12-C13-C15-C16
15	cB	819	CLA	C6-C7-C8-C10
15	cB	827	CLA	C6-C7-C8-C10
15	cB	828	CLA	C11-C12-C13-C15
15	cB	834	CLA	C6-C7-C8-C10
15	cB	836	CLA	C2-C3-C5-C6
15	cB	840	CLA	C11-C12-C13-C15
15	c1	403	CLA	C6-C7-C8-C10
15	c2	403	CLA	C6-C7-C8-C10
15	c3	402	CLA	C12-C13-C15-C16
15	c3	403	CLA	C6-C7-C8-C10
15	c3	404	CLA	C2-C3-C5-C6
15	c4	402	CLA	C12-C13-C15-C16
15	c4	417	CLA	C2-C3-C5-C6
15	c5	402	CLA	C12-C13-C15-C16
15	c5	403	CLA	C6-C7-C8-C10
15	c5	404	CLA	C2-C3-C5-C6
15	c6	404	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c6	418	CLA	C2-C3-C5-C6
15	aB	814	CLA	O1A-CGA-O2A-C1
15	aB	815	CLA	O1A-CGA-O2A-C1
15	bB	814	CLA	O1A-CGA-O2A-C1
15	bB	815	CLA	O1A-CGA-O2A-C1
15	cB	814	CLA	O1A-CGA-O2A-C1
15	cB	815	CLA	O1A-CGA-O2A-C1
15	c6	411	CLA	O1A-CGA-O2A-C1
15	a3	402	CLA	C13-C15-C16-C17
15	a4	403	CLA	C13-C15-C16-C17
15	b3	402	CLA	C13-C15-C16-C17
15	b5	402	CLA	C13-C15-C16-C17
15	c4	403	CLA	C13-C15-C16-C17
15	c5	403	CLA	C13-C15-C16-C17
18	aA	848	BCR	C15-C16-C17-C18
18	bA	849	BCR	C15-C16-C17-C18
18	cA	847	BCR	C15-C16-C17-C18
15	a1	409	CLA	CBD-CGD-O2D-CED
15	a3	411	CLA	CBD-CGD-O2D-CED
15	aB	806	CLA	C16-C17-C18-C20
15	bB	806	CLA	C16-C17-C18-C20
15	cB	806	CLA	C16-C17-C18-C20
15	aA	809	CLA	O1D-CGD-O2D-CED
15	aL	203	CLA	O1D-CGD-O2D-CED
15	bA	809	CLA	O1D-CGD-O2D-CED
15	bL	204	CLA	O1D-CGD-O2D-CED
15	cA	809	CLA	O1D-CGD-O2D-CED
19	aX	101	LHG	O9-C7-O7-C5
19	bX	101	LHG	O9-C7-O7-C5
19	cX	101	LHG	O9-C7-O7-C5
15	aB	820	CLA	CBA-CGA-O2A-C1
15	aB	834	CLA	CBA-CGA-O2A-C1
15	a5	402	CLA	CBA-CGA-O2A-C1
15	bB	820	CLA	CBA-CGA-O2A-C1
15	bB	834	CLA	CBA-CGA-O2A-C1
15	cB	820	CLA	CBA-CGA-O2A-C1
15	cB	834	CLA	CBA-CGA-O2A-C1
15	aA	809	CLA	C2A-CAA-CBA-CGA
15	aA	814	CLA	C2A-CAA-CBA-CGA
15	aB	813	CLA	C2A-CAA-CBA-CGA
15	aB	831	CLA	C2A-CAA-CBA-CGA
15	aB	835	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aL	203	CLA	C2A-CAA-CBA-CGA
15	bA	809	CLA	C2A-CAA-CBA-CGA
15	bA	814	CLA	C2A-CAA-CBA-CGA
15	bB	813	CLA	C2A-CAA-CBA-CGA
15	bB	831	CLA	C2A-CAA-CBA-CGA
15	bB	835	CLA	C2A-CAA-CBA-CGA
15	bL	204	CLA	C2A-CAA-CBA-CGA
15	cA	809	CLA	C2A-CAA-CBA-CGA
15	cA	814	CLA	C2A-CAA-CBA-CGA
15	cB	813	CLA	C2A-CAA-CBA-CGA
15	cB	831	CLA	C2A-CAA-CBA-CGA
15	cB	835	CLA	C2A-CAA-CBA-CGA
15	cL	203	CLA	C2A-CAA-CBA-CGA
15	cL	203	CLA	O1D-CGD-O2D-CED
15	aB	804	CLA	C13-C15-C16-C17
15	a5	403	CLA	C13-C15-C16-C17
15	bB	804	CLA	C13-C15-C16-C17
15	b1	402	CLA	C13-C15-C16-C17
15	b3	403	CLA	C13-C15-C16-C17
15	b4	403	CLA	C13-C15-C16-C17
15	b5	403	CLA	C13-C15-C16-C17
15	cB	804	CLA	C13-C15-C16-C17
15	c5	402	CLA	O1A-CGA-O2A-C1
15	c5	409	CLA	O1D-CGD-O2D-CED
15	a3	403	CLA	C13-C15-C16-C17
15	c3	402	CLA	C13-C15-C16-C17
15	bB	825	CLA	C3-C5-C6-C7
15	b5	409	CLA	C3-C5-C6-C7
15	c6	410	CLA	C3-C5-C6-C7
18	aF	201	BCR	C22-C23-C24-C25
18	bB	849	BCR	C22-C23-C24-C25
18	cF	202	BCR	C22-C23-C24-C25
15	aA	822	CLA	C16-C17-C18-C19
15	bA	822	CLA	C16-C17-C18-C19
15	cA	822	CLA	C16-C17-C18-C19
15	c1	403	CLA	C13-C15-C16-C17
15	aB	807	CLA	O1D-CGD-O2D-CED
15	a5	409	CLA	O1D-CGD-O2D-CED
15	bB	807	CLA	O1D-CGD-O2D-CED
15	b2	411	CLA	O1D-CGD-O2D-CED
15	cB	807	CLA	O1D-CGD-O2D-CED
19	aA	853	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	bA	854	LHG	C8-C7-O7-C5
19	cA	852	LHG	C8-C7-O7-C5
18	aB	848	BCR	C10-C11-C12-C13
18	a5	418	BCR	C18-C19-C20-C21
18	bB	848	BCR	C10-C11-C12-C13
18	b2	401	BCR	C10-C11-C12-C13
18	b5	418	BCR	C18-C19-C20-C21
18	cB	848	BCR	C10-C11-C12-C13
18	cF	205	BCR	C18-C19-C20-C21
15	a6	403	CLA	C13-C15-C16-C17
15	b6	403	CLA	C13-C15-C16-C17
15	c1	402	CLA	C13-C15-C16-C17
15	c6	403	CLA	C13-C15-C16-C17
15	aB	811	CLA	CBD-CGD-O2D-CED
15	bB	811	CLA	CBD-CGD-O2D-CED
15	cA	833	CLA	CBD-CGD-O2D-CED
15	cB	811	CLA	CBD-CGD-O2D-CED
15	aB	825	CLA	C3-C5-C6-C7
15	cB	825	CLA	C3-C5-C6-C7
19	aA	853	LHG	O7-C5-C6-O8
19	bA	854	LHG	O7-C5-C6-O8
19	cA	852	LHG	O7-C5-C6-O8
15	bA	833	CLA	CBD-CGD-O2D-CED
15	b5	402	CLA	O1A-CGA-O2A-C1
15	a1	401	CLA	C13-C15-C16-C17
15	a1	402	CLA	C13-C15-C16-C17
15	b1	403	CLA	C13-C15-C16-C17
15	b2	402	CLA	C13-C15-C16-C17
15	aA	821	CLA	C2-C3-C5-C6
15	a2	418	CLA	C2-C3-C5-C6
15	a3	417	CLA	C2-C3-C5-C6
15	a6	418	CLA	C2-C3-C5-C6
15	bA	821	CLA	C2-C3-C5-C6
15	b2	418	CLA	C2-C3-C5-C6
15	b3	417	CLA	C2-C3-C5-C6
15	b6	418	CLA	C2-C3-C5-C6
15	cA	821	CLA	C2-C3-C5-C6
15	c2	418	CLA	C2-C3-C5-C6
15	c3	417	CLA	C2-C3-C5-C6
15	aA	802	CLA	C11-C10-C8-C9
15	aA	822	CLA	C11-C10-C8-C9
15	aA	831	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	835	CLA	C14-C13-C15-C16
15	aB	828	CLA	C11-C12-C13-C14
15	aB	837	CLA	C6-C7-C8-C9
15	aB	840	CLA	C11-C12-C13-C14
15	aB	840	CLA	C14-C13-C15-C16
15	bA	802	CLA	C11-C10-C8-C9
15	bA	822	CLA	C11-C10-C8-C9
15	bA	831	CLA	C11-C10-C8-C9
15	bA	835	CLA	C14-C13-C15-C16
15	bB	828	CLA	C11-C12-C13-C14
15	bB	837	CLA	C6-C7-C8-C9
15	bB	840	CLA	C11-C12-C13-C14
15	bB	840	CLA	C14-C13-C15-C16
15	cA	802	CLA	C11-C10-C8-C9
15	cA	822	CLA	C11-C10-C8-C9
15	cA	831	CLA	C11-C10-C8-C9
15	cA	835	CLA	C14-C13-C15-C16
15	cB	828	CLA	C11-C12-C13-C14
15	cB	837	CLA	C6-C7-C8-C9
15	cB	840	CLA	C11-C12-C13-C14
15	cB	840	CLA	C14-C13-C15-C16
16	aA	846	PQN	C19-C18-C20-C21
16	bA	846	PQN	C19-C18-C20-C21
16	cA	845	PQN	C19-C18-C20-C21
15	aA	824	CLA	CBD-CGD-O2D-CED
15	aA	833	CLA	CBD-CGD-O2D-CED
15	a2	410	CLA	C3-C5-C6-C7
15	a5	402	CLA	C3-C5-C6-C7
15	b5	402	CLA	C3-C5-C6-C7
15	c2	410	CLA	C3-C5-C6-C7
15	c5	402	CLA	C3-C5-C6-C7
15	cA	834	CLA	O1D-CGD-O2D-CED
15	aA	803	CLA	C2A-CAA-CBA-CGA
15	aA	819	CLA	C2A-CAA-CBA-CGA
15	aA	821	CLA	C2A-CAA-CBA-CGA
15	bA	803	CLA	C2A-CAA-CBA-CGA
15	bA	819	CLA	C2A-CAA-CBA-CGA
15	bA	821	CLA	C2A-CAA-CBA-CGA
15	cA	803	CLA	C2A-CAA-CBA-CGA
15	cA	819	CLA	C2A-CAA-CBA-CGA
15	cA	821	CLA	C2A-CAA-CBA-CGA
18	a1	421	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a6	421	BCR	C11-C12-C13-C35
15	aA	834	CLA	O1D-CGD-O2D-CED
15	aB	826	CLA	O1D-CGD-O2D-CED
15	a2	411	CLA	O1D-CGD-O2D-CED
15	bA	834	CLA	O1D-CGD-O2D-CED
15	bB	826	CLA	O1D-CGD-O2D-CED
15	cB	826	CLA	O1D-CGD-O2D-CED
15	c2	402	CLA	C13-C15-C16-C17
15	cA	824	CLA	CBD-CGD-O2D-CED
19	cA	852	LHG	C27-C28-C29-C30
15	a5	402	CLA	O1A-CGA-O2A-C1
15	aA	805	CLA	C1A-C2A-CAA-CBA
15	aA	809	CLA	C1A-C2A-CAA-CBA
15	aA	810	CLA	C1A-C2A-CAA-CBA
15	aA	812	CLA	C1A-C2A-CAA-CBA
15	aA	819	CLA	C1A-C2A-CAA-CBA
15	aA	822	CLA	C1A-C2A-CAA-CBA
15	aA	831	CLA	C1A-C2A-CAA-CBA
15	aA	833	CLA	C1A-C2A-CAA-CBA
15	aA	835	CLA	C1A-C2A-CAA-CBA
15	aA	836	CLA	C1A-C2A-CAA-CBA
15	aA	845	CLA	C1A-C2A-CAA-CBA
15	aB	815	CLA	C1A-C2A-CAA-CBA
15	aB	830	CLA	C1A-C2A-CAA-CBA
15	aB	833	CLA	C1A-C2A-CAA-CBA
15	aK	102	CLA	C1A-C2A-CAA-CBA
15	a1	401	CLA	C1A-C2A-CAA-CBA
15	a1	404	CLA	C1A-C2A-CAA-CBA
15	a1	411	CLA	C1A-C2A-CAA-CBA
15	a2	402	CLA	C1A-C2A-CAA-CBA
15	a2	413	CLA	C1A-C2A-CAA-CBA
15	a3	402	CLA	C1A-C2A-CAA-CBA
15	a3	405	CLA	C1A-C2A-CAA-CBA
15	a4	402	CLA	C1A-C2A-CAA-CBA
15	a4	408	CLA	C1A-C2A-CAA-CBA
15	a4	412	CLA	C1A-C2A-CAA-CBA
15	a5	402	CLA	C1A-C2A-CAA-CBA
15	a5	405	CLA	C1A-C2A-CAA-CBA
15	a5	412	CLA	C1A-C2A-CAA-CBA
15	a5	420	CLA	C1A-C2A-CAA-CBA
15	a6	403	CLA	C1A-C2A-CAA-CBA
15	a6	406	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	409	CLA	C1A-C2A-CAA-CBA
15	a6	413	CLA	C1A-C2A-CAA-CBA
15	a6	422	CLA	C1A-C2A-CAA-CBA
15	bA	805	CLA	C1A-C2A-CAA-CBA
15	bA	809	CLA	C1A-C2A-CAA-CBA
15	bA	810	CLA	C1A-C2A-CAA-CBA
15	bA	812	CLA	C1A-C2A-CAA-CBA
15	bA	819	CLA	C1A-C2A-CAA-CBA
15	bA	822	CLA	C1A-C2A-CAA-CBA
15	bA	831	CLA	C1A-C2A-CAA-CBA
15	bA	833	CLA	C1A-C2A-CAA-CBA
15	bA	835	CLA	C1A-C2A-CAA-CBA
15	bA	836	CLA	C1A-C2A-CAA-CBA
15	bA	845	CLA	C1A-C2A-CAA-CBA
15	bB	815	CLA	C1A-C2A-CAA-CBA
15	bB	830	CLA	C1A-C2A-CAA-CBA
15	bB	833	CLA	C1A-C2A-CAA-CBA
15	bK	101	CLA	C1A-C2A-CAA-CBA
15	b1	402	CLA	C1A-C2A-CAA-CBA
15	b1	405	CLA	C1A-C2A-CAA-CBA
15	b1	412	CLA	C1A-C2A-CAA-CBA
15	b2	402	CLA	C1A-C2A-CAA-CBA
15	b2	405	CLA	C1A-C2A-CAA-CBA
15	b2	413	CLA	C1A-C2A-CAA-CBA
15	b3	402	CLA	C1A-C2A-CAA-CBA
15	b3	405	CLA	C1A-C2A-CAA-CBA
15	b4	402	CLA	C1A-C2A-CAA-CBA
15	b4	408	CLA	C1A-C2A-CAA-CBA
15	b4	412	CLA	C1A-C2A-CAA-CBA
15	b5	402	CLA	C1A-C2A-CAA-CBA
15	b5	405	CLA	C1A-C2A-CAA-CBA
15	b5	412	CLA	C1A-C2A-CAA-CBA
15	b5	420	CLA	C1A-C2A-CAA-CBA
15	b6	403	CLA	C1A-C2A-CAA-CBA
15	b6	406	CLA	C1A-C2A-CAA-CBA
15	b6	413	CLA	C1A-C2A-CAA-CBA
15	cA	805	CLA	C1A-C2A-CAA-CBA
15	cA	809	CLA	C1A-C2A-CAA-CBA
15	cA	810	CLA	C1A-C2A-CAA-CBA
15	cA	812	CLA	C1A-C2A-CAA-CBA
15	cA	819	CLA	C1A-C2A-CAA-CBA
15	cA	822	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	831	CLA	C1A-C2A-CAA-CBA
15	cA	833	CLA	C1A-C2A-CAA-CBA
15	cA	835	CLA	C1A-C2A-CAA-CBA
15	cA	836	CLA	C1A-C2A-CAA-CBA
15	cA	844	CLA	C1A-C2A-CAA-CBA
15	cB	815	CLA	C1A-C2A-CAA-CBA
15	cB	830	CLA	C1A-C2A-CAA-CBA
15	cB	833	CLA	C1A-C2A-CAA-CBA
15	cK	102	CLA	C1A-C2A-CAA-CBA
15	c1	402	CLA	C1A-C2A-CAA-CBA
15	c1	405	CLA	C1A-C2A-CAA-CBA
15	c1	412	CLA	C1A-C2A-CAA-CBA
15	c2	402	CLA	C1A-C2A-CAA-CBA
15	c2	405	CLA	C1A-C2A-CAA-CBA
15	c2	413	CLA	C1A-C2A-CAA-CBA
15	c3	402	CLA	C1A-C2A-CAA-CBA
15	c3	405	CLA	C1A-C2A-CAA-CBA
15	c4	402	CLA	C1A-C2A-CAA-CBA
15	c4	405	CLA	C1A-C2A-CAA-CBA
15	c4	408	CLA	C1A-C2A-CAA-CBA
15	c4	412	CLA	C1A-C2A-CAA-CBA
15	c5	402	CLA	C1A-C2A-CAA-CBA
15	c5	405	CLA	C1A-C2A-CAA-CBA
15	c5	412	CLA	C1A-C2A-CAA-CBA
15	c5	420	CLA	C1A-C2A-CAA-CBA
15	c6	403	CLA	C1A-C2A-CAA-CBA
15	c6	406	CLA	C1A-C2A-CAA-CBA
15	c6	413	CLA	C1A-C2A-CAA-CBA
19	aA	853	LHG	C27-C28-C29-C30
19	bA	854	LHG	C27-C28-C29-C30
20	aB	850	LMG	C31-C32-C33-C34
20	bB	851	LMG	C31-C32-C33-C34
20	cB	850	LMG	C31-C32-C33-C34
15	a2	402	CLA	C13-C15-C16-C17
19	cA	853	LHG	C4-O6-P-O3
19	aA	853	LHG	C17-C18-C19-C20
15	bA	824	CLA	CBD-CGD-O2D-CED
15	aA	804	CLA	O1D-CGD-O2D-CED
15	b3	409	CLA	O1D-CGD-O2D-CED
19	bA	854	LHG	C17-C18-C19-C20
19	cA	852	LHG	C17-C18-C19-C20
15	aB	807	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	840	CLA	C13-C15-C16-C17
15	bB	840	CLA	C13-C15-C16-C17
15	cB	807	CLA	C15-C16-C17-C18
15	cB	840	CLA	C13-C15-C16-C17
15	bA	804	CLA	O1D-CGD-O2D-CED
15	cA	804	CLA	O1D-CGD-O2D-CED
15	a3	409	CLA	O1D-CGD-O2D-CED
15	bB	807	CLA	C15-C16-C17-C18
15	aA	822	CLA	C16-C17-C18-C20
15	bA	822	CLA	C16-C17-C18-C20
15	cA	822	CLA	C16-C17-C18-C20
15	b2	410	CLA	C3-C5-C6-C7
15	aA	820	CLA	C8-C10-C11-C12
15	bA	820	CLA	C8-C10-C11-C12
15	cA	820	CLA	C8-C10-C11-C12
15	b2	404	CLA	CBA-CGA-O2A-C1
15	bA	836	CLA	C5-C6-C7-C8
19	aA	854	LHG	C11-C10-C9-C8
19	bA	855	LHG	C11-C10-C9-C8
19	cA	853	LHG	C11-C10-C9-C8
15	aA	822	CLA	C5-C6-C7-C8
15	cA	822	CLA	C5-C6-C7-C8
15	aA	836	CLA	C5-C6-C7-C8
15	cA	836	CLA	C5-C6-C7-C8
15	aB	834	CLA	O1A-CGA-O2A-C1
15	a6	422	CLA	O1A-CGA-O2A-C1
15	bB	834	CLA	O1A-CGA-O2A-C1
15	cB	834	CLA	O1A-CGA-O2A-C1
15	aA	810	CLA	C15-C16-C17-C18
15	bA	810	CLA	C15-C16-C17-C18
15	aB	822	CLA	C2A-CAA-CBA-CGA
15	bB	822	CLA	C2A-CAA-CBA-CGA
15	cB	822	CLA	C2A-CAA-CBA-CGA
15	aA	803	CLA	C16-C17-C18-C20
15	bA	803	CLA	C16-C17-C18-C20
15	cA	803	CLA	C16-C17-C18-C20
15	aA	822	CLA	O1D-CGD-O2D-CED
15	bA	822	CLA	O1D-CGD-O2D-CED
15	bA	826	CLA	O1D-CGD-O2D-CED
15	cA	822	CLA	O1D-CGD-O2D-CED
15	a6	403	CLA	C3-C5-C6-C7
15	b6	403	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	402	CLA	C3-C5-C6-C7
15	c6	403	CLA	C3-C5-C6-C7
15	cA	826	CLA	O1D-CGD-O2D-CED
15	bA	822	CLA	C5-C6-C7-C8
15	cA	810	CLA	C15-C16-C17-C18
20	aB	850	LMG	C35-C36-C37-C38
20	bB	851	LMG	C35-C36-C37-C38
15	aA	826	CLA	O1D-CGD-O2D-CED
15	c2	411	CLA	O1D-CGD-O2D-CED
20	cB	850	LMG	C35-C36-C37-C38
15	b6	412	CLA	CBD-CGD-O2D-CED
15	aA	831	CLA	C5-C6-C7-C8
15	bA	831	CLA	C5-C6-C7-C8
15	bL	202	CLA	C13-C15-C16-C17
15	cA	831	CLA	C5-C6-C7-C8
15	cL	201	CLA	C13-C15-C16-C17
19	aA	854	LHG	C10-C11-C12-C13
19	bA	855	LHG	C10-C11-C12-C13
19	cA	853	LHG	C10-C11-C12-C13
15	c4	409	CLA	C3-C5-C6-C7
15	aL	201	CLA	C13-C15-C16-C17
15	a6	412	CLA	CBD-CGD-O2D-CED
15	aB	828	CLA	CAA-CBA-CGA-O2A
15	bB	828	CLA	CAA-CBA-CGA-O2A
15	cB	828	CLA	CAA-CBA-CGA-O2A
15	c3	410	CLA	O1D-CGD-O2D-CED
15	aA	829	CLA	C10-C11-C12-C13
15	bA	829	CLA	C10-C11-C12-C13
15	cA	829	CLA	C10-C11-C12-C13
18	aB	848	BCR	C20-C21-C22-C37
18	aB	849	BCR	C11-C10-C9-C34
18	aI	101	BCR	C20-C21-C22-C37
18	a2	401	BCR	C20-C21-C22-C37
18	a2	419	BCR	C16-C17-C18-C36
18	a3	418	BCR	C20-C21-C22-C37
18	a4	418	BCR	C20-C21-C22-C37
18	bB	848	BCR	C20-C21-C22-C37
18	bB	850	BCR	C11-C10-C9-C34
18	bI	101	BCR	C20-C21-C22-C37
18	b2	419	BCR	C16-C17-C18-C36
18	b4	418	BCR	C20-C21-C22-C37
18	cB	848	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cB	849	BCR	C11-C10-C9-C34
18	cI	101	BCR	C20-C21-C22-C37
18	c2	401	BCR	C20-C21-C22-C37
18	c2	419	BCR	C16-C17-C18-C36
18	c2	419	BCR	C20-C21-C22-C37
18	c5	418	BCR	C20-C21-C22-C37
15	bB	826	CLA	O1A-CGA-O2A-C1
15	aB	828	CLA	C4-C3-C5-C6
15	bB	828	CLA	C4-C3-C5-C6
15	cB	828	CLA	C4-C3-C5-C6
20	bB	851	LMG	C39-C40-C41-C42
15	aA	812	CLA	CBA-CGA-O2A-C1
15	c2	404	CLA	CBA-CGA-O2A-C1
20	aB	850	LMG	C39-C40-C41-C42
15	a4	410	CLA	CBD-CGD-O2D-CED
15	bK	101	CLA	CBD-CGD-O2D-CED
15	b3	411	CLA	CBD-CGD-O2D-CED
15	cK	102	CLA	CBD-CGD-O2D-CED
15	c4	410	CLA	CBD-CGD-O2D-CED
15	aA	843	CLA	C15-C16-C17-C18
15	cA	842	CLA	C15-C16-C17-C18
20	cB	850	LMG	C39-C40-C41-C42
15	aB	826	CLA	O1A-CGA-O2A-C1
15	cB	826	CLA	O1A-CGA-O2A-C1
15	aB	821	CLA	C2A-CAA-CBA-CGA
15	bB	821	CLA	C2A-CAA-CBA-CGA
15	cB	821	CLA	C2A-CAA-CBA-CGA
15	bA	843	CLA	C15-C16-C17-C18
15	b5	403	CLA	C8-C10-C11-C12
15	a6	411	CLA	O1D-CGD-O2D-CED
15	b3	410	CLA	O1D-CGD-O2D-CED
15	c3	409	CLA	O1D-CGD-O2D-CED
15	aK	102	CLA	CBD-CGD-O2D-CED
15	a4	402	CLA	C3-C5-C6-C7
15	b4	402	CLA	C3-C5-C6-C7
15	b6	411	CLA	O1D-CGD-O2D-CED
15	c6	411	CLA	O1D-CGD-O2D-CED
15	aA	810	CLA	C8-C10-C11-C12
15	aB	828	CLA	C8-C10-C11-C12
15	bB	828	CLA	C8-C10-C11-C12
15	cB	828	CLA	C8-C10-C11-C12
16	aA	846	PQN	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	bA	846	PQN	C20-C21-C22-C23
16	cA	845	PQN	C20-C21-C22-C23
15	aB	828	CLA	CBA-CGA-O2A-C1
15	a2	404	CLA	CBA-CGA-O2A-C1
15	bA	812	CLA	CBA-CGA-O2A-C1
15	bB	828	CLA	CBA-CGA-O2A-C1
15	cA	812	CLA	CBA-CGA-O2A-C1
15	cB	828	CLA	CBA-CGA-O2A-C1
15	aB	820	CLA	O1A-CGA-O2A-C1
15	bB	820	CLA	O1A-CGA-O2A-C1
15	cB	820	CLA	O1A-CGA-O2A-C1
15	a3	410	CLA	O1D-CGD-O2D-CED
15	b4	410	CLA	CBD-CGD-O2D-CED
15	a5	403	CLA	C8-C10-C11-C12
15	bA	810	CLA	C8-C10-C11-C12
15	cA	810	CLA	C8-C10-C11-C12
16	aB	843	PQN	C18-C20-C21-C22
16	bB	843	PQN	C18-C20-C21-C22
16	cB	843	PQN	C18-C20-C21-C22
20	aB	850	LMG	C15-C16-C17-C18
20	bB	851	LMG	C15-C16-C17-C18
20	cB	850	LMG	C15-C16-C17-C18
15	b2	404	CLA	O1A-CGA-O2A-C1
15	aA	818	CLA	C6-C7-C8-C9
15	a1	402	CLA	C8-C10-C11-C12
15	a3	403	CLA	C8-C10-C11-C12
15	b1	403	CLA	C8-C10-C11-C12
15	b3	403	CLA	C8-C10-C11-C12
15	c1	403	CLA	C8-C10-C11-C12
15	c5	403	CLA	C8-C10-C11-C12
18	aB	846	BCR	C12-C13-C14-C15
18	a2	421	BCR	C20-C21-C22-C23
18	a6	420	BCR	C20-C21-C22-C23
18	bB	846	BCR	C12-C13-C14-C15
18	b3	420	BCR	C20-C21-C22-C23
18	b4	420	BCR	C20-C21-C22-C23
18	cB	846	BCR	C12-C13-C14-C15
18	c4	420	BCR	C20-C21-C22-C23
18	c6	420	BCR	C20-C21-C22-C23
15	bA	818	CLA	C6-C7-C8-C9
15	cA	818	CLA	C6-C7-C8-C9
19	aX	101	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	bX	101	LHG	O7-C5-C6-O8
19	cX	101	LHG	O7-C5-C6-O8
15	aA	812	CLA	C5-C6-C7-C8
15	a6	404	CLA	C8-C10-C11-C12
15	cA	812	CLA	C5-C6-C7-C8
15	c2	404	CLA	O1A-CGA-O2A-C1
15	aA	806	CLA	C15-C16-C17-C18
15	bA	806	CLA	C15-C16-C17-C18
15	bA	812	CLA	C5-C6-C7-C8
15	cA	806	CLA	C15-C16-C17-C18
15	c3	403	CLA	C8-C10-C11-C12
15	aA	806	CLA	C11-C12-C13-C15
15	aA	810	CLA	C11-C12-C13-C15
15	aA	812	CLA	C12-C13-C15-C16
15	aA	821	CLA	C6-C7-C8-C10
15	aA	821	CLA	C11-C12-C13-C15
15	aA	822	CLA	C11-C10-C8-C7
15	aA	826	CLA	C12-C13-C15-C16
15	aA	827	CLA	C12-C13-C15-C16
15	aA	829	CLA	C11-C12-C13-C15
15	aA	830	CLA	C12-C13-C15-C16
15	aA	834	CLA	C6-C7-C8-C10
15	aA	834	CLA	C12-C13-C15-C16
15	aA	835	CLA	C12-C13-C15-C16
15	aA	841	CLA	C6-C7-C8-C10
15	aB	804	CLA	C12-C13-C15-C16
15	aB	806	CLA	C11-C10-C8-C7
15	aB	814	CLA	C11-C10-C8-C7
15	aB	815	CLA	C11-C10-C8-C7
15	aB	827	CLA	C11-C12-C13-C15
15	aB	828	CLA	C2-C3-C5-C6
15	aB	833	CLA	C6-C7-C8-C10
15	aB	837	CLA	C6-C7-C8-C10
15	aL	202	CLA	C11-C12-C13-C15
15	a1	402	CLA	C11-C12-C13-C15
15	a1	422	CLA	C11-C12-C13-C15
15	a2	403	CLA	C11-C12-C13-C15
15	a2	406	CLA	C11-C12-C13-C15
15	a2	422	CLA	C11-C12-C13-C15
15	a3	421	CLA	C11-C12-C13-C15
15	a4	403	CLA	C11-C10-C8-C7
15	a4	421	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	403	CLA	C11-C10-C8-C7
15	a5	420	CLA	C11-C12-C13-C15
15	a6	404	CLA	C11-C12-C13-C15
15	a6	422	CLA	C11-C12-C13-C15
15	bA	806	CLA	C11-C12-C13-C15
15	bA	810	CLA	C11-C12-C13-C15
15	bA	812	CLA	C12-C13-C15-C16
15	bA	821	CLA	C6-C7-C8-C10
15	bA	821	CLA	C11-C12-C13-C15
15	bA	822	CLA	C11-C10-C8-C7
15	bA	826	CLA	C12-C13-C15-C16
15	bA	827	CLA	C12-C13-C15-C16
15	bA	829	CLA	C11-C12-C13-C15
15	bA	830	CLA	C12-C13-C15-C16
15	bA	834	CLA	C6-C7-C8-C10
15	bA	834	CLA	C12-C13-C15-C16
15	bA	835	CLA	C12-C13-C15-C16
15	bA	841	CLA	C6-C7-C8-C10
15	bB	804	CLA	C12-C13-C15-C16
15	bB	806	CLA	C11-C10-C8-C7
15	bB	815	CLA	C11-C10-C8-C7
15	bB	827	CLA	C11-C12-C13-C15
15	bB	828	CLA	C2-C3-C5-C6
15	bB	833	CLA	C6-C7-C8-C10
15	bB	837	CLA	C6-C7-C8-C10
15	bL	203	CLA	C11-C12-C13-C15
15	b1	403	CLA	C11-C10-C8-C7
15	b1	403	CLA	C11-C12-C13-C15
15	b2	403	CLA	C11-C12-C13-C15
15	b2	406	CLA	C11-C12-C13-C15
15	b2	422	CLA	C11-C12-C13-C15
15	b3	421	CLA	C11-C12-C13-C15
15	b4	403	CLA	C11-C10-C8-C7
15	b4	403	CLA	C11-C12-C13-C15
15	b4	421	CLA	C11-C12-C13-C15
15	b5	403	CLA	C11-C10-C8-C7
15	b5	420	CLA	C11-C12-C13-C15
15	b6	404	CLA	C11-C12-C13-C15
15	b6	422	CLA	C11-C12-C13-C15
15	cA	806	CLA	C11-C12-C13-C15
15	cA	810	CLA	C11-C12-C13-C15
15	cA	812	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	821	CLA	C6-C7-C8-C10
15	cA	821	CLA	C11-C12-C13-C15
15	cA	822	CLA	C11-C10-C8-C7
15	cA	826	CLA	C12-C13-C15-C16
15	cA	827	CLA	C12-C13-C15-C16
15	cA	829	CLA	C11-C12-C13-C15
15	cA	830	CLA	C12-C13-C15-C16
15	cA	834	CLA	C6-C7-C8-C10
15	cA	834	CLA	C12-C13-C15-C16
15	cA	835	CLA	C12-C13-C15-C16
15	cA	841	CLA	C6-C7-C8-C10
15	cB	804	CLA	C12-C13-C15-C16
15	cB	806	CLA	C11-C10-C8-C7
15	cB	815	CLA	C11-C10-C8-C7
15	cB	827	CLA	C11-C12-C13-C15
15	cB	828	CLA	C2-C3-C5-C6
15	cB	833	CLA	C6-C7-C8-C10
15	cB	837	CLA	C6-C7-C8-C10
15	cL	202	CLA	C11-C12-C13-C15
15	c1	402	CLA	C12-C13-C15-C16
15	c1	403	CLA	C11-C12-C13-C15
15	c2	403	CLA	C11-C12-C13-C15
15	c2	406	CLA	C11-C12-C13-C15
15	c2	422	CLA	C11-C12-C13-C15
15	c3	421	CLA	C11-C12-C13-C15
15	c4	403	CLA	C11-C10-C8-C7
15	c4	421	CLA	C11-C12-C13-C15
15	c5	403	CLA	C11-C10-C8-C7
15	c5	420	CLA	C11-C12-C13-C15
15	c6	404	CLA	C11-C12-C13-C15
16	aA	846	PQN	C17-C18-C20-C21
16	bA	846	PQN	C17-C18-C20-C21
16	cA	845	PQN	C17-C18-C20-C21
15	a2	404	CLA	O1A-CGA-O2A-C1
15	aA	806	CLA	C11-C12-C13-C14
15	aA	810	CLA	C11-C12-C13-C14
15	aA	834	CLA	C14-C13-C15-C16
15	aA	841	CLA	C6-C7-C8-C9
15	aB	803	CLA	C14-C13-C15-C16
15	aB	804	CLA	C14-C13-C15-C16
15	aB	806	CLA	C11-C10-C8-C9
15	aB	811	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	814	CLA	C11-C10-C8-C9
15	aB	820	CLA	C11-C10-C8-C9
15	aB	827	CLA	C11-C12-C13-C14
15	aB	833	CLA	C6-C7-C8-C9
15	aB	833	CLA	C11-C10-C8-C9
15	aB	837	CLA	C11-C12-C13-C14
15	aL	202	CLA	C6-C7-C8-C9
15	aL	202	CLA	C11-C12-C13-C14
15	a1	401	CLA	C11-C10-C8-C9
15	a1	401	CLA	C14-C13-C15-C16
15	a1	402	CLA	C11-C12-C13-C14
15	a2	402	CLA	C11-C10-C8-C9
15	a2	403	CLA	C11-C12-C13-C14
15	a3	402	CLA	C11-C10-C8-C9
15	a4	402	CLA	C11-C10-C8-C9
15	a5	402	CLA	C11-C10-C8-C9
15	a6	403	CLA	C11-C10-C8-C9
15	a6	404	CLA	C11-C12-C13-C14
15	bA	806	CLA	C11-C12-C13-C14
15	bA	810	CLA	C11-C12-C13-C14
15	bA	834	CLA	C14-C13-C15-C16
15	bA	841	CLA	C6-C7-C8-C9
15	bB	803	CLA	C14-C13-C15-C16
15	bB	804	CLA	C14-C13-C15-C16
15	bB	806	CLA	C11-C10-C8-C9
15	bB	811	CLA	C6-C7-C8-C9
15	bB	814	CLA	C11-C10-C8-C9
15	bB	820	CLA	C11-C10-C8-C9
15	bB	827	CLA	C11-C12-C13-C14
15	bB	833	CLA	C6-C7-C8-C9
15	bB	833	CLA	C11-C10-C8-C9
15	bB	837	CLA	C11-C12-C13-C14
15	bL	203	CLA	C6-C7-C8-C9
15	bL	203	CLA	C11-C12-C13-C14
15	b1	402	CLA	C11-C10-C8-C9
15	b1	402	CLA	C14-C13-C15-C16
15	b1	403	CLA	C11-C12-C13-C14
15	b2	402	CLA	C11-C10-C8-C9
15	b2	403	CLA	C11-C12-C13-C14
15	b3	402	CLA	C11-C10-C8-C9
15	b4	402	CLA	C11-C10-C8-C9
15	b5	402	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b6	403	CLA	C11-C10-C8-C9
15	b6	404	CLA	C11-C12-C13-C14
15	cA	806	CLA	C11-C12-C13-C14
15	cA	810	CLA	C11-C12-C13-C14
15	cA	834	CLA	C14-C13-C15-C16
15	cA	841	CLA	C6-C7-C8-C9
15	cB	803	CLA	C14-C13-C15-C16
15	cB	804	CLA	C14-C13-C15-C16
15	cB	806	CLA	C11-C10-C8-C9
15	cB	811	CLA	C6-C7-C8-C9
15	cB	814	CLA	C11-C10-C8-C9
15	cB	820	CLA	C11-C10-C8-C9
15	cB	827	CLA	C11-C12-C13-C14
15	cB	833	CLA	C6-C7-C8-C9
15	cB	833	CLA	C11-C10-C8-C9
15	cB	837	CLA	C11-C12-C13-C14
15	cL	202	CLA	C6-C7-C8-C9
15	cL	202	CLA	C11-C12-C13-C14
15	c1	402	CLA	C11-C10-C8-C9
15	c1	403	CLA	C11-C12-C13-C14
15	c2	402	CLA	C11-C10-C8-C9
15	c3	402	CLA	C11-C10-C8-C9
15	c4	402	CLA	C11-C10-C8-C9
15	c5	402	CLA	C11-C10-C8-C9
15	c5	403	CLA	C11-C12-C13-C14
15	c6	403	CLA	C11-C10-C8-C9
15	c6	404	CLA	C11-C12-C13-C14
15	a4	411	CLA	CBD-CGD-O2D-CED
15	c6	412	CLA	CBD-CGD-O2D-CED
15	a1	403	CLA	CBA-CGA-O2A-C1
15	a3	404	CLA	CBA-CGA-O2A-C1
15	a5	404	CLA	CBA-CGA-O2A-C1
15	a6	422	CLA	CBA-CGA-O2A-C1
15	b1	404	CLA	CBA-CGA-O2A-C1
15	b3	404	CLA	CBA-CGA-O2A-C1
15	b5	404	CLA	CBA-CGA-O2A-C1
15	c1	404	CLA	CBA-CGA-O2A-C1
15	c3	404	CLA	CBA-CGA-O2A-C1
15	c5	404	CLA	CBA-CGA-O2A-C1
15	b6	404	CLA	C8-C10-C11-C12
15	c6	404	CLA	C8-C10-C11-C12
18	aB	849	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bB	850	BCR	C11-C12-C13-C35
18	b6	402	BCR	C11-C12-C13-C35
18	cB	849	BCR	C11-C12-C13-C35
15	aA	830	CLA	C15-C16-C17-C18
15	bA	830	CLA	C15-C16-C17-C18
15	aB	823	CLA	C6-C7-C8-C10
15	a2	422	CLA	C16-C17-C18-C19
15	bB	823	CLA	C6-C7-C8-C10
15	b2	422	CLA	C16-C17-C18-C19
15	cB	823	CLA	C6-C7-C8-C10
15	c2	422	CLA	C16-C17-C18-C19
15	aA	805	CLA	C11-C12-C13-C14
15	bA	805	CLA	C11-C12-C13-C14
15	bA	819	CLA	C2C-C3C-CAC-CBC
15	cA	805	CLA	C11-C12-C13-C14
15	cA	819	CLA	C2C-C3C-CAC-CBC
15	a1	401	CLA	C3-C5-C6-C7
15	a2	402	CLA	C3-C5-C6-C7
15	a4	409	CLA	C3-C5-C6-C7
15	b1	402	CLA	C3-C5-C6-C7
15	b2	402	CLA	C3-C5-C6-C7
15	b4	409	CLA	C3-C5-C6-C7
15	c2	402	CLA	C3-C5-C6-C7
15	aB	801	CLA	O1D-CGD-O2D-CED
15	cB	801	CLA	O1D-CGD-O2D-CED
15	aB	819	CLA	C10-C11-C12-C13
15	aB	829	CLA	C10-C11-C12-C13
15	a4	403	CLA	C8-C10-C11-C12
15	bB	819	CLA	C10-C11-C12-C13
15	bB	829	CLA	C10-C11-C12-C13
15	cB	819	CLA	C10-C11-C12-C13
15	cB	829	CLA	C10-C11-C12-C13
15	aA	841	CLA	CBA-CGA-O2A-C1
15	aB	830	CLA	CBA-CGA-O2A-C1
15	a4	404	CLA	CBA-CGA-O2A-C1
15	a6	405	CLA	CBA-CGA-O2A-C1
15	bA	841	CLA	CBA-CGA-O2A-C1
15	bB	830	CLA	CBA-CGA-O2A-C1
15	b4	404	CLA	CBA-CGA-O2A-C1
15	b6	405	CLA	CBA-CGA-O2A-C1
15	cA	841	CLA	CBA-CGA-O2A-C1
15	cB	830	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	404	CLA	CBA-CGA-O2A-C1
15	c6	405	CLA	CBA-CGA-O2A-C1
15	bB	801	CLA	O1D-CGD-O2D-CED
15	aA	819	CLA	C2C-C3C-CAC-CBC
15	cA	830	CLA	C15-C16-C17-C18
18	aA	849	BCR	C22-C23-C24-C25
18	bA	850	BCR	C22-C23-C24-C25
18	cA	848	BCR	C22-C23-C24-C25
15	bB	805	CLA	CBD-CGD-O2D-CED
15	b4	411	CLA	CBD-CGD-O2D-CED
15	cB	805	CLA	CBD-CGD-O2D-CED
15	aA	826	CLA	C8-C10-C11-C12
15	aB	833	CLA	C13-C15-C16-C17
15	bA	826	CLA	C8-C10-C11-C12
15	bB	833	CLA	C13-C15-C16-C17
15	cA	826	CLA	C8-C10-C11-C12
15	cB	833	CLA	C13-C15-C16-C17
15	c1	402	CLA	C3-C5-C6-C7
19	aA	853	LHG	C34-C35-C36-C37
19	bA	854	LHG	C34-C35-C36-C37
19	cA	852	LHG	C34-C35-C36-C37
15	aA	814	CLA	CBA-CGA-O2A-C1
15	bA	814	CLA	CBA-CGA-O2A-C1
18	aI	102	BCR	C18-C19-C20-C21
18	cI	102	BCR	C18-C19-C20-C21
15	aA	820	CLA	C13-C15-C16-C17
15	aB	801	CLA	C8-C10-C11-C12
15	bA	820	CLA	C13-C15-C16-C17
15	bB	801	CLA	C8-C10-C11-C12
15	cA	820	CLA	C13-C15-C16-C17
15	cB	801	CLA	C8-C10-C11-C12
15	aA	820	CLA	C4-C3-C5-C6
15	aA	828	CLA	C4-C3-C5-C6
15	bA	820	CLA	C4-C3-C5-C6
15	bA	828	CLA	C4-C3-C5-C6
15	cA	820	CLA	C4-C3-C5-C6
15	cA	828	CLA	C4-C3-C5-C6
15	a5	410	CLA	O1D-CGD-O2D-CED
15	c3	402	CLA	C3-C5-C6-C7
15	c5	410	CLA	O1D-CGD-O2D-CED
15	aA	831	CLA	CBA-CGA-O2A-C1
15	aA	845	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	831	CLA	CBA-CGA-O2A-C1
15	bA	845	CLA	CBA-CGA-O2A-C1
15	cA	814	CLA	CBA-CGA-O2A-C1
15	cA	831	CLA	CBA-CGA-O2A-C1
15	cA	844	CLA	CBA-CGA-O2A-C1
15	aA	802	CLA	C3A-C2A-CAA-CBA
15	aA	807	CLA	C3A-C2A-CAA-CBA
15	aA	837	CLA	C3A-C2A-CAA-CBA
15	aA	843	CLA	C3A-C2A-CAA-CBA
15	aB	817	CLA	C3A-C2A-CAA-CBA
15	aB	818	CLA	C3A-C2A-CAA-CBA
15	aB	826	CLA	C3A-C2A-CAA-CBA
15	a2	406	CLA	C3A-C2A-CAA-CBA
15	a2	413	CLA	C3A-C2A-CAA-CBA
15	a3	412	CLA	C3A-C2A-CAA-CBA
15	a3	421	CLA	C3A-C2A-CAA-CBA
15	a4	412	CLA	C3A-C2A-CAA-CBA
15	a5	412	CLA	C3A-C2A-CAA-CBA
15	bA	802	CLA	C3A-C2A-CAA-CBA
15	bA	807	CLA	C3A-C2A-CAA-CBA
15	bA	837	CLA	C3A-C2A-CAA-CBA
15	bA	843	CLA	C3A-C2A-CAA-CBA
15	bB	817	CLA	C3A-C2A-CAA-CBA
15	bB	818	CLA	C3A-C2A-CAA-CBA
15	bB	826	CLA	C3A-C2A-CAA-CBA
15	b1	412	CLA	C3A-C2A-CAA-CBA
15	b2	406	CLA	C3A-C2A-CAA-CBA
15	b2	413	CLA	C3A-C2A-CAA-CBA
15	b3	412	CLA	C3A-C2A-CAA-CBA
15	b3	421	CLA	C3A-C2A-CAA-CBA
15	b4	412	CLA	C3A-C2A-CAA-CBA
15	b5	412	CLA	C3A-C2A-CAA-CBA
15	cA	802	CLA	C3A-C2A-CAA-CBA
15	cA	807	CLA	C3A-C2A-CAA-CBA
15	cA	837	CLA	C3A-C2A-CAA-CBA
15	cA	842	CLA	C3A-C2A-CAA-CBA
15	cA	843	CLA	C3A-C2A-CAA-CBA
15	cB	817	CLA	C3A-C2A-CAA-CBA
15	cB	818	CLA	C3A-C2A-CAA-CBA
15	cB	826	CLA	C3A-C2A-CAA-CBA
15	c1	412	CLA	C3A-C2A-CAA-CBA
15	c2	406	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c2	413	CLA	C3A-C2A-CAA-CBA
15	c3	412	CLA	C3A-C2A-CAA-CBA
15	c3	421	CLA	C3A-C2A-CAA-CBA
15	c4	412	CLA	C3A-C2A-CAA-CBA
15	c5	412	CLA	C3A-C2A-CAA-CBA
15	c6	413	CLA	C3A-C2A-CAA-CBA
15	b5	410	CLA	O1D-CGD-O2D-CED
18	aL	205	BCR	C15-C16-C17-C18
18	bL	201	BCR	C15-C16-C17-C18
18	bL	206	BCR	C15-C16-C17-C18
15	aB	805	CLA	CBD-CGD-O2D-CED
15	aB	827	CLA	C8-C10-C11-C12
15	cB	827	CLA	C8-C10-C11-C12
15	aB	829	CLA	CBA-CGA-O2A-C1
15	bB	829	CLA	CBA-CGA-O2A-C1
15	cB	829	CLA	CBA-CGA-O2A-C1
19	bA	854	LHG	C24-C25-C26-C27
15	a6	404	CLA	C13-C15-C16-C17
15	bB	827	CLA	C8-C10-C11-C12
15	b4	403	CLA	C8-C10-C11-C12
15	c4	403	CLA	C8-C10-C11-C12
15	c6	404	CLA	C13-C15-C16-C17
19	aX	101	LHG	C4-C5-C6-O8
19	bX	101	LHG	C4-C5-C6-O8
19	cX	101	LHG	C4-C5-C6-O8
15	c1	411	CLA	CBD-CGD-O2D-CED
15	aA	836	CLA	C6-C7-C8-C9
15	bA	836	CLA	C6-C7-C8-C9
15	cA	836	CLA	C6-C7-C8-C9
19	aA	853	LHG	C24-C25-C26-C27
19	aA	853	LHG	C30-C31-C32-C33
19	cA	852	LHG	C24-C25-C26-C27
19	cA	852	LHG	C30-C31-C32-C33
19	bA	854	LHG	C30-C31-C32-C33
15	b6	404	CLA	C13-C15-C16-C17
18	bB	848	BCR	C14-C15-C16-C17
18	cB	848	BCR	C14-C15-C16-C17
15	a3	402	CLA	C3-C5-C6-C7
15	b3	402	CLA	C3-C5-C6-C7
16	aB	843	PQN	C13-C15-C16-C17
16	bB	843	PQN	C13-C15-C16-C17
16	cB	843	PQN	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	805	CLA	C8-C10-C11-C12
15	cA	805	CLA	C8-C10-C11-C12
15	aA	841	CLA	C4-C3-C5-C6
15	bA	841	CLA	C4-C3-C5-C6
15	cA	841	CLA	C4-C3-C5-C6
15	aB	807	CLA	C16-C17-C18-C19
15	bB	807	CLA	C16-C17-C18-C19
15	cB	807	CLA	C16-C17-C18-C19
15	aA	828	CLA	C2-C3-C5-C6
15	bA	828	CLA	C2-C3-C5-C6
15	cA	828	CLA	C2-C3-C5-C6
15	c4	411	CLA	O1D-CGD-O2D-CED
15	aA	805	CLA	C8-C10-C11-C12
15	aA	812	CLA	O1A-CGA-O2A-C1
19	aA	853	LHG	O10-C23-O8-C6
19	bA	854	LHG	O10-C23-O8-C6
15	aB	810	CLA	C2A-CAA-CBA-CGA
15	bB	810	CLA	C2A-CAA-CBA-CGA
15	cB	810	CLA	C2A-CAA-CBA-CGA
15	bB	808	CLA	C8-C10-C11-C12
15	cB	808	CLA	C8-C10-C11-C12
20	aB	850	LMG	C30-C31-C32-C33
20	bB	851	LMG	C30-C31-C32-C33
15	aA	829	CLA	CBA-CGA-O2A-C1
15	bA	829	CLA	CBA-CGA-O2A-C1
15	cA	829	CLA	CBA-CGA-O2A-C1
20	cB	850	LMG	C30-C31-C32-C33
15	a1	409	CLA	O1D-CGD-O2D-CED
15	b1	410	CLA	O1D-CGD-O2D-CED
15	c1	410	CLA	O1D-CGD-O2D-CED
15	a1	403	CLA	O1A-CGA-O2A-C1
15	a3	404	CLA	O1A-CGA-O2A-C1
15	a5	404	CLA	O1A-CGA-O2A-C1
15	bA	812	CLA	O1A-CGA-O2A-C1
15	b3	404	CLA	O1A-CGA-O2A-C1
15	b5	404	CLA	O1A-CGA-O2A-C1
15	cA	812	CLA	O1A-CGA-O2A-C1
15	c3	404	CLA	O1A-CGA-O2A-C1
19	cA	852	LHG	O10-C23-O8-C6
20	aB	850	LMG	C28-C29-C30-C31
20	cB	850	LMG	C28-C29-C30-C31
15	aA	803	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	803	CLA	C16-C17-C18-C19
15	cA	803	CLA	C16-C17-C18-C19
15	cB	823	CLA	C6-C7-C8-C9
15	aB	808	CLA	C8-C10-C11-C12
15	bB	806	CLA	CAA-CBA-CGA-O2A
15	c3	411	CLA	O1D-CGD-O2D-CED
15	aB	828	CLA	O1A-CGA-O2A-C1
15	a6	405	CLA	O1A-CGA-O2A-C1
15	bB	828	CLA	O1A-CGA-O2A-C1
15	b1	404	CLA	O1A-CGA-O2A-C1
15	cB	828	CLA	O1A-CGA-O2A-C1
15	c1	404	CLA	O1A-CGA-O2A-C1
15	c5	404	CLA	O1A-CGA-O2A-C1
15	c6	405	CLA	O1A-CGA-O2A-C1
20	bB	851	LMG	C28-C29-C30-C31
15	a1	410	CLA	CBD-CGD-O2D-CED
15	aB	806	CLA	CAA-CBA-CGA-O2A
15	cB	806	CLA	CAA-CBA-CGA-O2A
15	aB	823	CLA	C6-C7-C8-C9
15	bB	823	CLA	C6-C7-C8-C9
15	c5	420	CLA	C16-C17-C18-C19
15	aA	825	CLA	C2-C1-O2A-CGA
15	aA	827	CLA	C2-C1-O2A-CGA
15	aB	803	CLA	C2-C1-O2A-CGA
15	bA	825	CLA	C2-C1-O2A-CGA
15	bA	827	CLA	C2-C1-O2A-CGA
15	bB	803	CLA	C2-C1-O2A-CGA
15	cA	825	CLA	C2-C1-O2A-CGA
15	cA	827	CLA	C2-C1-O2A-CGA
15	cB	803	CLA	C2-C1-O2A-CGA
15	aA	820	CLA	C2-C3-C5-C6
15	bA	820	CLA	C2-C3-C5-C6
15	cA	820	CLA	C2-C3-C5-C6
20	aB	850	LMG	C16-C17-C18-C19
20	bB	851	LMG	C41-C42-C43-C44
20	cB	850	LMG	C16-C17-C18-C19
15	b4	404	CLA	O1A-CGA-O2A-C1
15	b6	405	CLA	O1A-CGA-O2A-C1
15	aA	803	CLA	C10-C11-C12-C13
15	bA	803	CLA	C10-C11-C12-C13
15	cA	803	CLA	C10-C11-C12-C13
15	aA	805	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	820	CLA	C11-C12-C13-C14
15	aA	826	CLA	C14-C13-C15-C16
15	aA	827	CLA	C14-C13-C15-C16
15	aA	830	CLA	C14-C13-C15-C16
15	aA	839	CLA	C6-C7-C8-C9
15	aA	843	CLA	C11-C12-C13-C14
15	aB	808	CLA	C11-C10-C8-C9
15	aB	814	CLA	C6-C7-C8-C9
15	aB	828	CLA	C14-C13-C15-C16
15	aB	829	CLA	C14-C13-C15-C16
15	aB	833	CLA	C11-C12-C13-C14
15	a3	403	CLA	C11-C12-C13-C14
15	a4	403	CLA	C11-C12-C13-C14
15	a5	403	CLA	C11-C12-C13-C14
15	a6	403	CLA	C14-C13-C15-C16
15	bA	805	CLA	C11-C10-C8-C9
15	bA	820	CLA	C11-C12-C13-C14
15	bA	826	CLA	C14-C13-C15-C16
15	bA	827	CLA	C14-C13-C15-C16
15	bA	830	CLA	C14-C13-C15-C16
15	bA	839	CLA	C6-C7-C8-C9
15	bA	843	CLA	C11-C12-C13-C14
15	bB	808	CLA	C11-C10-C8-C9
15	bB	814	CLA	C6-C7-C8-C9
15	bB	828	CLA	C14-C13-C15-C16
15	bB	829	CLA	C14-C13-C15-C16
15	bB	833	CLA	C11-C12-C13-C14
15	b3	403	CLA	C11-C12-C13-C14
15	b4	403	CLA	C11-C12-C13-C14
15	b5	403	CLA	C11-C12-C13-C14
15	b6	403	CLA	C14-C13-C15-C16
15	cA	805	CLA	C11-C10-C8-C9
15	cA	820	CLA	C11-C12-C13-C14
15	cA	826	CLA	C14-C13-C15-C16
15	cA	827	CLA	C14-C13-C15-C16
15	cA	830	CLA	C14-C13-C15-C16
15	cA	839	CLA	C6-C7-C8-C9
15	cA	842	CLA	C11-C12-C13-C14
15	cB	808	CLA	C11-C10-C8-C9
15	cB	814	CLA	C6-C7-C8-C9
15	cB	828	CLA	C14-C13-C15-C16
15	cB	829	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	833	CLA	C11-C12-C13-C14
15	c2	403	CLA	C11-C12-C13-C14
15	c3	403	CLA	C11-C12-C13-C14
15	c4	403	CLA	C11-C12-C13-C14
15	c6	403	CLA	C14-C13-C15-C16
20	aB	850	LMG	C41-C42-C43-C44
20	bB	851	LMG	C16-C17-C18-C19
20	cB	850	LMG	C41-C42-C43-C44
15	aA	806	CLA	C10-C11-C12-C13
19	aX	101	LHG	C2-C3-O3-P
19	bX	101	LHG	C2-C3-O3-P
19	cX	101	LHG	C2-C3-O3-P
15	c4	404	CLA	O1A-CGA-O2A-C1
15	aA	820	CLA	C16-C17-C18-C20
15	aB	817	CLA	C6-C7-C8-C10
15	a5	420	CLA	C16-C17-C18-C19
15	bA	820	CLA	C16-C17-C18-C20
15	bB	817	CLA	C6-C7-C8-C10
15	b5	420	CLA	C16-C17-C18-C19
15	cA	820	CLA	C16-C17-C18-C20
15	cB	817	CLA	C6-C7-C8-C10
15	aA	820	CLA	C3-C5-C6-C7
15	bA	820	CLA	C3-C5-C6-C7
15	b2	403	CLA	C3-C5-C6-C7
15	cA	820	CLA	C3-C5-C6-C7
18	aA	852	BCR	C5-C6-C7-C8
18	aA	852	BCR	C23-C24-C25-C26
18	aA	852	BCR	C23-C24-C25-C30
18	aB	845	BCR	C1-C6-C7-C8
18	aB	846	BCR	C23-C24-C25-C26
18	aB	847	BCR	C23-C24-C25-C30
18	aB	849	BCR	C23-C24-C25-C26
18	aB	849	BCR	C23-C24-C25-C30
18	aF	201	BCR	C23-C24-C25-C26
18	aF	203	BCR	C5-C6-C7-C8
18	aI	102	BCR	C23-C24-C25-C30
18	aM	101	BCR	C23-C24-C25-C26
18	aM	101	BCR	C23-C24-C25-C30
18	a1	418	BCR	C23-C24-C25-C26
18	a1	420	BCR	C23-C24-C25-C26
18	a1	421	BCR	C23-C24-C25-C26
18	a1	421	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a2	401	BCR	C23-C24-C25-C26
18	a2	401	BCR	C23-C24-C25-C30
18	a2	420	BCR	C23-C24-C25-C30
18	a3	401	BCR	C23-C24-C25-C26
18	a3	401	BCR	C23-C24-C25-C30
18	a3	419	BCR	C23-C24-C25-C26
18	a4	401	BCR	C1-C6-C7-C8
18	a4	401	BCR	C5-C6-C7-C8
18	a4	401	BCR	C23-C24-C25-C26
18	a4	401	BCR	C23-C24-C25-C30
18	a4	419	BCR	C23-C24-C25-C26
18	a5	401	BCR	C1-C6-C7-C8
18	a5	401	BCR	C5-C6-C7-C8
18	a5	401	BCR	C23-C24-C25-C26
18	a6	401	BCR	C23-C24-C25-C26
18	a6	402	BCR	C23-C24-C25-C26
18	a6	402	BCR	C23-C24-C25-C30
18	a6	421	BCR	C23-C24-C25-C26
18	a6	421	BCR	C23-C24-C25-C30
18	bA	853	BCR	C5-C6-C7-C8
18	bA	853	BCR	C23-C24-C25-C26
18	bA	853	BCR	C23-C24-C25-C30
18	bB	845	BCR	C1-C6-C7-C8
18	bB	846	BCR	C23-C24-C25-C26
18	bB	847	BCR	C23-C24-C25-C30
18	bB	849	BCR	C23-C24-C25-C26
18	bB	850	BCR	C23-C24-C25-C26
18	bB	850	BCR	C23-C24-C25-C30
18	bI	102	BCR	C23-C24-C25-C30
18	bJ	105	BCR	C5-C6-C7-C8
18	bM	101	BCR	C23-C24-C25-C26
18	bM	101	BCR	C23-C24-C25-C30
18	b1	401	BCR	C23-C24-C25-C26
18	b1	419	BCR	C23-C24-C25-C26
18	b1	420	BCR	C5-C6-C7-C8
18	b2	401	BCR	C23-C24-C25-C26
18	b2	401	BCR	C23-C24-C25-C30
18	b2	420	BCR	C23-C24-C25-C30
18	b3	401	BCR	C23-C24-C25-C30
18	b3	419	BCR	C23-C24-C25-C26
18	b4	401	BCR	C1-C6-C7-C8
18	b4	401	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b4	401	BCR	C23-C24-C25-C26
18	b4	401	BCR	C23-C24-C25-C30
18	b4	419	BCR	C23-C24-C25-C26
18	b5	401	BCR	C1-C6-C7-C8
18	b5	401	BCR	C5-C6-C7-C8
18	b5	401	BCR	C23-C24-C25-C26
18	b6	401	BCR	C23-C24-C25-C26
18	b6	402	BCR	C23-C24-C25-C26
18	b6	402	BCR	C23-C24-C25-C30
18	b6	421	BCR	C23-C24-C25-C26
18	b6	421	BCR	C23-C24-C25-C30
18	cA	851	BCR	C5-C6-C7-C8
18	cA	851	BCR	C23-C24-C25-C26
18	cA	851	BCR	C23-C24-C25-C30
18	cB	845	BCR	C1-C6-C7-C8
18	cB	846	BCR	C23-C24-C25-C26
18	cB	847	BCR	C23-C24-C25-C30
18	cB	849	BCR	C23-C24-C25-C26
18	cB	849	BCR	C23-C24-C25-C30
18	cF	202	BCR	C23-C24-C25-C26
18	cF	205	BCR	C5-C6-C7-C8
18	cI	102	BCR	C23-C24-C25-C30
18	cM	101	BCR	C23-C24-C25-C26
18	cM	101	BCR	C23-C24-C25-C30
18	c1	401	BCR	C5-C6-C7-C8
18	c1	401	BCR	C23-C24-C25-C26
18	c1	419	BCR	C23-C24-C25-C26
18	c2	401	BCR	C23-C24-C25-C26
18	c2	401	BCR	C23-C24-C25-C30
18	c2	420	BCR	C23-C24-C25-C26
18	c2	420	BCR	C23-C24-C25-C30
18	c3	401	BCR	C23-C24-C25-C26
18	c3	401	BCR	C23-C24-C25-C30
18	c3	419	BCR	C23-C24-C25-C26
18	c4	401	BCR	C1-C6-C7-C8
18	c4	401	BCR	C5-C6-C7-C8
18	c4	401	BCR	C23-C24-C25-C26
18	c4	401	BCR	C23-C24-C25-C30
18	c4	419	BCR	C23-C24-C25-C26
18	c5	401	BCR	C1-C6-C7-C8
18	c5	401	BCR	C5-C6-C7-C8
18	c5	401	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c6	401	BCR	C23-C24-C25-C26
18	c6	402	BCR	C23-C24-C25-C30
15	bA	806	CLA	C10-C11-C12-C13
15	b2	403	CLA	C8-C10-C11-C12
15	aA	829	CLA	CAA-CBA-CGA-O2A
15	bA	829	CLA	CAA-CBA-CGA-O2A
15	cA	829	CLA	CAA-CBA-CGA-O2A
18	b1	401	BCR	C7-C8-C9-C34
18	b6	421	BCR	C11-C12-C13-C35
15	a4	404	CLA	O1A-CGA-O2A-C1
18	aB	847	BCR	C35-C13-C14-C15
18	aB	849	BCR	C21-C22-C23-C24
18	a4	401	BCR	C11-C12-C13-C14
18	bB	847	BCR	C35-C13-C14-C15
18	bB	850	BCR	C21-C22-C23-C24
18	b4	401	BCR	C11-C12-C13-C14
18	cB	847	BCR	C35-C13-C14-C15
18	cB	849	BCR	C21-C22-C23-C24
15	aA	827	CLA	C5-C6-C7-C8
15	aB	807	CLA	C5-C6-C7-C8
15	aB	815	CLA	C10-C11-C12-C13
15	aB	828	CLA	C5-C6-C7-C8
15	a2	403	CLA	C8-C10-C11-C12
15	bA	827	CLA	C5-C6-C7-C8
15	bB	807	CLA	C5-C6-C7-C8
15	bB	815	CLA	C10-C11-C12-C13
15	bB	828	CLA	C5-C6-C7-C8
15	cA	827	CLA	C5-C6-C7-C8
15	cB	807	CLA	C5-C6-C7-C8
15	cB	815	CLA	C10-C11-C12-C13
15	cB	828	CLA	C5-C6-C7-C8
18	aB	848	BCR	C14-C15-C16-C17
18	aF	203	BCR	C14-C15-C16-C17
18	bJ	105	BCR	C14-C15-C16-C17
18	cF	205	BCR	C14-C15-C16-C17
15	cA	806	CLA	C10-C11-C12-C13
15	aB	828	CLA	C16-C17-C18-C20
15	bB	828	CLA	C16-C17-C18-C20
15	cB	828	CLA	C16-C17-C18-C20
15	cB	833	CLA	O1D-CGD-O2D-CED
15	aB	833	CLA	O1D-CGD-O2D-CED
15	a3	411	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	833	CLA	O1D-CGD-O2D-CED
15	c2	403	CLA	C8-C10-C11-C12
15	aB	829	CLA	O1D-CGD-O2D-CED
15	aA	805	CLA	C11-C10-C8-C7
15	aA	807	CLA	C6-C7-C8-C10
15	aA	807	CLA	C12-C13-C15-C16
15	aA	828	CLA	C11-C10-C8-C7
15	aA	829	CLA	C11-C10-C8-C7
15	aA	839	CLA	C6-C7-C8-C10
15	aA	839	CLA	C12-C13-C15-C16
15	aB	803	CLA	C12-C13-C15-C16
15	aB	809	CLA	C11-C10-C8-C7
15	aB	820	CLA	C11-C10-C8-C7
15	aB	829	CLA	C12-C13-C15-C16
15	aB	833	CLA	C11-C10-C8-C7
15	aB	833	CLA	C12-C13-C15-C16
15	aB	837	CLA	C11-C12-C13-C15
15	aB	840	CLA	C11-C10-C8-C7
15	a1	401	CLA	C11-C10-C8-C7
15	a1	401	CLA	C12-C13-C15-C16
15	a1	402	CLA	C11-C10-C8-C7
15	a2	402	CLA	C11-C10-C8-C7
15	a2	403	CLA	C11-C10-C8-C7
15	a3	402	CLA	C11-C10-C8-C7
15	a3	403	CLA	C11-C10-C8-C7
15	a4	402	CLA	C11-C10-C8-C7
15	a4	403	CLA	C11-C12-C13-C15
15	a5	402	CLA	C11-C10-C8-C7
15	a5	403	CLA	C11-C12-C13-C15
15	a6	403	CLA	C11-C10-C8-C7
15	a6	404	CLA	C11-C10-C8-C7
15	bA	805	CLA	C11-C10-C8-C7
15	bA	807	CLA	C6-C7-C8-C10
15	bA	807	CLA	C12-C13-C15-C16
15	bA	828	CLA	C11-C10-C8-C7
15	bA	829	CLA	C11-C10-C8-C7
15	bA	839	CLA	C6-C7-C8-C10
15	bA	839	CLA	C12-C13-C15-C16
15	bB	803	CLA	C12-C13-C15-C16
15	bB	809	CLA	C11-C10-C8-C7
15	bB	820	CLA	C11-C10-C8-C7
15	bB	829	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	833	CLA	C11-C10-C8-C7
15	bB	833	CLA	C12-C13-C15-C16
15	bB	837	CLA	C11-C12-C13-C15
15	bB	840	CLA	C11-C10-C8-C7
15	b1	402	CLA	C11-C10-C8-C7
15	b2	402	CLA	C11-C10-C8-C7
15	b2	403	CLA	C11-C10-C8-C7
15	b3	402	CLA	C11-C10-C8-C7
15	b3	403	CLA	C11-C10-C8-C7
15	b4	402	CLA	C11-C10-C8-C7
15	b5	402	CLA	C11-C10-C8-C7
15	b5	403	CLA	C11-C12-C13-C15
15	b6	403	CLA	C11-C10-C8-C7
15	b6	404	CLA	C11-C10-C8-C7
15	cA	805	CLA	C11-C10-C8-C7
15	cA	807	CLA	C6-C7-C8-C10
15	cA	807	CLA	C12-C13-C15-C16
15	cA	828	CLA	C11-C10-C8-C7
15	cA	829	CLA	C11-C10-C8-C7
15	cA	839	CLA	C6-C7-C8-C10
15	cA	839	CLA	C12-C13-C15-C16
15	cB	803	CLA	C12-C13-C15-C16
15	cB	809	CLA	C11-C10-C8-C7
15	cB	820	CLA	C11-C10-C8-C7
15	cB	829	CLA	C12-C13-C15-C16
15	cB	833	CLA	C11-C10-C8-C7
15	cB	833	CLA	C12-C13-C15-C16
15	cB	837	CLA	C11-C12-C13-C15
15	cB	840	CLA	C11-C10-C8-C7
15	c1	402	CLA	C11-C10-C8-C7
15	c1	403	CLA	C11-C10-C8-C7
15	c2	402	CLA	C11-C10-C8-C7
15	c2	403	CLA	C11-C10-C8-C7
15	c3	402	CLA	C11-C10-C8-C7
15	c3	403	CLA	C11-C10-C8-C7
15	c4	402	CLA	C11-C10-C8-C7
15	c4	403	CLA	C11-C12-C13-C15
15	c5	402	CLA	C11-C10-C8-C7
15	c5	403	CLA	C11-C12-C13-C15
15	c6	403	CLA	C11-C10-C8-C7
15	c6	404	CLA	C11-C10-C8-C7
15	b6	412	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	829	CLA	O1D-CGD-O2D-CED
15	bA	821	CLA	C10-C11-C12-C13
15	cA	821	CLA	C10-C11-C12-C13
18	aB	845	BCR	C19-C20-C21-C22
18	bB	845	BCR	C19-C20-C21-C22
18	cB	845	BCR	C19-C20-C21-C22
15	a6	422	CLA	C16-C17-C18-C20
15	aA	809	CLA	C13-C15-C16-C17
15	aA	821	CLA	C10-C11-C12-C13
15	aA	839	CLA	C10-C11-C12-C13
15	aB	837	CLA	C5-C6-C7-C8
15	bA	839	CLA	C10-C11-C12-C13
15	bB	837	CLA	C5-C6-C7-C8
15	cA	809	CLA	C13-C15-C16-C17
15	cA	839	CLA	C10-C11-C12-C13
15	cB	837	CLA	C5-C6-C7-C8
15	aA	841	CLA	C2A-CAA-CBA-CGA
15	bA	841	CLA	C2A-CAA-CBA-CGA
15	cA	841	CLA	C2A-CAA-CBA-CGA
15	bA	809	CLA	C13-C15-C16-C17
18	aF	202	BCR	C20-C21-C22-C37
18	aI	101	BCR	C11-C10-C9-C34
18	aL	205	BCR	C16-C17-C18-C36
18	a1	421	BCR	C11-C10-C9-C34
18	a1	421	BCR	C20-C21-C22-C37
18	a3	418	BCR	C16-C17-C18-C36
18	a4	418	BCR	C16-C17-C18-C36
18	a5	401	BCR	C35-C13-C14-C15
18	a5	418	BCR	C16-C17-C18-C36
18	a5	418	BCR	C20-C21-C22-C37
18	a6	402	BCR	C20-C21-C22-C37
18	a6	419	BCR	C20-C21-C22-C37
18	bF	202	BCR	C20-C21-C22-C37
18	bI	101	BCR	C11-C10-C9-C34
18	bL	201	BCR	C16-C17-C18-C36
18	bL	206	BCR	C16-C17-C18-C36
18	b1	418	BCR	C20-C21-C22-C37
18	b2	401	BCR	C20-C21-C22-C37
18	b3	401	BCR	C35-C13-C14-C15
18	b3	418	BCR	C16-C17-C18-C36
18	b3	418	BCR	C20-C21-C22-C37
18	b5	401	BCR	C35-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b5	418	BCR	C16-C17-C18-C36
18	b5	418	BCR	C20-C21-C22-C37
18	b6	402	BCR	C20-C21-C22-C37
18	b6	419	BCR	C20-C21-C22-C37
18	cF	204	BCR	C20-C21-C22-C37
18	cI	101	BCR	C11-C10-C9-C34
18	c3	418	BCR	C16-C17-C18-C36
18	c3	418	BCR	C20-C21-C22-C37
18	c5	401	BCR	C35-C13-C14-C15
18	c6	402	BCR	C20-C21-C22-C37
18	c6	419	BCR	C20-C21-C22-C37
15	a2	403	CLA	C3-C5-C6-C7
15	c2	403	CLA	C3-C5-C6-C7
15	cB	807	CLA	C16-C17-C18-C20
15	aA	806	CLA	C13-C15-C16-C17
15	bA	806	CLA	C13-C15-C16-C17
15	aA	817	CLA	CBA-CGA-O2A-C1
15	bA	817	CLA	CBA-CGA-O2A-C1
15	cA	817	CLA	CBA-CGA-O2A-C1
15	bB	829	CLA	O1D-CGD-O2D-CED
15	aB	825	CLA	C5-C6-C7-C8
15	bB	825	CLA	C5-C6-C7-C8
15	cB	825	CLA	C5-C6-C7-C8
15	cB	810	CLA	O1D-CGD-O2D-CED
15	aB	806	CLA	C13-C15-C16-C17
15	bB	806	CLA	C13-C15-C16-C17
15	cA	806	CLA	C13-C15-C16-C17
15	cB	806	CLA	C13-C15-C16-C17
15	aA	802	CLA	CAD-CBD-CGD-O2D
15	aA	806	CLA	CAD-CBD-CGD-O2D
15	aA	813	CLA	CAD-CBD-CGD-O2D
15	aA	818	CLA	CAD-CBD-CGD-O2D
15	aA	827	CLA	CAD-CBD-CGD-O2D
15	aB	811	CLA	CAD-CBD-CGD-O2D
15	aB	830	CLA	CAD-CBD-CGD-O2D
15	aB	838	CLA	CAD-CBD-CGD-O2D
15	aB	840	CLA	CAD-CBD-CGD-O2D
15	a1	409	CLA	CAD-CBD-CGD-O2D
15	a2	411	CLA	CAD-CBD-CGD-O2D
15	a2	412	CLA	CAD-CBD-CGD-O2D
15	a3	410	CLA	CAD-CBD-CGD-O2D
15	a4	405	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a4	410	CLA	CAD-CBD-CGD-O2D
15	a5	410	CLA	CAD-CBD-CGD-O2D
15	a5	411	CLA	CAD-CBD-CGD-O2D
15	bA	802	CLA	CAD-CBD-CGD-O2D
15	bA	806	CLA	CAD-CBD-CGD-O2D
15	bA	813	CLA	CAD-CBD-CGD-O2D
15	bA	818	CLA	CAD-CBD-CGD-O2D
15	bA	827	CLA	CAD-CBD-CGD-O2D
15	bB	811	CLA	CAD-CBD-CGD-O2D
15	bB	830	CLA	CAD-CBD-CGD-O2D
15	bB	838	CLA	CAD-CBD-CGD-O2D
15	bB	840	CLA	CAD-CBD-CGD-O2D
15	b1	410	CLA	CAD-CBD-CGD-O2D
15	b2	411	CLA	CAD-CBD-CGD-O2D
15	b2	412	CLA	CAD-CBD-CGD-O2D
15	b3	410	CLA	CAD-CBD-CGD-O2D
15	b3	411	CLA	CAD-CBD-CGD-O2D
15	b4	405	CLA	CAD-CBD-CGD-O2D
15	b4	410	CLA	CAD-CBD-CGD-O2D
15	b5	410	CLA	CAD-CBD-CGD-O2D
15	b5	411	CLA	CAD-CBD-CGD-O2D
15	b6	411	CLA	CAD-CBD-CGD-O2D
15	cA	802	CLA	CAD-CBD-CGD-O2D
15	cA	806	CLA	CAD-CBD-CGD-O2D
15	cA	813	CLA	CAD-CBD-CGD-O2D
15	cA	818	CLA	CAD-CBD-CGD-O2D
15	cA	827	CLA	CAD-CBD-CGD-O2D
15	cB	811	CLA	CAD-CBD-CGD-O2D
15	cB	830	CLA	CAD-CBD-CGD-O2D
15	cB	838	CLA	CAD-CBD-CGD-O2D
15	cB	840	CLA	CAD-CBD-CGD-O2D
15	c1	410	CLA	CAD-CBD-CGD-O2D
15	c2	411	CLA	CAD-CBD-CGD-O2D
15	c2	412	CLA	CAD-CBD-CGD-O2D
15	c3	410	CLA	CAD-CBD-CGD-O2D
15	c4	405	CLA	CAD-CBD-CGD-O2D
15	c4	410	CLA	CAD-CBD-CGD-O2D
15	c5	410	CLA	CAD-CBD-CGD-O2D
15	c5	411	CLA	CAD-CBD-CGD-O2D
15	a6	412	CLA	O1D-CGD-O2D-CED
15	bB	810	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	830	CLA	C10-C11-C12-C13
15	bA	825	CLA	C5-C6-C7-C8
15	bA	830	CLA	C10-C11-C12-C13
15	cA	825	CLA	C5-C6-C7-C8
15	cA	830	CLA	C10-C11-C12-C13
15	aB	810	CLA	O1D-CGD-O2D-CED
15	bA	833	CLA	O1D-CGD-O2D-CED
18	aI	102	BCR	C22-C23-C24-C25
18	bI	102	BCR	C22-C23-C24-C25
18	b3	418	BCR	C22-C23-C24-C25
18	cI	102	BCR	C22-C23-C24-C25
15	aB	830	CLA	O1A-CGA-O2A-C1
15	aB	808	CLA	CBA-CGA-O2A-C1
15	bB	808	CLA	CBA-CGA-O2A-C1
15	cB	808	CLA	CBA-CGA-O2A-C1
15	cA	833	CLA	O1D-CGD-O2D-CED
15	aB	807	CLA	C16-C17-C18-C20
15	bB	807	CLA	C16-C17-C18-C20
20	aB	850	LMG	O1-C7-C8-C9
20	bB	851	LMG	O1-C7-C8-C9
20	cB	850	LMG	O1-C7-C8-C9
15	bB	817	CLA	CBD-CGD-O2D-CED
15	cB	817	CLA	CBD-CGD-O2D-CED
15	a1	422	CLA	O1A-CGA-O2A-C1
15	bB	830	CLA	O1A-CGA-O2A-C1
15	cB	830	CLA	O1A-CGA-O2A-C1
15	aA	802	CLA	C13-C15-C16-C17
15	aA	807	CLA	C10-C11-C12-C13
15	bA	802	CLA	C13-C15-C16-C17
15	bA	807	CLA	C10-C11-C12-C13
15	cA	802	CLA	C13-C15-C16-C17
15	cA	807	CLA	C10-C11-C12-C13
15	aL	203	CLA	CAA-CBA-CGA-O2A
15	bL	204	CLA	CAA-CBA-CGA-O2A
15	cL	203	CLA	CAA-CBA-CGA-O2A
18	bI	102	BCR	C18-C19-C20-C21
15	aB	817	CLA	CBD-CGD-O2D-CED
15	cB	829	CLA	O1A-CGA-O2A-C1
15	aB	817	CLA	C6-C7-C8-C9
15	a5	420	CLA	C16-C17-C18-C20
15	bB	817	CLA	C6-C7-C8-C9
15	b5	409	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b5	420	CLA	C16-C17-C18-C20
15	cB	817	CLA	C6-C7-C8-C9
15	c5	409	CLA	C16-C17-C18-C19
15	c5	420	CLA	C16-C17-C18-C20
15	c6	410	CLA	C16-C17-C18-C19
15	aA	833	CLA	O1D-CGD-O2D-CED
15	aA	805	CLA	CHA-CBD-CGD-O1D
15	aA	805	CLA	CHA-CBD-CGD-O2D
15	aA	814	CLA	CHA-CBD-CGD-O1D
15	aA	814	CLA	CHA-CBD-CGD-O2D
15	aA	828	CLA	CHA-CBD-CGD-O1D
15	aA	835	CLA	CHA-CBD-CGD-O1D
15	aA	835	CLA	CHA-CBD-CGD-O2D
15	aA	837	CLA	CHA-CBD-CGD-O1D
15	aA	837	CLA	CHA-CBD-CGD-O2D
15	aA	838	CLA	CHA-CBD-CGD-O1D
15	aA	842	CLA	CHA-CBD-CGD-O1D
15	aB	808	CLA	CHA-CBD-CGD-O1D
15	aB	815	CLA	CHA-CBD-CGD-O1D
15	aB	815	CLA	CHA-CBD-CGD-O2D
15	aB	825	CLA	CHA-CBD-CGD-O1D
15	aB	825	CLA	CHA-CBD-CGD-O2D
15	aB	826	CLA	CHA-CBD-CGD-O1D
15	aB	827	CLA	CHA-CBD-CGD-O1D
15	aB	836	CLA	CHA-CBD-CGD-O1D
15	aB	836	CLA	CHA-CBD-CGD-O2D
15	aJ	202	CLA	CHA-CBD-CGD-O2D
15	aK	102	CLA	CHA-CBD-CGD-O1D
15	aL	201	CLA	CHA-CBD-CGD-O1D
15	aL	201	CLA	CHA-CBD-CGD-O2D
15	aX	102	CLA	CHA-CBD-CGD-O1D
15	aX	102	CLA	CHA-CBD-CGD-O2D
15	a1	406	CLA	CHA-CBD-CGD-O1D
15	a1	406	CLA	CHA-CBD-CGD-O2D
15	a1	411	CLA	CHA-CBD-CGD-O1D
15	a1	415	CLA	CHA-CBD-CGD-O1D
15	a1	415	CLA	CHA-CBD-CGD-O2D
15	a1	422	CLA	CHA-CBD-CGD-O1D
15	a2	408	CLA	CHA-CBD-CGD-O1D
15	a2	408	CLA	CHA-CBD-CGD-O2D
15	a2	413	CLA	CHA-CBD-CGD-O1D
15	a2	417	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a2	417	CLA	CHA-CBD-CGD-O2D
15	a2	422	CLA	CHA-CBD-CGD-O1D
15	a3	407	CLA	CHA-CBD-CGD-O1D
15	a3	407	CLA	CHA-CBD-CGD-O2D
15	a3	412	CLA	CHA-CBD-CGD-O1D
15	a3	416	CLA	CHA-CBD-CGD-O1D
15	a3	416	CLA	CHA-CBD-CGD-O2D
15	a4	407	CLA	CHA-CBD-CGD-O1D
15	a4	407	CLA	CHA-CBD-CGD-O2D
15	a4	412	CLA	CHA-CBD-CGD-O1D
15	a4	416	CLA	CHA-CBD-CGD-O1D
15	a4	416	CLA	CHA-CBD-CGD-O2D
15	a5	407	CLA	CHA-CBD-CGD-O1D
15	a5	407	CLA	CHA-CBD-CGD-O2D
15	a5	412	CLA	CHA-CBD-CGD-O1D
15	a5	416	CLA	CHA-CBD-CGD-O1D
15	a5	416	CLA	CHA-CBD-CGD-O2D
15	a6	408	CLA	CHA-CBD-CGD-O1D
15	a6	408	CLA	CHA-CBD-CGD-O2D
15	a6	413	CLA	CHA-CBD-CGD-O1D
15	a6	413	CLA	CHA-CBD-CGD-O2D
15	a6	417	CLA	CHA-CBD-CGD-O1D
15	a6	417	CLA	CHA-CBD-CGD-O2D
15	bA	803	CLA	CHA-CBD-CGD-O2D
15	bA	805	CLA	CHA-CBD-CGD-O1D
15	bA	805	CLA	CHA-CBD-CGD-O2D
15	bA	814	CLA	CHA-CBD-CGD-O1D
15	bA	814	CLA	CHA-CBD-CGD-O2D
15	bA	828	CLA	CHA-CBD-CGD-O1D
15	bA	835	CLA	CHA-CBD-CGD-O1D
15	bA	835	CLA	CHA-CBD-CGD-O2D
15	bA	837	CLA	CHA-CBD-CGD-O1D
15	bA	837	CLA	CHA-CBD-CGD-O2D
15	bA	838	CLA	CHA-CBD-CGD-O1D
15	bA	842	CLA	CHA-CBD-CGD-O1D
15	bB	808	CLA	CHA-CBD-CGD-O1D
15	bB	815	CLA	CHA-CBD-CGD-O1D
15	bB	815	CLA	CHA-CBD-CGD-O2D
15	bB	825	CLA	CHA-CBD-CGD-O1D
15	bB	825	CLA	CHA-CBD-CGD-O2D
15	bB	826	CLA	CHA-CBD-CGD-O1D
15	bB	827	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	836	CLA	CHA-CBD-CGD-O1D
15	bB	836	CLA	CHA-CBD-CGD-O2D
15	bJ	101	CLA	CHA-CBD-CGD-O2D
15	bK	101	CLA	CHA-CBD-CGD-O1D
15	bL	202	CLA	CHA-CBD-CGD-O1D
15	bL	202	CLA	CHA-CBD-CGD-O2D
15	bX	102	CLA	CHA-CBD-CGD-O1D
15	bX	102	CLA	CHA-CBD-CGD-O2D
15	b1	407	CLA	CHA-CBD-CGD-O1D
15	b1	407	CLA	CHA-CBD-CGD-O2D
15	b1	412	CLA	CHA-CBD-CGD-O1D
15	b1	416	CLA	CHA-CBD-CGD-O1D
15	b1	416	CLA	CHA-CBD-CGD-O2D
15	b2	408	CLA	CHA-CBD-CGD-O1D
15	b2	408	CLA	CHA-CBD-CGD-O2D
15	b2	413	CLA	CHA-CBD-CGD-O1D
15	b2	417	CLA	CHA-CBD-CGD-O1D
15	b2	417	CLA	CHA-CBD-CGD-O2D
15	b3	407	CLA	CHA-CBD-CGD-O1D
15	b3	407	CLA	CHA-CBD-CGD-O2D
15	b3	412	CLA	CHA-CBD-CGD-O1D
15	b3	416	CLA	CHA-CBD-CGD-O1D
15	b3	416	CLA	CHA-CBD-CGD-O2D
15	b4	407	CLA	CHA-CBD-CGD-O1D
15	b4	407	CLA	CHA-CBD-CGD-O2D
15	b4	412	CLA	CHA-CBD-CGD-O1D
15	b4	416	CLA	CHA-CBD-CGD-O1D
15	b4	416	CLA	CHA-CBD-CGD-O2D
15	b5	407	CLA	CHA-CBD-CGD-O1D
15	b5	407	CLA	CHA-CBD-CGD-O2D
15	b5	412	CLA	CHA-CBD-CGD-O1D
15	b5	416	CLA	CHA-CBD-CGD-O1D
15	b5	416	CLA	CHA-CBD-CGD-O2D
15	b6	408	CLA	CHA-CBD-CGD-O1D
15	b6	408	CLA	CHA-CBD-CGD-O2D
15	b6	413	CLA	CHA-CBD-CGD-O1D
15	b6	413	CLA	CHA-CBD-CGD-O2D
15	b6	417	CLA	CHA-CBD-CGD-O1D
15	b6	417	CLA	CHA-CBD-CGD-O2D
15	cA	803	CLA	CHA-CBD-CGD-O2D
15	cA	805	CLA	CHA-CBD-CGD-O1D
15	cA	805	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	814	CLA	CHA-CBD-CGD-O1D
15	cA	814	CLA	CHA-CBD-CGD-O2D
15	cA	828	CLA	CHA-CBD-CGD-O1D
15	cA	835	CLA	CHA-CBD-CGD-O1D
15	cA	835	CLA	CHA-CBD-CGD-O2D
15	cA	837	CLA	CHA-CBD-CGD-O1D
15	cA	837	CLA	CHA-CBD-CGD-O2D
15	cA	838	CLA	CHA-CBD-CGD-O1D
15	cB	808	CLA	CHA-CBD-CGD-O1D
15	cB	815	CLA	CHA-CBD-CGD-O1D
15	cB	815	CLA	CHA-CBD-CGD-O2D
15	cB	825	CLA	CHA-CBD-CGD-O1D
15	cB	826	CLA	CHA-CBD-CGD-O1D
15	cB	827	CLA	CHA-CBD-CGD-O1D
15	cB	836	CLA	CHA-CBD-CGD-O1D
15	cB	836	CLA	CHA-CBD-CGD-O2D
15	cF	201	CLA	CHA-CBD-CGD-O1D
15	cJ	101	CLA	CHA-CBD-CGD-O2D
15	cK	102	CLA	CHA-CBD-CGD-O1D
15	cL	201	CLA	CHA-CBD-CGD-O1D
15	cL	201	CLA	CHA-CBD-CGD-O2D
15	cX	102	CLA	CHA-CBD-CGD-O1D
15	cX	102	CLA	CHA-CBD-CGD-O2D
15	c1	407	CLA	CHA-CBD-CGD-O1D
15	c1	407	CLA	CHA-CBD-CGD-O2D
15	c1	412	CLA	CHA-CBD-CGD-O1D
15	c1	416	CLA	CHA-CBD-CGD-O1D
15	c1	416	CLA	CHA-CBD-CGD-O2D
15	c2	408	CLA	CHA-CBD-CGD-O1D
15	c2	408	CLA	CHA-CBD-CGD-O2D
15	c2	413	CLA	CHA-CBD-CGD-O1D
15	c2	417	CLA	CHA-CBD-CGD-O1D
15	c2	417	CLA	CHA-CBD-CGD-O2D
15	c2	422	CLA	CHA-CBD-CGD-O1D
15	c3	407	CLA	CHA-CBD-CGD-O1D
15	c3	407	CLA	CHA-CBD-CGD-O2D
15	c3	412	CLA	CHA-CBD-CGD-O1D
15	c3	416	CLA	CHA-CBD-CGD-O1D
15	c3	416	CLA	CHA-CBD-CGD-O2D
15	c4	407	CLA	CHA-CBD-CGD-O1D
15	c4	407	CLA	CHA-CBD-CGD-O2D
15	c4	412	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	416	CLA	CHA-CBD-CGD-O1D
15	c4	416	CLA	CHA-CBD-CGD-O2D
15	c5	407	CLA	CHA-CBD-CGD-O1D
15	c5	407	CLA	CHA-CBD-CGD-O2D
15	c5	412	CLA	CHA-CBD-CGD-O1D
15	c5	416	CLA	CHA-CBD-CGD-O1D
15	c5	416	CLA	CHA-CBD-CGD-O2D
15	c6	408	CLA	CHA-CBD-CGD-O1D
15	c6	408	CLA	CHA-CBD-CGD-O2D
15	c6	413	CLA	CHA-CBD-CGD-O1D
15	c6	413	CLA	CHA-CBD-CGD-O2D
15	c6	417	CLA	CHA-CBD-CGD-O1D
15	c6	417	CLA	CHA-CBD-CGD-O2D
15	a4	410	CLA	O1D-CGD-O2D-CED
15	a4	403	CLA	C3-C5-C6-C7
15	b4	403	CLA	C3-C5-C6-C7
15	aA	814	CLA	O1A-CGA-O2A-C1
15	aA	829	CLA	O1A-CGA-O2A-C1
15	aA	831	CLA	O1A-CGA-O2A-C1
15	aB	829	CLA	O1A-CGA-O2A-C1
15	bA	814	CLA	O1A-CGA-O2A-C1
15	bA	829	CLA	O1A-CGA-O2A-C1
15	bA	831	CLA	O1A-CGA-O2A-C1
15	bB	829	CLA	O1A-CGA-O2A-C1
15	cA	829	CLA	O1A-CGA-O2A-C1
15	cA	831	CLA	O1A-CGA-O2A-C1
18	aB	845	BCR	C11-C10-C9-C8
18	aF	202	BCR	C11-C10-C9-C8
18	bB	845	BCR	C11-C10-C9-C8
18	bF	202	BCR	C11-C10-C9-C8
18	cB	845	BCR	C11-C10-C9-C8
18	cF	204	BCR	C11-C10-C9-C8
15	bA	832	CLA	O1D-CGD-O2D-CED
15	cA	832	CLA	O1D-CGD-O2D-CED
15	cA	814	CLA	O1A-CGA-O2A-C1
15	aA	833	CLA	C16-C17-C18-C19
15	a5	409	CLA	C16-C17-C18-C19
15	bA	833	CLA	C16-C17-C18-C19
15	cA	833	CLA	C16-C17-C18-C19
15	c4	409	CLA	C16-C17-C18-C19
15	aA	832	CLA	O1D-CGD-O2D-CED
15	b4	410	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	410	CLA	O1D-CGD-O2D-CED
15	c6	412	CLA	O1D-CGD-O2D-CED
15	b1	411	CLA	CBD-CGD-O2D-CED
15	aA	807	CLA	C14-C13-C15-C16
15	aA	828	CLA	C11-C10-C8-C9
15	aA	839	CLA	C14-C13-C15-C16
15	aA	841	CLA	C11-C10-C8-C9
15	aB	802	CLA	C11-C12-C13-C14
15	aB	827	CLA	C11-C10-C8-C9
15	aB	840	CLA	C11-C10-C8-C9
15	a2	402	CLA	C14-C13-C15-C16
15	bA	807	CLA	C14-C13-C15-C16
15	bA	839	CLA	C14-C13-C15-C16
15	bA	841	CLA	C11-C10-C8-C9
15	bB	802	CLA	C11-C12-C13-C14
15	bB	827	CLA	C11-C10-C8-C9
15	bB	840	CLA	C11-C10-C8-C9
15	b2	402	CLA	C14-C13-C15-C16
15	cA	807	CLA	C14-C13-C15-C16
15	cA	828	CLA	C11-C10-C8-C9
15	cA	839	CLA	C14-C13-C15-C16
15	cA	841	CLA	C11-C10-C8-C9
15	cB	802	CLA	C11-C12-C13-C14
15	cB	827	CLA	C11-C10-C8-C9
15	cB	840	CLA	C11-C10-C8-C9
15	c2	402	CLA	C14-C13-C15-C16
15	bA	824	CLA	O1D-CGD-O2D-CED
15	cA	844	CLA	O1A-CGA-O2A-C1
15	aA	824	CLA	O1D-CGD-O2D-CED
15	cA	824	CLA	O1D-CGD-O2D-CED
15	aB	814	CLA	C2A-CAA-CBA-CGA
15	bB	814	CLA	C2A-CAA-CBA-CGA
15	cB	814	CLA	C2A-CAA-CBA-CGA
15	aB	811	CLA	O1D-CGD-O2D-CED
15	c1	411	CLA	O1D-CGD-O2D-CED
15	aA	845	CLA	O1A-CGA-O2A-C1
15	bA	845	CLA	O1A-CGA-O2A-C1
15	b6	422	CLA	O1A-CGA-O2A-C1
18	c1	401	BCR	C7-C8-C9-C34
15	a1	410	CLA	O1D-CGD-O2D-CED
15	aA	841	CLA	C10-C11-C12-C13
15	bA	841	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	802	CLA	C15-C16-C17-C18
18	c4	401	BCR	C11-C12-C13-C14
15	b1	403	CLA	C3-C5-C6-C7
15	c4	403	CLA	C3-C5-C6-C7
20	cB	850	LMG	C38-C39-C40-C41
15	aA	813	CLA	C1A-C2A-CAA-CBA
15	aA	827	CLA	C1A-C2A-CAA-CBA
15	aA	832	CLA	C1A-C2A-CAA-CBA
15	aA	844	CLA	C1A-C2A-CAA-CBA
15	aB	812	CLA	C1A-C2A-CAA-CBA
15	aB	813	CLA	C1A-C2A-CAA-CBA
15	aB	818	CLA	C1A-C2A-CAA-CBA
15	a2	405	CLA	C1A-C2A-CAA-CBA
15	a3	412	CLA	C1A-C2A-CAA-CBA
15	a4	405	CLA	C1A-C2A-CAA-CBA
15	a5	413	CLA	C1A-C2A-CAA-CBA
15	a6	414	CLA	C1A-C2A-CAA-CBA
15	bA	813	CLA	C1A-C2A-CAA-CBA
15	bA	827	CLA	C1A-C2A-CAA-CBA
15	bA	844	CLA	C1A-C2A-CAA-CBA
15	bB	812	CLA	C1A-C2A-CAA-CBA
15	bB	813	CLA	C1A-C2A-CAA-CBA
15	bB	818	CLA	C1A-C2A-CAA-CBA
15	b3	412	CLA	C1A-C2A-CAA-CBA
15	b4	405	CLA	C1A-C2A-CAA-CBA
15	b5	413	CLA	C1A-C2A-CAA-CBA
15	b6	414	CLA	C1A-C2A-CAA-CBA
15	cA	813	CLA	C1A-C2A-CAA-CBA
15	cA	827	CLA	C1A-C2A-CAA-CBA
15	cA	832	CLA	C1A-C2A-CAA-CBA
15	cA	843	CLA	C1A-C2A-CAA-CBA
15	cB	812	CLA	C1A-C2A-CAA-CBA
15	cB	813	CLA	C1A-C2A-CAA-CBA
15	cB	818	CLA	C1A-C2A-CAA-CBA
15	c3	412	CLA	C1A-C2A-CAA-CBA
15	c5	413	CLA	C1A-C2A-CAA-CBA
15	c6	414	CLA	C1A-C2A-CAA-CBA
15	a1	408	CLA	C16-C17-C18-C19
15	b1	409	CLA	C16-C17-C18-C19
15	b2	410	CLA	C16-C17-C18-C19
15	b4	409	CLA	C16-C17-C18-C19
15	b6	410	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b6	422	CLA	C16-C17-C18-C20
15	c1	409	CLA	C16-C17-C18-C19
15	aA	802	CLA	C15-C16-C17-C18
15	bA	802	CLA	C15-C16-C17-C18
15	cA	841	CLA	C10-C11-C12-C13
20	aB	850	LMG	C38-C39-C40-C41
20	bB	851	LMG	C38-C39-C40-C41
15	bB	811	CLA	O1D-CGD-O2D-CED
15	b3	411	CLA	O1D-CGD-O2D-CED
15	cB	805	CLA	O1D-CGD-O2D-CED
15	cB	811	CLA	O1D-CGD-O2D-CED
15	bA	817	CLA	O1A-CGA-O2A-C1
19	aA	853	LHG	C3-O3-P-O6
19	bA	854	LHG	C3-O3-P-O6
19	cA	852	LHG	C3-O3-P-O6
15	aB	805	CLA	O1D-CGD-O2D-CED
15	a4	411	CLA	O1D-CGD-O2D-CED
15	bB	805	CLA	O1D-CGD-O2D-CED
15	aB	840	CLA	C2C-C3C-CAC-CBC
15	bB	840	CLA	C2C-C3C-CAC-CBC
15	cB	840	CLA	C2C-C3C-CAC-CBC
15	aA	825	CLA	C3-C5-C6-C7
15	bA	825	CLA	C3-C5-C6-C7
15	cA	825	CLA	C3-C5-C6-C7
15	aA	817	CLA	O1A-CGA-O2A-C1
15	cA	817	CLA	O1A-CGA-O2A-C1
15	cA	841	CLA	O1A-CGA-O2A-C1
19	aA	854	LHG	C3-O3-P-O4
19	bA	855	LHG	C3-O3-P-O4
19	bA	855	LHG	C4-O6-P-O5
19	cA	853	LHG	C3-O3-P-O4
19	cA	853	LHG	C4-O6-P-O5
15	a4	409	CLA	C16-C17-C18-C19
15	a6	410	CLA	C16-C17-C18-C19
15	aB	806	CLA	CBA-CGA-O2A-C1
15	bB	806	CLA	CBA-CGA-O2A-C1
15	cB	806	CLA	CBA-CGA-O2A-C1
15	aA	841	CLA	O1A-CGA-O2A-C1
15	bA	841	CLA	O1A-CGA-O2A-C1
15	aA	822	CLA	C3-C5-C6-C7
15	bA	822	CLA	C3-C5-C6-C7
15	cA	822	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	403	CLA	C3-C5-C6-C7
15	b4	411	CLA	O1D-CGD-O2D-CED
20	aB	850	LMG	C32-C33-C34-C35
20	bB	851	LMG	C32-C33-C34-C35
15	aA	833	CLA	C16-C17-C18-C20
15	bA	833	CLA	C16-C17-C18-C20
15	cA	833	CLA	C16-C17-C18-C20
20	cB	850	LMG	C32-C33-C34-C35
15	aA	814	CLA	CAD-CBD-CGD-O1D
15	aA	838	CLA	CAD-CBD-CGD-O1D
15	aB	803	CLA	CAD-CBD-CGD-O1D
15	aB	806	CLA	CAD-CBD-CGD-O1D
15	aB	814	CLA	CAD-CBD-CGD-O1D
15	aB	836	CLA	CAD-CBD-CGD-O1D
15	aL	201	CLA	CAD-CBD-CGD-O1D
15	a1	411	CLA	CAD-CBD-CGD-O1D
15	a2	413	CLA	CAD-CBD-CGD-O1D
15	a3	412	CLA	CAD-CBD-CGD-O1D
15	a4	412	CLA	CAD-CBD-CGD-O1D
15	a5	412	CLA	CAD-CBD-CGD-O1D
15	a5	415	CLA	CAD-CBD-CGD-O1D
15	a6	413	CLA	CAD-CBD-CGD-O1D
15	bA	814	CLA	CAD-CBD-CGD-O1D
15	bA	838	CLA	CAD-CBD-CGD-O1D
15	bB	803	CLA	CAD-CBD-CGD-O1D
15	bB	806	CLA	CAD-CBD-CGD-O1D
15	bB	814	CLA	CAD-CBD-CGD-O1D
15	bB	836	CLA	CAD-CBD-CGD-O1D
15	bL	202	CLA	CAD-CBD-CGD-O1D
15	b1	412	CLA	CAD-CBD-CGD-O1D
15	b2	413	CLA	CAD-CBD-CGD-O1D
15	b3	412	CLA	CAD-CBD-CGD-O1D
15	b4	412	CLA	CAD-CBD-CGD-O1D
15	b5	412	CLA	CAD-CBD-CGD-O1D
15	b5	415	CLA	CAD-CBD-CGD-O1D
15	b6	413	CLA	CAD-CBD-CGD-O1D
15	cA	814	CLA	CAD-CBD-CGD-O1D
15	cA	815	CLA	CAD-CBD-CGD-O1D
15	cA	838	CLA	CAD-CBD-CGD-O1D
15	cB	803	CLA	CAD-CBD-CGD-O1D
15	cB	806	CLA	CAD-CBD-CGD-O1D
15	cB	814	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	836	CLA	CAD-CBD-CGD-O1D
15	cL	201	CLA	CAD-CBD-CGD-O1D
15	c1	412	CLA	CAD-CBD-CGD-O1D
15	c2	413	CLA	CAD-CBD-CGD-O1D
15	c3	412	CLA	CAD-CBD-CGD-O1D
15	c4	412	CLA	CAD-CBD-CGD-O1D
15	c5	412	CLA	CAD-CBD-CGD-O1D
15	c5	415	CLA	CAD-CBD-CGD-O1D
15	c6	413	CLA	CAD-CBD-CGD-O1D
15	aB	810	CLA	C13-C15-C16-C17
15	bB	810	CLA	C13-C15-C16-C17
15	cB	810	CLA	C13-C15-C16-C17
15	aB	806	CLA	O1A-CGA-O2A-C1
15	bB	806	CLA	O1A-CGA-O2A-C1
15	cB	806	CLA	O1A-CGA-O2A-C1
15	a1	402	CLA	C3-C5-C6-C7
15	a3	403	CLA	C3-C5-C6-C7
15	b3	403	CLA	C3-C5-C6-C7
15	c3	403	CLA	C3-C5-C6-C7
15	aA	832	CLA	CBA-CGA-O2A-C1
15	bA	832	CLA	CBA-CGA-O2A-C1
15	cA	832	CLA	CBA-CGA-O2A-C1
15	aA	835	CLA	C16-C17-C18-C20
15	a1	422	CLA	C16-C17-C18-C20
15	a3	409	CLA	C16-C17-C18-C19
15	bA	835	CLA	C16-C17-C18-C20
15	b3	409	CLA	C16-C17-C18-C19
15	cA	835	CLA	C16-C17-C18-C20
15	c2	410	CLA	C16-C17-C18-C19
15	c3	409	CLA	C16-C17-C18-C19
15	aA	820	CLA	C11-C12-C13-C15
15	aA	825	CLA	C11-C10-C8-C7
15	aA	828	CLA	C6-C7-C8-C10
15	aA	841	CLA	C11-C10-C8-C7
15	aA	844	CLA	C3A-C2A-CAA-CBA
15	aB	814	CLA	C6-C7-C8-C10
15	aB	834	CLA	C3A-C2A-CAA-CBA
15	aB	837	CLA	C12-C13-C15-C16
15	aB	839	CLA	C11-C12-C13-C15
15	aL	203	CLA	C6-C7-C8-C10
15	a3	403	CLA	C11-C12-C13-C15
15	bA	820	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	825	CLA	C11-C10-C8-C7
15	bA	828	CLA	C6-C7-C8-C10
15	bA	841	CLA	C11-C10-C8-C7
15	bA	844	CLA	C3A-C2A-CAA-CBA
15	bB	814	CLA	C6-C7-C8-C10
15	bB	834	CLA	C3A-C2A-CAA-CBA
15	bB	837	CLA	C12-C13-C15-C16
15	bB	839	CLA	C11-C12-C13-C15
15	bL	204	CLA	C6-C7-C8-C10
15	b3	403	CLA	C11-C12-C13-C15
15	cA	820	CLA	C11-C12-C13-C15
15	cA	825	CLA	C11-C10-C8-C7
15	cA	828	CLA	C6-C7-C8-C10
15	cA	841	CLA	C11-C10-C8-C7
15	cB	814	CLA	C6-C7-C8-C10
15	cB	834	CLA	C3A-C2A-CAA-CBA
15	cB	837	CLA	C12-C13-C15-C16
15	cB	839	CLA	C11-C12-C13-C15
15	cL	203	CLA	C6-C7-C8-C10
15	c3	403	CLA	C11-C12-C13-C15
20	cB	850	LMG	C36-C37-C38-C39
20	aB	850	LMG	C36-C37-C38-C39
20	bB	851	LMG	C36-C37-C38-C39
20	aB	850	LMG	O1-C7-C8-O7
20	bB	851	LMG	O1-C7-C8-O7
20	cB	850	LMG	O1-C7-C8-O7
15	b1	411	CLA	O1D-CGD-O2D-CED
15	aB	818	CLA	O1D-CGD-O2D-CED
15	cB	818	CLA	O1D-CGD-O2D-CED
19	aA	853	LHG	C11-C10-C9-C8
19	bA	854	LHG	C11-C10-C9-C8
15	aA	834	CLA	C4-C3-C5-C6
15	bA	834	CLA	C4-C3-C5-C6
15	cA	834	CLA	C4-C3-C5-C6
19	cA	852	LHG	C11-C10-C9-C8
15	aA	806	CLA	C11-C10-C8-C9
15	aA	810	CLA	C11-C10-C8-C9
15	aA	829	CLA	C11-C12-C13-C14
15	aA	829	CLA	C14-C13-C15-C16
15	aA	833	CLA	C11-C10-C8-C9
15	aB	808	CLA	C11-C12-C13-C14
15	aB	809	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	837	CLA	C14-C13-C15-C16
15	a2	403	CLA	C11-C10-C8-C9
15	bA	806	CLA	C11-C10-C8-C9
15	bA	810	CLA	C11-C10-C8-C9
15	bA	828	CLA	C11-C10-C8-C9
15	bA	829	CLA	C11-C12-C13-C14
15	bA	829	CLA	C14-C13-C15-C16
15	bA	833	CLA	C11-C10-C8-C9
15	bB	808	CLA	C11-C12-C13-C14
15	bB	809	CLA	C11-C10-C8-C9
15	bB	837	CLA	C14-C13-C15-C16
15	cA	806	CLA	C11-C10-C8-C9
15	cA	810	CLA	C11-C10-C8-C9
15	cA	829	CLA	C11-C12-C13-C14
15	cA	829	CLA	C14-C13-C15-C16
15	cA	833	CLA	C11-C10-C8-C9
15	cB	808	CLA	C11-C12-C13-C14
15	cB	809	CLA	C11-C10-C8-C9
15	cB	837	CLA	C14-C13-C15-C16
16	aB	843	PQN	C19-C18-C20-C21
16	bB	843	PQN	C19-C18-C20-C21
16	cB	843	PQN	C19-C18-C20-C21
15	bB	818	CLA	O1D-CGD-O2D-CED
18	aK	101	BCR	C22-C23-C24-C25
18	aL	205	BCR	C6-C7-C8-C9
18	a3	418	BCR	C22-C23-C24-C25
18	a6	419	BCR	C22-C23-C24-C25
18	bA	848	BCR	C22-C23-C24-C25
18	bL	201	BCR	C6-C7-C8-C9
18	bL	206	BCR	C6-C7-C8-C9
18	b2	419	BCR	C22-C23-C24-C25
18	b6	419	BCR	C22-C23-C24-C25
18	cK	101	BCR	C22-C23-C24-C25
18	c6	419	BCR	C22-C23-C24-C25
15	cA	834	CLA	O1A-CGA-O2A-C1
15	c5	403	CLA	C3-C5-C6-C7
15	c6	404	CLA	C3-C5-C6-C7
15	a6	422	CLA	C16-C17-C18-C19
15	aA	834	CLA	O1A-CGA-O2A-C1
15	bA	834	CLA	O1A-CGA-O2A-C1
15	a5	403	CLA	C3-C5-C6-C7
15	aB	815	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	815	CLA	C16-C17-C18-C20
15	cB	815	CLA	C16-C17-C18-C20
18	c4	418	BCR	C16-C17-C18-C36
15	bA	832	CLA	O1A-CGA-O2A-C1
15	cA	832	CLA	O1A-CGA-O2A-C1
15	aA	820	CLA	C16-C17-C18-C19
15	a2	410	CLA	C16-C17-C18-C19
15	bA	820	CLA	C16-C17-C18-C19
15	cA	820	CLA	C16-C17-C18-C19
15	aA	823	CLA	C1-C2-C3-C4
15	aB	832	CLA	C1-C2-C3-C4
15	bA	823	CLA	C1-C2-C3-C4
15	bB	832	CLA	C1-C2-C3-C4
15	cA	823	CLA	C1-C2-C3-C4
15	cB	832	CLA	C1-C2-C3-C4
15	aA	832	CLA	O1A-CGA-O2A-C1
15	a6	404	CLA	C3-C5-C6-C7
15	bB	806	CLA	C3-C5-C6-C7
15	b5	403	CLA	C3-C5-C6-C7
15	b6	404	CLA	C3-C5-C6-C7
15	cB	806	CLA	C3-C5-C6-C7
15	aA	829	CLA	C2A-CAA-CBA-CGA
15	a1	409	CLA	C2A-CAA-CBA-CGA
15	a5	410	CLA	C2A-CAA-CBA-CGA
15	bA	829	CLA	C2A-CAA-CBA-CGA
15	b5	410	CLA	C2A-CAA-CBA-CGA
15	cA	829	CLA	C2A-CAA-CBA-CGA
15	c1	410	CLA	C2A-CAA-CBA-CGA
15	c5	410	CLA	C2A-CAA-CBA-CGA
15	aA	814	CLA	C2-C1-O2A-CGA
15	aA	841	CLA	C2-C1-O2A-CGA
15	aB	807	CLA	C2-C1-O2A-CGA
15	aB	829	CLA	C2-C1-O2A-CGA
15	bA	814	CLA	C2-C1-O2A-CGA
15	bA	841	CLA	C2-C1-O2A-CGA
15	bB	807	CLA	C2-C1-O2A-CGA
15	bB	829	CLA	C2-C1-O2A-CGA
15	cA	814	CLA	C2-C1-O2A-CGA
15	cA	841	CLA	C2-C1-O2A-CGA
15	cB	807	CLA	C2-C1-O2A-CGA
15	cB	829	CLA	C2-C1-O2A-CGA
15	aB	802	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	802	CLA	CAA-CBA-CGA-O2A
15	cB	802	CLA	CAA-CBA-CGA-O2A
15	cB	808	CLA	O1A-CGA-O2A-C1
15	aB	806	CLA	C3-C5-C6-C7
15	aA	834	CLA	CBA-CGA-O2A-C1
15	a1	422	CLA	CBA-CGA-O2A-C1
15	bA	834	CLA	CBA-CGA-O2A-C1
15	cA	834	CLA	CBA-CGA-O2A-C1
18	cI	101	BCR	C9-C10-C11-C12
15	aB	808	CLA	O1A-CGA-O2A-C1
15	bB	808	CLA	O1A-CGA-O2A-C1
15	b6	404	CLA	O1A-CGA-O2A-C1
15	cA	834	CLA	C16-C17-C18-C20
15	aA	822	CLA	C4-C3-C5-C6
15	cA	822	CLA	C4-C3-C5-C6
18	aA	849	BCR	C23-C24-C25-C26
18	aA	852	BCR	C1-C6-C7-C8
18	aB	847	BCR	C23-C24-C25-C26
18	aI	102	BCR	C23-C24-C25-C26
18	aL	205	BCR	C23-C24-C25-C26
18	a1	418	BCR	C23-C24-C25-C30
18	a1	420	BCR	C23-C24-C25-C30
18	a2	420	BCR	C23-C24-C25-C26
18	a3	419	BCR	C23-C24-C25-C30
18	a4	419	BCR	C23-C24-C25-C30
18	a5	401	BCR	C23-C24-C25-C30
18	a6	401	BCR	C23-C24-C25-C30
18	a6	402	BCR	C1-C6-C7-C8
18	bA	850	BCR	C23-C24-C25-C26
18	bA	853	BCR	C1-C6-C7-C8
18	bB	847	BCR	C23-C24-C25-C26
18	bI	102	BCR	C23-C24-C25-C26
18	bL	201	BCR	C23-C24-C25-C26
18	bL	206	BCR	C23-C24-C25-C26
18	b1	401	BCR	C23-C24-C25-C30
18	b1	419	BCR	C23-C24-C25-C30
18	b2	420	BCR	C23-C24-C25-C26
18	b3	401	BCR	C23-C24-C25-C26
18	b3	419	BCR	C23-C24-C25-C30
18	b4	419	BCR	C23-C24-C25-C30
18	b5	401	BCR	C23-C24-C25-C30
18	b6	401	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b6	402	BCR	C1-C6-C7-C8
18	cA	848	BCR	C23-C24-C25-C26
18	cA	851	BCR	C1-C6-C7-C8
18	cB	847	BCR	C23-C24-C25-C26
18	cI	102	BCR	C23-C24-C25-C26
18	c1	401	BCR	C23-C24-C25-C30
18	c1	419	BCR	C23-C24-C25-C30
18	c3	419	BCR	C23-C24-C25-C30
18	c4	419	BCR	C23-C24-C25-C30
18	c5	401	BCR	C23-C24-C25-C30
18	c6	401	BCR	C23-C24-C25-C30
18	c6	402	BCR	C1-C6-C7-C8
15	aA	834	CLA	C16-C17-C18-C20
15	bA	834	CLA	C16-C17-C18-C20
15	bA	822	CLA	C15-C16-C17-C18
15	cA	822	CLA	C15-C16-C17-C18
15	b1	410	CLA	C2A-CAA-CBA-CGA
18	aF	203	BCR	C16-C17-C18-C19
18	bJ	105	BCR	C16-C17-C18-C19
18	cF	205	BCR	C16-C17-C18-C19
19	aA	854	LHG	O7-C5-C6-O8
19	bA	855	LHG	O7-C5-C6-O8
19	cA	853	LHG	O7-C5-C6-O8
15	aA	822	CLA	C15-C16-C17-C18
19	aA	853	LHG	C11-C12-C13-C14
19	bA	854	LHG	C11-C12-C13-C14
19	cA	852	LHG	C11-C12-C13-C14
15	b6	404	CLA	CBA-CGA-O2A-C1
19	aA	853	LHG	C4-C5-C6-O8
19	aA	854	LHG	C4-C5-C6-O8
19	bA	854	LHG	C4-C5-C6-O8
19	bA	855	LHG	C4-C5-C6-O8
19	cA	852	LHG	C4-C5-C6-O8
19	cA	853	LHG	C4-C5-C6-O8
14	aA	801	CL0	C12-C13-C15-C16
14	bA	801	CL0	C12-C13-C15-C16
14	cA	801	CL0	C12-C13-C15-C16
15	aA	841	CLA	C2-C3-C5-C6
15	aB	828	CLA	C12-C13-C15-C16
15	a2	402	CLA	C12-C13-C15-C16
15	a6	403	CLA	C12-C13-C15-C16
15	bA	841	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	828	CLA	C12-C13-C15-C16
15	b1	402	CLA	C12-C13-C15-C16
15	b2	402	CLA	C12-C13-C15-C16
15	b6	403	CLA	C12-C13-C15-C16
15	cA	841	CLA	C2-C3-C5-C6
15	cB	828	CLA	C12-C13-C15-C16
15	c2	402	CLA	C12-C13-C15-C16
15	c6	403	CLA	C12-C13-C15-C16
15	aB	815	CLA	C11-C10-C8-C9
15	a1	402	CLA	C11-C10-C8-C9
15	a3	403	CLA	C11-C10-C8-C9
15	a5	403	CLA	C11-C10-C8-C9
15	a6	404	CLA	C11-C10-C8-C9
15	bB	815	CLA	C11-C10-C8-C9
15	bB	839	CLA	C11-C12-C13-C14
15	b1	403	CLA	C11-C10-C8-C9
15	b2	403	CLA	C11-C10-C8-C9
15	b3	403	CLA	C11-C10-C8-C9
15	b4	403	CLA	C11-C10-C8-C9
15	b5	403	CLA	C11-C10-C8-C9
15	b6	404	CLA	C11-C10-C8-C9
15	cB	815	CLA	C11-C10-C8-C9
15	cB	839	CLA	C11-C12-C13-C14
15	c1	403	CLA	C11-C10-C8-C9
15	c2	403	CLA	C11-C10-C8-C9
15	c3	403	CLA	C11-C10-C8-C9
15	c5	403	CLA	C11-C10-C8-C9
15	c6	404	CLA	C11-C10-C8-C9
15	aB	810	CLA	C8-C10-C11-C12
18	aF	203	BCR	C15-C16-C17-C18
18	aI	101	BCR	C9-C10-C11-C12
18	aL	205	BCR	C9-C10-C11-C12
18	bI	101	BCR	C9-C10-C11-C12
18	bJ	105	BCR	C15-C16-C17-C18
18	bL	201	BCR	C9-C10-C11-C12
18	bL	206	BCR	C9-C10-C11-C12
18	cF	205	BCR	C15-C16-C17-C18
15	aA	835	CLA	C16-C17-C18-C19
15	bA	835	CLA	C16-C17-C18-C19
15	cA	835	CLA	C16-C17-C18-C19
16	aB	843	PQN	C23-C25-C26-C27
16	bB	843	PQN	C23-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	cB	843	PQN	C23-C25-C26-C27
15	bB	810	CLA	C8-C10-C11-C12
15	cB	810	CLA	C8-C10-C11-C12
15	a6	404	CLA	O1A-CGA-O2A-C1
15	c6	404	CLA	O1A-CGA-O2A-C1
15	b2	422	CLA	C16-C17-C18-C20
15	b6	422	CLA	C16-C17-C18-C19
15	c2	422	CLA	C16-C17-C18-C20
15	b3	403	CLA	CBA-CGA-O2A-C1
19	aA	854	LHG	C2-C3-O3-P
19	bA	855	LHG	C2-C3-O3-P
19	cA	853	LHG	C2-C3-O3-P
15	bA	822	CLA	C4-C3-C5-C6
15	aA	822	CLA	C2-C3-C5-C6
15	aA	834	CLA	C2-C3-C5-C6
15	bA	822	CLA	C2-C3-C5-C6
15	bA	834	CLA	C2-C3-C5-C6
15	cA	822	CLA	C2-C3-C5-C6
15	cA	834	CLA	C2-C3-C5-C6
15	aA	834	CLA	C16-C17-C18-C19
15	a2	422	CLA	C16-C17-C18-C20
15	bA	834	CLA	C16-C17-C18-C19
15	cA	834	CLA	C16-C17-C18-C19
15	aB	833	CLA	CBA-CGA-O2A-C1
15	a2	403	CLA	CBA-CGA-O2A-C1
15	a3	403	CLA	CBA-CGA-O2A-C1
15	a6	404	CLA	CBA-CGA-O2A-C1
15	bB	833	CLA	CBA-CGA-O2A-C1
15	b2	403	CLA	CBA-CGA-O2A-C1
15	b4	403	CLA	CBA-CGA-O2A-C1
15	cB	833	CLA	CBA-CGA-O2A-C1
15	c2	403	CLA	CBA-CGA-O2A-C1
15	c6	404	CLA	CBA-CGA-O2A-C1
15	a4	403	CLA	O1A-CGA-O2A-C1
15	aB	835	CLA	CAA-CBA-CGA-O2A
15	bB	835	CLA	CAA-CBA-CGA-O2A
15	cB	835	CLA	CAA-CBA-CGA-O2A
14	aA	801	CL0	CAA-CBA-CGA-O2A
14	bA	801	CL0	CAA-CBA-CGA-O2A
14	cA	801	CL0	CAA-CBA-CGA-O2A
15	cA	803	CLA	O1D-CGD-O2D-CED
18	a5	418	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a3	403	CLA	O1A-CGA-O2A-C1
15	a4	403	CLA	CBA-CGA-O2A-C1
15	c3	403	CLA	CBA-CGA-O2A-C1
15	bB	808	CLA	C2A-CAA-CBA-CGA
15	cB	808	CLA	C2A-CAA-CBA-CGA
18	aB	847	BCR	C15-C16-C17-C18
18	bB	847	BCR	C15-C16-C17-C18
18	cB	847	BCR	C15-C16-C17-C18
20	cB	850	LMG	C29-C30-C31-C32
18	a1	418	BCR	C18-C19-C20-C21
18	a4	419	BCR	C10-C11-C12-C13
18	b1	419	BCR	C18-C19-C20-C21
18	b4	419	BCR	C10-C11-C12-C13
18	c1	419	BCR	C18-C19-C20-C21
18	c2	401	BCR	C10-C11-C12-C13
18	c2	420	BCR	C18-C19-C20-C21
18	c3	418	BCR	C18-C19-C20-C21
18	c4	419	BCR	C10-C11-C12-C13
18	c5	418	BCR	C18-C19-C20-C21
15	a2	403	CLA	O1A-CGA-O2A-C1
15	b2	403	CLA	O1A-CGA-O2A-C1
15	b4	403	CLA	O1A-CGA-O2A-C1
15	c2	403	CLA	O1A-CGA-O2A-C1
15	aB	818	CLA	C10-C11-C12-C13
15	bB	818	CLA	C10-C11-C12-C13
15	cB	818	CLA	C10-C11-C12-C13
20	aB	850	LMG	C29-C30-C31-C32
20	bB	851	LMG	C29-C30-C31-C32
15	aB	809	CLA	C4-C3-C5-C6
15	bB	809	CLA	C4-C3-C5-C6
15	cB	809	CLA	C4-C3-C5-C6
15	aB	833	CLA	O1A-CGA-O2A-C1
15	bB	833	CLA	O1A-CGA-O2A-C1
15	b3	403	CLA	O1A-CGA-O2A-C1
15	c3	403	CLA	O1A-CGA-O2A-C1
15	aA	809	CLA	C8-C10-C11-C12
15	aB	802	CLA	C15-C16-C17-C18
15	a5	410	CLA	C13-C15-C16-C17
15	bA	809	CLA	C8-C10-C11-C12
15	bB	802	CLA	C15-C16-C17-C18
15	c2	416	CLA	CAA-CBA-CGA-O1A
15	aA	808	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	812	CLA	C2-C1-O2A-CGA
15	aA	829	CLA	C2-C1-O2A-CGA
15	bA	808	CLA	C2-C1-O2A-CGA
15	bA	812	CLA	C2-C1-O2A-CGA
15	bA	829	CLA	C2-C1-O2A-CGA
15	cA	808	CLA	C2-C1-O2A-CGA
15	cA	812	CLA	C2-C1-O2A-CGA
15	cA	829	CLA	C2-C1-O2A-CGA
15	cA	809	CLA	C8-C10-C11-C12
15	cB	802	CLA	C15-C16-C17-C18
15	c6	410	CLA	C16-C17-C18-C20
15	cB	833	CLA	O1A-CGA-O2A-C1
15	a2	416	CLA	CAA-CBA-CGA-O1A
15	a5	415	CLA	CAA-CBA-CGA-O1A
15	bB	835	CLA	CAA-CBA-CGA-O1A
15	cB	835	CLA	CAA-CBA-CGA-O1A
15	aA	837	CLA	C2A-CAA-CBA-CGA
15	aB	808	CLA	C2A-CAA-CBA-CGA
15	aX	102	CLA	C2A-CAA-CBA-CGA
15	a2	411	CLA	C2A-CAA-CBA-CGA
15	a3	410	CLA	C2A-CAA-CBA-CGA
15	a4	410	CLA	C2A-CAA-CBA-CGA
15	a6	411	CLA	C2A-CAA-CBA-CGA
15	bA	837	CLA	C2A-CAA-CBA-CGA
15	bX	102	CLA	C2A-CAA-CBA-CGA
15	b2	411	CLA	C2A-CAA-CBA-CGA
15	b3	410	CLA	C2A-CAA-CBA-CGA
15	b4	410	CLA	C2A-CAA-CBA-CGA
15	b6	411	CLA	C2A-CAA-CBA-CGA
15	cA	837	CLA	C2A-CAA-CBA-CGA
15	cX	102	CLA	C2A-CAA-CBA-CGA
15	c2	411	CLA	C2A-CAA-CBA-CGA
15	c3	410	CLA	C2A-CAA-CBA-CGA
15	c4	410	CLA	C2A-CAA-CBA-CGA
15	c6	411	CLA	C2A-CAA-CBA-CGA
15	cA	818	CLA	C5-C6-C7-C8
15	aB	828	CLA	CAA-CBA-CGA-O1A
15	bB	828	CLA	CAA-CBA-CGA-O1A
15	cB	828	CLA	CAA-CBA-CGA-O1A
15	bA	803	CLA	O1D-CGD-O2D-CED
15	aA	818	CLA	C5-C6-C7-C8
15	bA	818	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	835	CLA	CAA-CBA-CGA-O1A
15	a3	415	CLA	CAA-CBA-CGA-O1A
15	c3	415	CLA	CAA-CBA-CGA-O1A
15	c4	409	CLA	C16-C17-C18-C20
18	aA	852	BCR	C19-C20-C21-C22
18	bA	853	BCR	C19-C20-C21-C22
18	cA	851	BCR	C19-C20-C21-C22
15	a3	410	CLA	C13-C15-C16-C17
15	aA	803	CLA	O1D-CGD-O2D-CED
15	aB	824	CLA	CAA-CBA-CGA-O1A
15	bB	824	CLA	CAA-CBA-CGA-O1A
15	cB	824	CLA	CAA-CBA-CGA-O1A
15	aA	809	CLA	C6-C7-C8-C9
15	aB	815	CLA	C11-C12-C13-C14
15	aB	839	CLA	C11-C12-C13-C14
15	a4	403	CLA	C11-C10-C8-C9
15	bA	809	CLA	C6-C7-C8-C9
15	bB	815	CLA	C11-C12-C13-C14
15	cA	809	CLA	C6-C7-C8-C9
15	cB	815	CLA	C11-C12-C13-C14
15	c4	403	CLA	C11-C10-C8-C9
20	aB	850	LMG	C13-C14-C15-C16
20	bB	851	LMG	C13-C14-C15-C16
20	cB	850	LMG	C13-C14-C15-C16
15	b5	415	CLA	CAA-CBA-CGA-O1A
15	b3	410	CLA	C13-C15-C16-C17
18	aA	852	BCR	C11-C10-C9-C34
18	aB	846	BCR	C11-C10-C9-C34
18	aB	846	BCR	C20-C21-C22-C37
18	aB	849	BCR	C35-C13-C14-C15
18	a1	417	BCR	C20-C21-C22-C37
18	a6	421	BCR	C20-C21-C22-C37
18	bA	853	BCR	C11-C10-C9-C34
18	bB	846	BCR	C11-C10-C9-C34
18	bB	846	BCR	C20-C21-C22-C37
18	bB	850	BCR	C35-C13-C14-C15
18	b6	421	BCR	C20-C21-C22-C37
18	cA	851	BCR	C11-C10-C9-C34
18	cB	846	BCR	C11-C10-C9-C34
18	cB	846	BCR	C20-C21-C22-C37
18	cB	849	BCR	C35-C13-C14-C15
18	c3	401	BCR	C35-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c5	418	BCR	C16-C17-C18-C36
15	a6	416	CLA	CAA-CBA-CGA-O1A
15	bB	831	CLA	CAA-CBA-CGA-O1A
15	b5	415	CLA	CAA-CBA-CGA-O2A
15	b6	416	CLA	CAA-CBA-CGA-O1A
15	cB	831	CLA	CAA-CBA-CGA-O1A
15	c5	415	CLA	CAA-CBA-CGA-O1A
15	c5	415	CLA	CAA-CBA-CGA-O2A
15	aA	809	CLA	C16-C17-C18-C20
15	aB	815	CLA	C16-C17-C18-C19
15	bA	809	CLA	C16-C17-C18-C20
15	bB	815	CLA	C16-C17-C18-C19
15	b2	406	CLA	C16-C17-C18-C19
15	cA	809	CLA	C16-C17-C18-C20
15	cB	815	CLA	C16-C17-C18-C19
15	aA	806	CLA	O2A-C1-C2-C3
15	bA	806	CLA	O2A-C1-C2-C3
15	cA	806	CLA	O2A-C1-C2-C3
15	c4	403	CLA	CBA-CGA-O2A-C1
15	aB	831	CLA	CAA-CBA-CGA-O1A
15	aK	102	CLA	CAA-CBA-CGA-O1A
15	a3	415	CLA	CAA-CBA-CGA-O2A
15	a4	415	CLA	CAA-CBA-CGA-O1A
15	bK	101	CLA	CAA-CBA-CGA-O1A
15	b4	415	CLA	CAA-CBA-CGA-O1A
15	c4	415	CLA	CAA-CBA-CGA-O1A
20	aB	850	LMG	C33-C34-C35-C36
20	bB	851	LMG	C33-C34-C35-C36
20	cB	850	LMG	C33-C34-C35-C36
18	aF	201	BCR	C7-C8-C9-C10
18	aL	205	BCR	C21-C22-C23-C24
18	bB	849	BCR	C7-C8-C9-C10
18	bL	201	BCR	C21-C22-C23-C24
18	bL	206	BCR	C21-C22-C23-C24
18	cF	202	BCR	C7-C8-C9-C10
15	a1	414	CLA	CAA-CBA-CGA-O1A
15	a2	416	CLA	CAA-CBA-CGA-O2A
15	a5	415	CLA	CAA-CBA-CGA-O2A
15	b1	415	CLA	CAA-CBA-CGA-O1A
15	b1	415	CLA	CAA-CBA-CGA-O2A
15	b2	416	CLA	CAA-CBA-CGA-O1A
15	b2	416	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b3	415	CLA	CAA-CBA-CGA-O1A
15	cB	824	CLA	CAA-CBA-CGA-O2A
15	cK	102	CLA	CAA-CBA-CGA-O1A
15	aA	802	CLA	C1A-C2A-CAA-CBA
15	aA	808	CLA	C1A-C2A-CAA-CBA
15	aA	817	CLA	C1A-C2A-CAA-CBA
15	aA	825	CLA	C1A-C2A-CAA-CBA
15	aA	837	CLA	C1A-C2A-CAA-CBA
15	aA	842	CLA	C1A-C2A-CAA-CBA
15	aB	811	CLA	C1A-C2A-CAA-CBA
15	aB	838	CLA	C1A-C2A-CAA-CBA
15	a1	403	CLA	C1A-C2A-CAA-CBA
15	a1	412	CLA	C1A-C2A-CAA-CBA
15	a3	404	CLA	C1A-C2A-CAA-CBA
15	a4	404	CLA	C1A-C2A-CAA-CBA
15	bA	802	CLA	C1A-C2A-CAA-CBA
15	bA	808	CLA	C1A-C2A-CAA-CBA
15	bA	817	CLA	C1A-C2A-CAA-CBA
15	bA	825	CLA	C1A-C2A-CAA-CBA
15	bA	832	CLA	C1A-C2A-CAA-CBA
15	bA	837	CLA	C1A-C2A-CAA-CBA
15	bA	842	CLA	C1A-C2A-CAA-CBA
15	bB	811	CLA	C1A-C2A-CAA-CBA
15	bB	838	CLA	C1A-C2A-CAA-CBA
15	b1	413	CLA	C1A-C2A-CAA-CBA
15	b4	413	CLA	C1A-C2A-CAA-CBA
15	cA	802	CLA	C1A-C2A-CAA-CBA
15	cA	808	CLA	C1A-C2A-CAA-CBA
15	cA	817	CLA	C1A-C2A-CAA-CBA
15	cA	825	CLA	C1A-C2A-CAA-CBA
15	cA	837	CLA	C1A-C2A-CAA-CBA
15	cB	811	CLA	C1A-C2A-CAA-CBA
15	cB	838	CLA	C1A-C2A-CAA-CBA
15	cF	201	CLA	C1A-C2A-CAA-CBA
15	c1	404	CLA	C1A-C2A-CAA-CBA
15	c1	413	CLA	C1A-C2A-CAA-CBA
15	c4	413	CLA	C1A-C2A-CAA-CBA
15	aA	802	CLA	C6-C7-C8-C10
15	aA	829	CLA	C12-C13-C15-C16
15	aA	833	CLA	C6-C7-C8-C10
15	aB	802	CLA	C11-C12-C13-C15
15	bA	802	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	829	CLA	C12-C13-C15-C16
15	bA	833	CLA	C6-C7-C8-C10
15	bB	802	CLA	C11-C12-C13-C15
15	cA	802	CLA	C6-C7-C8-C10
15	cA	829	CLA	C12-C13-C15-C16
15	cA	833	CLA	C6-C7-C8-C10
15	cB	802	CLA	C11-C12-C13-C15
15	aB	824	CLA	CAA-CBA-CGA-O2A
15	bB	824	CLA	CAA-CBA-CGA-O2A
15	b3	415	CLA	CAA-CBA-CGA-O2A
15	a1	414	CLA	CAA-CBA-CGA-O2A
15	b2	409	CLA	CAA-CBA-CGA-O2A
15	b3	408	CLA	CAA-CBA-CGA-O2A
15	b6	409	CLA	CAA-CBA-CGA-O2A
15	c1	415	CLA	CAA-CBA-CGA-O1A
15	c5	408	CLA	CAA-CBA-CGA-O2A
15	c6	409	CLA	CAA-CBA-CGA-O2A
15	c6	416	CLA	CAA-CBA-CGA-O1A
15	aL	201	CLA	C8-C10-C11-C12
15	bL	202	CLA	C8-C10-C11-C12
15	cA	833	CLA	C5-C6-C7-C8
15	cB	814	CLA	C5-C6-C7-C8
15	cL	201	CLA	C8-C10-C11-C12
15	aA	835	CLA	C2A-CAA-CBA-CGA
15	aB	829	CLA	C2A-CAA-CBA-CGA
15	a2	418	CLA	C2A-CAA-CBA-CGA
15	bA	835	CLA	C2A-CAA-CBA-CGA
15	bB	829	CLA	C2A-CAA-CBA-CGA
15	cA	835	CLA	C2A-CAA-CBA-CGA
15	cB	829	CLA	C2A-CAA-CBA-CGA
15	c2	418	CLA	C2A-CAA-CBA-CGA
15	bB	814	CLA	C5-C6-C7-C8
15	b5	410	CLA	C13-C15-C16-C17
15	c5	410	CLA	C13-C15-C16-C17
15	aA	823	CLA	CAA-CBA-CGA-O2A
15	aB	833	CLA	CAA-CBA-CGA-O2A
15	bA	823	CLA	CAA-CBA-CGA-O2A
15	bB	833	CLA	CAA-CBA-CGA-O2A
15	cA	823	CLA	CAA-CBA-CGA-O2A
15	cB	833	CLA	CAA-CBA-CGA-O2A
15	a3	408	CLA	CAA-CBA-CGA-O2A
15	a6	409	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	415	CLA	CAA-CBA-CGA-O2A
15	c2	409	CLA	CAA-CBA-CGA-O2A
15	aA	833	CLA	C5-C6-C7-C8
15	aB	814	CLA	C5-C6-C7-C8
15	bA	830	CLA	C5-C6-C7-C8
15	bA	833	CLA	C5-C6-C7-C8
15	bL	204	CLA	C13-C15-C16-C17
15	b2	411	CLA	C13-C15-C16-C17
15	aB	809	CLA	CBA-CGA-O2A-C1
15	a4	409	CLA	C16-C17-C18-C20
15	a6	410	CLA	C16-C17-C18-C20
15	b4	409	CLA	C16-C17-C18-C20
15	b5	409	CLA	C16-C17-C18-C20
15	b6	410	CLA	C16-C17-C18-C20
15	aL	203	CLA	C13-C15-C16-C17
15	a1	407	CLA	CAA-CBA-CGA-O1A
15	a2	409	CLA	CAA-CBA-CGA-O2A
15	a4	408	CLA	CAA-CBA-CGA-O2A
15	a5	408	CLA	CAA-CBA-CGA-O2A
15	b1	408	CLA	CAA-CBA-CGA-O2A
15	b5	408	CLA	CAA-CBA-CGA-O2A
15	c3	408	CLA	CAA-CBA-CGA-O2A
15	aA	830	CLA	C5-C6-C7-C8
15	cA	830	CLA	C5-C6-C7-C8
15	cL	203	CLA	C13-C15-C16-C17
15	c3	410	CLA	C13-C15-C16-C17
15	bB	809	CLA	CBA-CGA-O2A-C1
15	b1	408	CLA	CAA-CBA-CGA-O1A
15	b4	408	CLA	CAA-CBA-CGA-O2A
15	c1	408	CLA	CAA-CBA-CGA-O1A
15	c4	403	CLA	O1A-CGA-O2A-C1
15	c5	409	CLA	C16-C17-C18-C20
18	aB	846	BCR	C11-C10-C9-C8
18	bB	846	BCR	C11-C10-C9-C8
18	cB	846	BCR	C11-C10-C9-C8
15	a2	411	CLA	C13-C15-C16-C17
15	a4	408	CLA	CAA-CBA-CGA-O1A
15	a4	415	CLA	CAA-CBA-CGA-O2A
15	a6	416	CLA	CAA-CBA-CGA-O2A
15	b4	415	CLA	CAA-CBA-CGA-O2A
15	b6	416	CLA	CAA-CBA-CGA-O2A
15	c3	415	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	408	CLA	CAA-CBA-CGA-O2A
15	c4	415	CLA	CAA-CBA-CGA-O2A
15	c6	416	CLA	CAA-CBA-CGA-O2A
15	a5	403	CLA	O1A-CGA-O2A-C1
15	a5	403	CLA	CBA-CGA-O2A-C1
15	cB	809	CLA	CBA-CGA-O2A-C1
15	b2	418	CLA	C2A-CAA-CBA-CGA
20	aB	850	LMG	C42-C43-C44-C45
20	bB	851	LMG	C42-C43-C44-C45
20	cB	850	LMG	C42-C43-C44-C45
18	aF	201	BCR	C13-C14-C15-C16
18	aJ	204	BCR	C13-C14-C15-C16
18	bB	849	BCR	C13-C14-C15-C16
18	bJ	103	BCR	C13-C14-C15-C16
18	cF	202	BCR	C13-C14-C15-C16
18	cJ	103	BCR	C13-C14-C15-C16
15	c2	416	CLA	CAA-CBA-CGA-O2A
18	a2	419	BCR	C22-C23-C24-C25
18	c2	419	BCR	C22-C23-C24-C25
18	c3	418	BCR	C22-C23-C24-C25
15	a5	409	CLA	C16-C17-C18-C20
15	c4	421	CLA	C16-C17-C18-C20
15	b5	403	CLA	O1A-CGA-O2A-C1
15	a1	407	CLA	CAA-CBA-CGA-O2A
15	c1	408	CLA	CAA-CBA-CGA-O2A
15	c4	408	CLA	CAA-CBA-CGA-O1A
15	aA	839	CLA	C4-C3-C5-C6
15	aB	811	CLA	C4-C3-C5-C6
15	aB	837	CLA	C4-C3-C5-C6
15	bA	839	CLA	C4-C3-C5-C6
15	bB	811	CLA	C4-C3-C5-C6
15	bB	837	CLA	C4-C3-C5-C6
15	cA	839	CLA	C4-C3-C5-C6
15	cB	811	CLA	C4-C3-C5-C6
15	cB	837	CLA	C4-C3-C5-C6
15	bB	809	CLA	C2-C3-C5-C6
15	c5	403	CLA	O1A-CGA-O2A-C1
18	a2	420	BCR	C18-C19-C20-C21
15	a2	409	CLA	CAA-CBA-CGA-O1A
15	a3	408	CLA	CAA-CBA-CGA-O1A
15	b3	408	CLA	CAA-CBA-CGA-O1A
15	b5	408	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	831	CLA	CAA-CBA-CGA-O2A
15	c5	408	CLA	CAA-CBA-CGA-O1A
15	aA	805	CLA	CAA-CBA-CGA-O2A
15	cA	805	CLA	CAA-CBA-CGA-O2A
15	a5	408	CLA	CAA-CBA-CGA-O1A
15	a6	409	CLA	CAA-CBA-CGA-O1A
15	b2	409	CLA	CAA-CBA-CGA-O1A
15	b4	408	CLA	CAA-CBA-CGA-O1A
15	b6	409	CLA	CAA-CBA-CGA-O1A
15	c2	409	CLA	CAA-CBA-CGA-O1A
15	bA	826	CLA	C15-C16-C17-C18
15	cA	826	CLA	C15-C16-C17-C18
15	b2	410	CLA	C16-C17-C18-C20
18	aA	849	BCR	C23-C24-C25-C30
18	aB	845	BCR	C23-C24-C25-C26
18	aB	845	BCR	C23-C24-C25-C30
18	aB	846	BCR	C23-C24-C25-C30
18	aF	201	BCR	C23-C24-C25-C30
18	aF	202	BCR	C23-C24-C25-C30
18	aF	203	BCR	C1-C6-C7-C8
18	aI	101	BCR	C23-C24-C25-C30
18	aI	102	BCR	C1-C6-C7-C8
18	aJ	204	BCR	C23-C24-C25-C26
18	aJ	204	BCR	C23-C24-C25-C30
18	aK	101	BCR	C23-C24-C25-C30
18	aL	205	BCR	C23-C24-C25-C30
18	a2	401	BCR	C1-C6-C7-C8
18	a6	402	BCR	C5-C6-C7-C8
18	bA	848	BCR	C23-C24-C25-C30
18	bA	850	BCR	C23-C24-C25-C30
18	bB	845	BCR	C23-C24-C25-C26
18	bB	845	BCR	C23-C24-C25-C30
18	bB	846	BCR	C23-C24-C25-C30
18	bB	849	BCR	C23-C24-C25-C30
18	bF	202	BCR	C23-C24-C25-C30
18	bI	101	BCR	C23-C24-C25-C30
18	bI	102	BCR	C1-C6-C7-C8
18	bJ	103	BCR	C23-C24-C25-C26
18	bJ	103	BCR	C23-C24-C25-C30
18	bJ	105	BCR	C1-C6-C7-C8
18	bL	201	BCR	C23-C24-C25-C30
18	bL	206	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b2	401	BCR	C1-C6-C7-C8
18	cA	848	BCR	C23-C24-C25-C30
18	cB	845	BCR	C23-C24-C25-C26
18	cB	845	BCR	C23-C24-C25-C30
18	cB	846	BCR	C23-C24-C25-C30
18	cF	202	BCR	C23-C24-C25-C30
18	cF	204	BCR	C23-C24-C25-C30
18	cF	205	BCR	C1-C6-C7-C8
18	cI	101	BCR	C23-C24-C25-C30
18	cI	102	BCR	C1-C6-C7-C8
18	cJ	103	BCR	C23-C24-C25-C26
18	cJ	103	BCR	C23-C24-C25-C30
18	cK	101	BCR	C23-C24-C25-C30
18	c2	401	BCR	C1-C6-C7-C8
18	c6	402	BCR	C5-C6-C7-C8
15	aA	826	CLA	C15-C16-C17-C18
15	bA	805	CLA	CAA-CBA-CGA-O2A
15	aB	831	CLA	CAA-CBA-CGA-O2A
15	aK	102	CLA	CAA-CBA-CGA-O2A
15	bB	831	CLA	CAA-CBA-CGA-O2A
15	bK	101	CLA	CAA-CBA-CGA-O2A
15	cK	102	CLA	CAA-CBA-CGA-O2A
15	aA	810	CLA	C4-C3-C5-C6
15	bA	810	CLA	C4-C3-C5-C6
15	cA	810	CLA	C4-C3-C5-C6
18	aB	846	BCR	C7-C8-C9-C10
18	bB	846	BCR	C7-C8-C9-C10
18	cB	846	BCR	C7-C8-C9-C10
15	aA	812	CLA	C13-C15-C16-C17
15	bA	812	CLA	C13-C15-C16-C17
15	cA	812	CLA	C13-C15-C16-C17
15	c2	411	CLA	C13-C15-C16-C17
15	aB	809	CLA	C2-C3-C5-C6
15	cB	809	CLA	C2-C3-C5-C6
15	aB	841	CLA	CAA-CBA-CGA-O2A
15	bB	841	CLA	CAA-CBA-CGA-O2A
15	cB	841	CLA	CAA-CBA-CGA-O2A
15	c6	409	CLA	CAA-CBA-CGA-O1A
15	b5	403	CLA	CBA-CGA-O2A-C1
15	cA	819	CLA	CAA-CBA-CGA-O2A
15	b4	421	CLA	C16-C17-C18-C20
15	aA	835	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	820	CLA	C13-C15-C16-C17
15	bA	835	CLA	C13-C15-C16-C17
15	bB	820	CLA	C13-C15-C16-C17
15	cA	835	CLA	C13-C15-C16-C17
15	cB	806	CLA	C10-C11-C12-C13
15	cK	102	CLA	O1D-CGD-O2D-CED
15	aA	844	CLA	CAA-CBA-CGA-O2A
15	a1	406	CLA	CAA-CBA-CGA-O2A
15	bA	844	CLA	CAA-CBA-CGA-O2A
15	b1	407	CLA	CAA-CBA-CGA-O2A
15	cA	843	CLA	CAA-CBA-CGA-O2A
15	aB	816	CLA	C2A-CAA-CBA-CGA
15	aB	824	CLA	C2A-CAA-CBA-CGA
15	a6	418	CLA	C2A-CAA-CBA-CGA
15	bB	824	CLA	C2A-CAA-CBA-CGA
15	b6	418	CLA	C2A-CAA-CBA-CGA
15	cB	816	CLA	C2A-CAA-CBA-CGA
15	cB	824	CLA	C2A-CAA-CBA-CGA
15	c6	418	CLA	C2A-CAA-CBA-CGA
15	cB	820	CLA	C13-C15-C16-C17
15	aA	819	CLA	CAA-CBA-CGA-O2A
15	bA	819	CLA	CAA-CBA-CGA-O2A
15	c5	403	CLA	CBA-CGA-O2A-C1
15	aB	813	CLA	CAA-CBA-CGA-O1A
15	aB	841	CLA	CAA-CBA-CGA-O1A
15	a1	411	CLA	CAA-CBA-CGA-O2A
15	bB	813	CLA	CAA-CBA-CGA-O1A
15	bB	841	CLA	CAA-CBA-CGA-O1A
15	b4	407	CLA	CAA-CBA-CGA-O2A
15	cB	813	CLA	CAA-CBA-CGA-O1A
15	cB	841	CLA	CAA-CBA-CGA-O1A
15	c1	407	CLA	CAA-CBA-CGA-O2A
15	c3	408	CLA	CAA-CBA-CGA-O1A
15	c5	407	CLA	CAA-CBA-CGA-O2A
15	a4	421	CLA	C16-C17-C18-C20
15	bK	101	CLA	O1D-CGD-O2D-CED
15	aA	830	CLA	CAA-CBA-CGA-O2A
15	bA	830	CLA	CAA-CBA-CGA-O2A
15	cA	830	CLA	CAA-CBA-CGA-O2A
15	aA	802	CLA	C4-C3-C5-C6
15	aB	818	CLA	C4-C3-C5-C6
15	bA	802	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	818	CLA	C4-C3-C5-C6
15	cA	802	CLA	C4-C3-C5-C6
15	cB	818	CLA	C4-C3-C5-C6
15	a1	401	CLA	C6-C7-C8-C10
15	a4	402	CLA	C6-C7-C8-C10
15	a5	402	CLA	C6-C7-C8-C10
15	a6	403	CLA	C6-C7-C8-C10
15	b1	402	CLA	C6-C7-C8-C10
15	b2	402	CLA	C6-C7-C8-C10
15	b4	402	CLA	C6-C7-C8-C10
15	b5	402	CLA	C6-C7-C8-C10
15	b6	403	CLA	C6-C7-C8-C10
15	c1	402	CLA	C6-C7-C8-C10
15	c3	402	CLA	C6-C7-C8-C10
15	c4	402	CLA	C6-C7-C8-C10
15	c5	402	CLA	C6-C7-C8-C10
15	c6	403	CLA	C6-C7-C8-C10
15	c4	407	CLA	CAA-CBA-CGA-O2A
15	b6	422	CLA	CBA-CGA-O2A-C1
15	cB	827	CLA	CBD-CGD-O2D-CED
15	aB	806	CLA	C10-C11-C12-C13
15	bB	806	CLA	C10-C11-C12-C13
18	aM	101	BCR	C15-C16-C17-C18
18	bM	101	BCR	C15-C16-C17-C18
18	cM	101	BCR	C15-C16-C17-C18
15	c2	418	CLA	CAA-CBA-CGA-O2A
15	c5	417	CLA	CAA-CBA-CGA-O2A
15	c6	418	CLA	CAA-CBA-CGA-O2A
15	aB	827	CLA	CBD-CGD-O2D-CED
15	bB	827	CLA	CBD-CGD-O2D-CED
15	a5	407	CLA	CAA-CBA-CGA-O2A
15	a1	402	CLA	O1A-CGA-O2A-C1
15	aK	102	CLA	O1D-CGD-O2D-CED
15	a4	407	CLA	CAA-CBA-CGA-O2A
15	b1	412	CLA	CAA-CBA-CGA-O2A
15	b5	407	CLA	CAA-CBA-CGA-O2A
15	c1	412	CLA	CAA-CBA-CGA-O2A
15	a2	418	CLA	CAA-CBA-CGA-O2A
15	a5	417	CLA	CAA-CBA-CGA-O2A
15	a6	418	CLA	CAA-CBA-CGA-O2A
15	b5	417	CLA	CAA-CBA-CGA-O2A
15	b6	418	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	417	CLA	CAA-CBA-CGA-O2A
15	c4	417	CLA	CAA-CBA-CGA-O2A
15	a3	417	CLA	C2A-CAA-CBA-CGA
15	bB	816	CLA	C2A-CAA-CBA-CGA
15	a1	422	CLA	C16-C17-C18-C19
15	c2	406	CLA	C16-C17-C18-C19
15	aA	811	CLA	CAA-CBA-CGA-O2A
15	bA	811	CLA	CAA-CBA-CGA-O2A
15	b3	407	CLA	CAA-CBA-CGA-O2A
15	cA	811	CLA	CAA-CBA-CGA-O2A
18	aB	845	BCR	C11-C10-C9-C34
18	aB	846	BCR	C16-C17-C18-C36
18	bB	845	BCR	C11-C10-C9-C34
18	bB	846	BCR	C16-C17-C18-C36
18	b4	418	BCR	C16-C17-C18-C36
18	cB	845	BCR	C11-C10-C9-C34
18	cB	846	BCR	C16-C17-C18-C36
15	a1	422	CLA	CAA-CBA-CGA-O2A
15	a3	417	CLA	CAA-CBA-CGA-O2A
15	a4	417	CLA	CAA-CBA-CGA-O2A
15	b1	417	CLA	CAA-CBA-CGA-O2A
15	b3	417	CLA	CAA-CBA-CGA-O2A
15	b4	417	CLA	CAA-CBA-CGA-O2A
15	aA	830	CLA	C4-C3-C5-C6
15	bA	830	CLA	C4-C3-C5-C6
15	cA	830	CLA	C4-C3-C5-C6
16	aB	843	PQN	C14-C13-C15-C16
16	cB	843	PQN	C14-C13-C15-C16
15	b5	412	CLA	CAA-CBA-CGA-O2A
15	c3	407	CLA	CAA-CBA-CGA-O2A
15	aA	809	CLA	C16-C17-C18-C19
15	bA	809	CLA	C16-C17-C18-C19
15	cA	809	CLA	C16-C17-C18-C19
15	a1	416	CLA	CAA-CBA-CGA-O2A
14	aA	801	CL0	C11-C12-C13-C14
14	bA	801	CL0	C11-C12-C13-C14
14	cA	801	CL0	C11-C12-C13-C14
15	aA	803	CLA	C6-C7-C8-C9
15	aA	826	CLA	C11-C10-C8-C9
15	aA	833	CLA	C6-C7-C8-C9
15	aB	810	CLA	C11-C10-C8-C9
15	aB	834	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aL	203	CLA	C6-C7-C8-C9
15	a2	402	CLA	C6-C7-C8-C9
15	a3	402	CLA	C6-C7-C8-C9
15	bA	803	CLA	C6-C7-C8-C9
15	bA	826	CLA	C11-C10-C8-C9
15	bA	833	CLA	C6-C7-C8-C9
15	bB	810	CLA	C11-C10-C8-C9
15	bB	834	CLA	C6-C7-C8-C9
15	bL	204	CLA	C6-C7-C8-C9
15	cA	803	CLA	C6-C7-C8-C9
15	cA	826	CLA	C11-C10-C8-C9
15	cA	833	CLA	C6-C7-C8-C9
15	cB	810	CLA	C11-C10-C8-C9
15	cB	834	CLA	C6-C7-C8-C9
15	cL	203	CLA	C6-C7-C8-C9
15	a3	407	CLA	CAA-CBA-CGA-O2A
15	a5	412	CLA	CAA-CBA-CGA-O2A
15	b2	408	CLA	CAA-CBA-CGA-O2A
15	c2	408	CLA	CAA-CBA-CGA-O2A
15	aA	824	CLA	C3A-C2A-CAA-CBA
15	aA	827	CLA	C3A-C2A-CAA-CBA
15	aB	828	CLA	C3A-C2A-CAA-CBA
15	aL	202	CLA	C3A-C2A-CAA-CBA
15	a2	422	CLA	C3A-C2A-CAA-CBA
15	bA	824	CLA	C3A-C2A-CAA-CBA
15	bA	827	CLA	C3A-C2A-CAA-CBA
15	bB	828	CLA	C3A-C2A-CAA-CBA
15	bL	203	CLA	C3A-C2A-CAA-CBA
15	b2	422	CLA	C3A-C2A-CAA-CBA
15	cA	824	CLA	C3A-C2A-CAA-CBA
15	cA	827	CLA	C3A-C2A-CAA-CBA
15	cB	828	CLA	C3A-C2A-CAA-CBA
15	cL	202	CLA	C3A-C2A-CAA-CBA
15	c2	422	CLA	C3A-C2A-CAA-CBA
15	b2	418	CLA	CAA-CBA-CGA-O2A
15	c1	417	CLA	CAA-CBA-CGA-O2A
15	aA	811	CLA	CAA-CBA-CGA-O1A
15	aA	844	CLA	CAA-CBA-CGA-O1A
15	a1	406	CLA	CAA-CBA-CGA-O1A
15	a2	408	CLA	CAA-CBA-CGA-O2A
15	a4	412	CLA	CAA-CBA-CGA-O2A
15	bA	844	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b1	407	CLA	CAA-CBA-CGA-O1A
15	cA	843	CLA	CAA-CBA-CGA-O1A
15	c5	412	CLA	CAA-CBA-CGA-O2A
15	c6	408	CLA	CAA-CBA-CGA-O2A
15	aA	822	CLA	CAD-CBD-CGD-O2D
15	aA	823	CLA	CAD-CBD-CGD-O2D
15	aA	839	CLA	CAD-CBD-CGD-O2D
15	aA	845	CLA	CAD-CBD-CGD-O2D
15	aB	819	CLA	CAD-CBD-CGD-O2D
15	aB	823	CLA	CAD-CBD-CGD-O2D
15	aB	833	CLA	CAD-CBD-CGD-O2D
15	aB	834	CLA	CAD-CBD-CGD-O2D
15	a1	401	CLA	CAD-CBD-CGD-O2D
15	a1	408	CLA	CAD-CBD-CGD-O2D
15	a1	412	CLA	CAD-CBD-CGD-O2D
15	a2	402	CLA	CAD-CBD-CGD-O2D
15	a2	405	CLA	CAD-CBD-CGD-O2D
15	a2	406	CLA	CAD-CBD-CGD-O2D
15	a2	414	CLA	CAD-CBD-CGD-O2D
15	a3	402	CLA	CAD-CBD-CGD-O2D
15	a3	404	CLA	CAD-CBD-CGD-O2D
15	a3	411	CLA	CAD-CBD-CGD-O2D
15	a4	402	CLA	CAD-CBD-CGD-O2D
15	a4	411	CLA	CAD-CBD-CGD-O2D
15	a4	413	CLA	CAD-CBD-CGD-O2D
15	a4	421	CLA	CAD-CBD-CGD-O2D
15	a5	402	CLA	CAD-CBD-CGD-O2D
15	a5	405	CLA	CAD-CBD-CGD-O2D
15	a5	409	CLA	CAD-CBD-CGD-O2D
15	a5	420	CLA	CAD-CBD-CGD-O2D
15	a6	403	CLA	CAD-CBD-CGD-O2D
15	a6	411	CLA	CAD-CBD-CGD-O2D
15	a6	414	CLA	CAD-CBD-CGD-O2D
15	a6	422	CLA	CAD-CBD-CGD-O2D
15	bA	822	CLA	CAD-CBD-CGD-O2D
15	bA	823	CLA	CAD-CBD-CGD-O2D
15	bA	839	CLA	CAD-CBD-CGD-O2D
15	bA	845	CLA	CAD-CBD-CGD-O2D
15	bB	819	CLA	CAD-CBD-CGD-O2D
15	bB	823	CLA	CAD-CBD-CGD-O2D
15	bB	833	CLA	CAD-CBD-CGD-O2D
15	bB	834	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b1	402	CLA	CAD-CBD-CGD-O2D
15	b1	404	CLA	CAD-CBD-CGD-O2D
15	b1	409	CLA	CAD-CBD-CGD-O2D
15	b1	411	CLA	CAD-CBD-CGD-O2D
15	b1	413	CLA	CAD-CBD-CGD-O2D
15	b2	402	CLA	CAD-CBD-CGD-O2D
15	b2	405	CLA	CAD-CBD-CGD-O2D
15	b3	402	CLA	CAD-CBD-CGD-O2D
15	b4	402	CLA	CAD-CBD-CGD-O2D
15	b4	409	CLA	CAD-CBD-CGD-O2D
15	b4	411	CLA	CAD-CBD-CGD-O2D
15	b4	413	CLA	CAD-CBD-CGD-O2D
15	b4	421	CLA	CAD-CBD-CGD-O2D
15	b5	402	CLA	CAD-CBD-CGD-O2D
15	b5	405	CLA	CAD-CBD-CGD-O2D
15	b5	409	CLA	CAD-CBD-CGD-O2D
15	b5	420	CLA	CAD-CBD-CGD-O2D
15	b6	403	CLA	CAD-CBD-CGD-O2D
15	b6	414	CLA	CAD-CBD-CGD-O2D
15	cA	822	CLA	CAD-CBD-CGD-O2D
15	cA	823	CLA	CAD-CBD-CGD-O2D
15	cA	839	CLA	CAD-CBD-CGD-O2D
15	cA	844	CLA	CAD-CBD-CGD-O2D
15	cB	819	CLA	CAD-CBD-CGD-O2D
15	cB	823	CLA	CAD-CBD-CGD-O2D
15	cB	833	CLA	CAD-CBD-CGD-O2D
15	cB	834	CLA	CAD-CBD-CGD-O2D
15	c1	402	CLA	CAD-CBD-CGD-O2D
15	c1	409	CLA	CAD-CBD-CGD-O2D
15	c1	411	CLA	CAD-CBD-CGD-O2D
15	c1	413	CLA	CAD-CBD-CGD-O2D
15	c2	402	CLA	CAD-CBD-CGD-O2D
15	c2	406	CLA	CAD-CBD-CGD-O2D
15	c2	414	CLA	CAD-CBD-CGD-O2D
15	c3	402	CLA	CAD-CBD-CGD-O2D
15	c3	411	CLA	CAD-CBD-CGD-O2D
15	c3	413	CLA	CAD-CBD-CGD-O2D
15	c4	402	CLA	CAD-CBD-CGD-O2D
15	c4	413	CLA	CAD-CBD-CGD-O2D
15	c4	421	CLA	CAD-CBD-CGD-O2D
15	c5	402	CLA	CAD-CBD-CGD-O2D
15	c5	405	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c5	409	CLA	CAD-CBD-CGD-O2D
15	c5	420	CLA	CAD-CBD-CGD-O2D
15	c6	403	CLA	CAD-CBD-CGD-O2D
15	c6	411	CLA	CAD-CBD-CGD-O2D
15	c6	414	CLA	CAD-CBD-CGD-O2D
15	b3	417	CLA	C2A-CAA-CBA-CGA
15	aB	806	CLA	C2-C1-O2A-CGA
15	bB	806	CLA	C2-C1-O2A-CGA
15	cB	806	CLA	C2-C1-O2A-CGA
15	a6	408	CLA	CAA-CBA-CGA-O2A
15	bA	811	CLA	CAA-CBA-CGA-O1A
15	b6	408	CLA	CAA-CBA-CGA-O2A
15	cA	811	CLA	CAA-CBA-CGA-O1A
15	aA	809	CLA	CAA-CBA-CGA-O2A
15	bA	809	CLA	CAA-CBA-CGA-O2A
15	cA	809	CLA	CAA-CBA-CGA-O2A
18	b5	418	BCR	C22-C23-C24-C25
18	c5	418	BCR	C22-C23-C24-C25
15	aB	814	CLA	C4-C3-C5-C6
15	bB	814	CLA	C4-C3-C5-C6
15	cB	814	CLA	C4-C3-C5-C6
16	bB	843	PQN	C14-C13-C15-C16
15	b1	409	CLA	C16-C17-C18-C20
15	a5	407	CLA	CAA-CBA-CGA-O1A
15	c2	413	CLA	CAA-CBA-CGA-O2A
15	c6	413	CLA	CAA-CBA-CGA-O2A
15	aA	810	CLA	C2-C3-C5-C6
15	aB	811	CLA	C2-C3-C5-C6
15	aB	818	CLA	C2-C3-C5-C6
15	aB	837	CLA	C2-C3-C5-C6
15	bA	810	CLA	C2-C3-C5-C6
15	bB	811	CLA	C2-C3-C5-C6
15	bB	818	CLA	C2-C3-C5-C6
15	bB	837	CLA	C2-C3-C5-C6
15	cA	810	CLA	C2-C3-C5-C6
15	cB	811	CLA	C2-C3-C5-C6
15	cB	818	CLA	C2-C3-C5-C6
15	cB	837	CLA	C2-C3-C5-C6
15	aA	806	CLA	CAA-CBA-CGA-O2A
15	aB	807	CLA	CAA-CBA-CGA-O2A
15	bA	806	CLA	CAA-CBA-CGA-O2A
15	bB	807	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	806	CLA	CAA-CBA-CGA-O2A
15	cB	807	CLA	CAA-CBA-CGA-O2A
18	aA	852	BCR	C11-C12-C13-C14
18	aB	845	BCR	C11-C12-C13-C14
18	aJ	205	BCR	C21-C22-C23-C24
18	bA	853	BCR	C11-C12-C13-C14
18	bB	845	BCR	C11-C12-C13-C14
18	bJ	104	BCR	C21-C22-C23-C24
18	cA	851	BCR	C11-C12-C13-C14
18	cB	845	BCR	C11-C12-C13-C14
18	cJ	104	BCR	C21-C22-C23-C24
15	a2	408	CLA	CAA-CBA-CGA-O1A
15	a3	407	CLA	CAA-CBA-CGA-O1A
15	a3	412	CLA	CAA-CBA-CGA-O2A
15	b3	412	CLA	CAA-CBA-CGA-O2A
15	b6	413	CLA	CAA-CBA-CGA-O2A
15	c1	407	CLA	CAA-CBA-CGA-O1A
15	c5	407	CLA	CAA-CBA-CGA-O1A
15	aA	818	CLA	C3-C5-C6-C7
15	bA	818	CLA	C3-C5-C6-C7
15	bB	806	CLA	CAA-CBA-CGA-O1A
15	cB	806	CLA	CAA-CBA-CGA-O1A
15	a2	413	CLA	CAA-CBA-CGA-O2A
15	a6	413	CLA	CAA-CBA-CGA-O2A
15	b2	408	CLA	CAA-CBA-CGA-O1A
15	b2	413	CLA	CAA-CBA-CGA-O2A
15	b4	412	CLA	CAA-CBA-CGA-O2A
15	c3	407	CLA	CAA-CBA-CGA-O1A
15	c3	412	CLA	CAA-CBA-CGA-O2A
15	c4	412	CLA	CAA-CBA-CGA-O2A
15	aA	803	CLA	O2A-C1-C2-C3
15	aA	827	CLA	O2A-C1-C2-C3
15	aA	829	CLA	O2A-C1-C2-C3
15	aB	805	CLA	O2A-C1-C2-C3
15	aB	825	CLA	O2A-C1-C2-C3
15	a2	410	CLA	O2A-C1-C2-C3
15	bA	803	CLA	O2A-C1-C2-C3
15	bA	827	CLA	O2A-C1-C2-C3
15	bA	829	CLA	O2A-C1-C2-C3
15	bB	805	CLA	O2A-C1-C2-C3
15	bB	825	CLA	O2A-C1-C2-C3
15	b2	410	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	803	CLA	O2A-C1-C2-C3
15	cA	827	CLA	O2A-C1-C2-C3
15	cA	829	CLA	O2A-C1-C2-C3
15	cB	805	CLA	O2A-C1-C2-C3
15	cB	825	CLA	O2A-C1-C2-C3
15	c4	409	CLA	O2A-C1-C2-C3
15	c3	417	CLA	C2A-CAA-CBA-CGA
15	aB	806	CLA	CAA-CBA-CGA-O1A
15	b1	417	CLA	C3-C5-C6-C7
15	cA	818	CLA	C3-C5-C6-C7
15	aA	837	CLA	CAA-CBA-CGA-O2A
15	a1	411	CLA	CAA-CBA-CGA-O1A
15	a2	413	CLA	CAA-CBA-CGA-O1A
15	a4	407	CLA	CAA-CBA-CGA-O1A
15	a6	408	CLA	CAA-CBA-CGA-O1A
15	a6	413	CLA	CAA-CBA-CGA-O1A
15	bA	837	CLA	CAA-CBA-CGA-O2A
15	b2	413	CLA	CAA-CBA-CGA-O1A
15	b3	407	CLA	CAA-CBA-CGA-O1A
15	b4	407	CLA	CAA-CBA-CGA-O1A
15	b5	407	CLA	CAA-CBA-CGA-O1A
15	b6	408	CLA	CAA-CBA-CGA-O1A
15	b6	413	CLA	CAA-CBA-CGA-O1A
15	cA	837	CLA	CAA-CBA-CGA-O2A
15	c1	412	CLA	CAA-CBA-CGA-O1A
15	c2	408	CLA	CAA-CBA-CGA-O1A
15	c4	407	CLA	CAA-CBA-CGA-O1A
15	c6	408	CLA	CAA-CBA-CGA-O1A
15	aB	839	CLA	C13-C15-C16-C17
15	c2	418	CLA	C5-C6-C7-C8
15	a1	408	CLA	C16-C17-C18-C20
14	aA	801	CL0	CHA-CBD-CGD-O1D
14	aA	801	CL0	CHA-CBD-CGD-O2D
14	bA	801	CL0	CHA-CBD-CGD-O1D
14	bA	801	CL0	CHA-CBD-CGD-O2D
14	cA	801	CL0	CHA-CBD-CGD-O1D
14	cA	801	CL0	CHA-CBD-CGD-O2D
15	aA	803	CLA	CHA-CBD-CGD-O1D
15	aA	803	CLA	CHA-CBD-CGD-O2D
15	aA	815	CLA	CHA-CBD-CGD-O1D
15	aA	828	CLA	CHA-CBD-CGD-O2D
15	aA	838	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	804	CLA	CHA-CBD-CGD-O1D
15	aB	804	CLA	CHA-CBD-CGD-O2D
15	aB	805	CLA	CHA-CBD-CGD-O1D
15	aB	808	CLA	CHA-CBD-CGD-O2D
15	aB	810	CLA	CHA-CBD-CGD-O1D
15	aB	810	CLA	CHA-CBD-CGD-O2D
15	aB	811	CLA	CHA-CBD-CGD-O2D
15	aB	821	CLA	CHA-CBD-CGD-O1D
15	aB	821	CLA	CHA-CBD-CGD-O2D
15	aB	824	CLA	CHA-CBD-CGD-O1D
15	aB	824	CLA	CHA-CBD-CGD-O2D
15	aB	826	CLA	CHA-CBD-CGD-O2D
15	aB	827	CLA	CHA-CBD-CGD-O2D
15	aB	831	CLA	CHA-CBD-CGD-O2D
15	aJ	201	CLA	CHA-CBD-CGD-O1D
15	aJ	201	CLA	CHA-CBD-CGD-O2D
15	aK	102	CLA	CHA-CBD-CGD-O2D
15	aL	203	CLA	CHA-CBD-CGD-O1D
15	aL	203	CLA	CHA-CBD-CGD-O2D
15	a1	402	CLA	CHA-CBD-CGD-O2D
15	a1	403	CLA	CHA-CBD-CGD-O1D
15	a1	405	CLA	CHA-CBD-CGD-O1D
15	a1	405	CLA	CHA-CBD-CGD-O2D
15	a1	411	CLA	CHA-CBD-CGD-O2D
15	a2	403	CLA	CHA-CBD-CGD-O2D
15	a2	404	CLA	CHA-CBD-CGD-O1D
15	a2	407	CLA	CHA-CBD-CGD-O1D
15	a2	407	CLA	CHA-CBD-CGD-O2D
15	a2	413	CLA	CHA-CBD-CGD-O2D
15	a3	406	CLA	CHA-CBD-CGD-O1D
15	a3	406	CLA	CHA-CBD-CGD-O2D
15	a3	412	CLA	CHA-CBD-CGD-O2D
15	a4	403	CLA	CHA-CBD-CGD-O2D
15	a4	404	CLA	CHA-CBD-CGD-O1D
15	a4	406	CLA	CHA-CBD-CGD-O1D
15	a4	406	CLA	CHA-CBD-CGD-O2D
15	a4	412	CLA	CHA-CBD-CGD-O2D
15	a5	403	CLA	CHA-CBD-CGD-O2D
15	a5	404	CLA	CHA-CBD-CGD-O1D
15	a5	406	CLA	CHA-CBD-CGD-O1D
15	a5	406	CLA	CHA-CBD-CGD-O2D
15	a5	412	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	404	CLA	CHA-CBD-CGD-O2D
15	a6	405	CLA	CHA-CBD-CGD-O1D
15	a6	407	CLA	CHA-CBD-CGD-O1D
15	a6	407	CLA	CHA-CBD-CGD-O2D
15	bA	803	CLA	CHA-CBD-CGD-O1D
15	bA	815	CLA	CHA-CBD-CGD-O1D
15	bA	828	CLA	CHA-CBD-CGD-O2D
15	bA	838	CLA	CHA-CBD-CGD-O2D
15	bB	804	CLA	CHA-CBD-CGD-O1D
15	bB	804	CLA	CHA-CBD-CGD-O2D
15	bB	805	CLA	CHA-CBD-CGD-O1D
15	bB	808	CLA	CHA-CBD-CGD-O2D
15	bB	810	CLA	CHA-CBD-CGD-O1D
15	bB	810	CLA	CHA-CBD-CGD-O2D
15	bB	811	CLA	CHA-CBD-CGD-O2D
15	bB	821	CLA	CHA-CBD-CGD-O1D
15	bB	821	CLA	CHA-CBD-CGD-O2D
15	bB	824	CLA	CHA-CBD-CGD-O1D
15	bB	824	CLA	CHA-CBD-CGD-O2D
15	bB	826	CLA	CHA-CBD-CGD-O2D
15	bB	827	CLA	CHA-CBD-CGD-O2D
15	bB	831	CLA	CHA-CBD-CGD-O2D
15	bF	201	CLA	CHA-CBD-CGD-O1D
15	bF	201	CLA	CHA-CBD-CGD-O2D
15	bK	101	CLA	CHA-CBD-CGD-O2D
15	bL	204	CLA	CHA-CBD-CGD-O1D
15	bL	204	CLA	CHA-CBD-CGD-O2D
15	b1	403	CLA	CHA-CBD-CGD-O2D
15	b1	404	CLA	CHA-CBD-CGD-O1D
15	b1	406	CLA	CHA-CBD-CGD-O1D
15	b1	406	CLA	CHA-CBD-CGD-O2D
15	b1	412	CLA	CHA-CBD-CGD-O2D
15	b2	403	CLA	CHA-CBD-CGD-O2D
15	b2	404	CLA	CHA-CBD-CGD-O1D
15	b2	407	CLA	CHA-CBD-CGD-O1D
15	b2	407	CLA	CHA-CBD-CGD-O2D
15	b2	413	CLA	CHA-CBD-CGD-O2D
15	b3	406	CLA	CHA-CBD-CGD-O1D
15	b3	406	CLA	CHA-CBD-CGD-O2D
15	b3	412	CLA	CHA-CBD-CGD-O2D
15	b4	403	CLA	CHA-CBD-CGD-O2D
15	b4	404	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b4	406	CLA	CHA-CBD-CGD-O1D
15	b4	406	CLA	CHA-CBD-CGD-O2D
15	b4	412	CLA	CHA-CBD-CGD-O2D
15	b5	403	CLA	CHA-CBD-CGD-O2D
15	b5	404	CLA	CHA-CBD-CGD-O1D
15	b5	406	CLA	CHA-CBD-CGD-O1D
15	b5	406	CLA	CHA-CBD-CGD-O2D
15	b5	412	CLA	CHA-CBD-CGD-O2D
15	b6	404	CLA	CHA-CBD-CGD-O2D
15	b6	405	CLA	CHA-CBD-CGD-O1D
15	b6	407	CLA	CHA-CBD-CGD-O1D
15	b6	407	CLA	CHA-CBD-CGD-O2D
15	b6	422	CLA	CHA-CBD-CGD-O1D
15	cA	803	CLA	CHA-CBD-CGD-O1D
15	cA	815	CLA	CHA-CBD-CGD-O1D
15	cA	828	CLA	CHA-CBD-CGD-O2D
15	cA	838	CLA	CHA-CBD-CGD-O2D
15	cB	804	CLA	CHA-CBD-CGD-O1D
15	cB	804	CLA	CHA-CBD-CGD-O2D
15	cB	805	CLA	CHA-CBD-CGD-O1D
15	cB	808	CLA	CHA-CBD-CGD-O2D
15	cB	810	CLA	CHA-CBD-CGD-O1D
15	cB	810	CLA	CHA-CBD-CGD-O2D
15	cB	811	CLA	CHA-CBD-CGD-O2D
15	cB	821	CLA	CHA-CBD-CGD-O1D
15	cB	821	CLA	CHA-CBD-CGD-O2D
15	cB	824	CLA	CHA-CBD-CGD-O1D
15	cB	824	CLA	CHA-CBD-CGD-O2D
15	cB	826	CLA	CHA-CBD-CGD-O2D
15	cB	827	CLA	CHA-CBD-CGD-O2D
15	cB	831	CLA	CHA-CBD-CGD-O2D
15	cF	203	CLA	CHA-CBD-CGD-O1D
15	cF	203	CLA	CHA-CBD-CGD-O2D
15	cK	102	CLA	CHA-CBD-CGD-O2D
15	cL	203	CLA	CHA-CBD-CGD-O1D
15	cL	203	CLA	CHA-CBD-CGD-O2D
15	c1	403	CLA	CHA-CBD-CGD-O2D
15	c1	404	CLA	CHA-CBD-CGD-O1D
15	c1	406	CLA	CHA-CBD-CGD-O1D
15	c1	406	CLA	CHA-CBD-CGD-O2D
15	c1	412	CLA	CHA-CBD-CGD-O2D
15	c2	403	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c2	404	CLA	CHA-CBD-CGD-O1D
15	c2	407	CLA	CHA-CBD-CGD-O1D
15	c2	407	CLA	CHA-CBD-CGD-O2D
15	c2	413	CLA	CHA-CBD-CGD-O2D
15	c3	406	CLA	CHA-CBD-CGD-O1D
15	c3	406	CLA	CHA-CBD-CGD-O2D
15	c3	412	CLA	CHA-CBD-CGD-O2D
15	c4	403	CLA	CHA-CBD-CGD-O2D
15	c4	406	CLA	CHA-CBD-CGD-O1D
15	c4	406	CLA	CHA-CBD-CGD-O2D
15	c4	412	CLA	CHA-CBD-CGD-O2D
15	c5	403	CLA	CHA-CBD-CGD-O2D
15	c5	404	CLA	CHA-CBD-CGD-O1D
15	c5	406	CLA	CHA-CBD-CGD-O1D
15	c5	406	CLA	CHA-CBD-CGD-O2D
15	c5	412	CLA	CHA-CBD-CGD-O2D
15	c6	404	CLA	CHA-CBD-CGD-O2D
15	c6	405	CLA	CHA-CBD-CGD-O1D
15	c6	407	CLA	CHA-CBD-CGD-O1D
15	c6	407	CLA	CHA-CBD-CGD-O2D
15	bB	839	CLA	C13-C15-C16-C17
15	b2	418	CLA	C5-C6-C7-C8
15	cB	839	CLA	C13-C15-C16-C17
15	a3	412	CLA	CAA-CBA-CGA-O1A
15	b4	412	CLA	CAA-CBA-CGA-O1A
15	cA	837	CLA	CAA-CBA-CGA-O1A
15	c3	412	CLA	CAA-CBA-CGA-O1A
15	c6	413	CLA	CAA-CBA-CGA-O1A
15	aB	821	CLA	CAA-CBA-CGA-O2A
15	bB	821	CLA	CAA-CBA-CGA-O2A
15	a1	402	CLA	CBA-CGA-O2A-C1
15	bB	808	CLA	C3-C5-C6-C7
15	aA	837	CLA	CAA-CBA-CGA-O1A
15	a4	412	CLA	CAA-CBA-CGA-O1A
15	bA	837	CLA	CAA-CBA-CGA-O1A
15	b3	412	CLA	CAA-CBA-CGA-O1A
15	c2	413	CLA	CAA-CBA-CGA-O1A
15	c4	412	CLA	CAA-CBA-CGA-O1A
15	c5	412	CLA	CAA-CBA-CGA-O1A
15	aB	823	CLA	CAA-CBA-CGA-O2A
15	a6	422	CLA	CAA-CBA-CGA-O2A
15	bB	823	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	821	CLA	CAA-CBA-CGA-O2A
15	b1	403	CLA	O1A-CGA-O2A-C1
15	b1	412	CLA	CAA-CBA-CGA-O1A
15	c1	403	CLA	O1A-CGA-O2A-C1
15	aA	824	CLA	CAA-CBA-CGA-O2A
15	bA	824	CLA	CAA-CBA-CGA-O2A
15	bB	834	CLA	CAA-CBA-CGA-O2A
15	cA	824	CLA	CAA-CBA-CGA-O2A
15	cB	823	CLA	CAA-CBA-CGA-O2A
15	cB	834	CLA	CAA-CBA-CGA-O2A
15	c1	409	CLA	C16-C17-C18-C20
15	a2	418	CLA	C5-C6-C7-C8
15	cA	819	CLA	C5-C6-C7-C8
15	aB	808	CLA	C3-C5-C6-C7
15	cB	808	CLA	C3-C5-C6-C7
15	aB	834	CLA	CAA-CBA-CGA-O2A
15	b6	422	CLA	CAA-CBA-CGA-O2A
15	aB	806	CLA	C4-C3-C5-C6
15	bB	806	CLA	C4-C3-C5-C6
15	cB	806	CLA	C4-C3-C5-C6
15	aA	819	CLA	C5-C6-C7-C8
15	bA	819	CLA	C5-C6-C7-C8
15	bB	807	CLA	CAA-CBA-CGA-O1A
15	aB	806	CLA	C6-C7-C8-C10
15	aL	201	CLA	C2-C3-C5-C6
15	a2	402	CLA	C6-C7-C8-C10
15	a3	402	CLA	C6-C7-C8-C10
15	bB	806	CLA	C6-C7-C8-C10
15	bL	202	CLA	C2-C3-C5-C6
15	b3	402	CLA	C6-C7-C8-C10
15	b3	421	CLA	C12-C13-C15-C16
15	cB	806	CLA	C6-C7-C8-C10
15	cL	201	CLA	C2-C3-C5-C6
15	c2	402	CLA	C6-C7-C8-C10
15	c2	410	CLA	C16-C17-C18-C20
15	a4	410	CLA	C13-C15-C16-C17
15	c4	410	CLA	C13-C15-C16-C17
15	b5	412	CLA	CAA-CBA-CGA-O1A
15	aA	802	CLA	C6-C7-C8-C9
15	aA	825	CLA	C11-C10-C8-C9
15	aL	201	CLA	C11-C10-C8-C9
15	a1	401	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a3	421	CLA	C14-C13-C15-C16
15	a4	402	CLA	C6-C7-C8-C9
15	a5	402	CLA	C6-C7-C8-C9
15	a6	403	CLA	C6-C7-C8-C9
15	bA	802	CLA	C6-C7-C8-C9
15	bA	825	CLA	C11-C10-C8-C9
15	bL	202	CLA	C11-C10-C8-C9
15	b1	402	CLA	C6-C7-C8-C9
15	b2	402	CLA	C6-C7-C8-C9
15	b3	402	CLA	C6-C7-C8-C9
15	b3	421	CLA	C14-C13-C15-C16
15	b4	402	CLA	C6-C7-C8-C9
15	b5	402	CLA	C6-C7-C8-C9
15	b6	403	CLA	C6-C7-C8-C9
15	cA	802	CLA	C6-C7-C8-C9
15	cA	825	CLA	C11-C10-C8-C9
15	cL	201	CLA	C11-C10-C8-C9
15	c1	402	CLA	C6-C7-C8-C9
15	c2	402	CLA	C6-C7-C8-C9
15	c3	402	CLA	C6-C7-C8-C9
15	c3	421	CLA	C14-C13-C15-C16
15	c4	402	CLA	C6-C7-C8-C9
15	c5	402	CLA	C6-C7-C8-C9
15	c6	403	CLA	C6-C7-C8-C9
15	cB	807	CLA	CAA-CBA-CGA-O1A
18	aA	848	BCR	C19-C20-C21-C22
18	bA	849	BCR	C19-C20-C21-C22
18	cA	847	BCR	C19-C20-C21-C22
15	a5	417	CLA	CAA-CBA-CGA-O1A
15	a3	417	CLA	C3-C5-C6-C7
15	cA	807	CLA	C3-C5-C6-C7
15	c3	417	CLA	C3-C5-C6-C7
15	a5	412	CLA	CAA-CBA-CGA-O1A
15	aA	806	CLA	CAA-CBA-CGA-O1A
15	aB	807	CLA	CAA-CBA-CGA-O1A
15	bA	806	CLA	CAA-CBA-CGA-O1A
15	cA	806	CLA	CAA-CBA-CGA-O1A
15	c5	417	CLA	CAA-CBA-CGA-O1A
15	aB	804	CLA	C4C-C3C-CAC-CBC
15	cB	804	CLA	C4C-C3C-CAC-CBC
15	aA	807	CLA	C3-C5-C6-C7
15	bA	807	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	417	CLA	CAA-CBA-CGA-O1A
15	a5	410	CLA	C5-C6-C7-C8
15	a5	410	CLA	C8-C10-C11-C12
15	b4	410	CLA	C5-C6-C7-C8
15	b6	411	CLA	C5-C6-C7-C8
15	aA	829	CLA	C4-C3-C5-C6
15	bA	829	CLA	C4-C3-C5-C6
15	cA	829	CLA	C4-C3-C5-C6
15	bB	804	CLA	C4C-C3C-CAC-CBC
15	b1	403	CLA	CBA-CGA-O2A-C1
15	c1	403	CLA	CBA-CGA-O2A-C1
15	aB	810	CLA	C15-C16-C17-C18
15	a4	410	CLA	C5-C6-C7-C8
15	bB	810	CLA	C15-C16-C17-C18
15	cB	810	CLA	C15-C16-C17-C18
15	c6	411	CLA	C5-C6-C7-C8
15	b6	418	CLA	C3-C5-C6-C7
15	aA	803	CLA	C1A-C2A-CAA-CBA
15	aA	814	CLA	C1A-C2A-CAA-CBA
15	aA	824	CLA	C1A-C2A-CAA-CBA
15	aA	830	CLA	C1A-C2A-CAA-CBA
15	aB	816	CLA	C1A-C2A-CAA-CBA
15	aB	822	CLA	C1A-C2A-CAA-CBA
15	aB	828	CLA	C1A-C2A-CAA-CBA
15	aL	202	CLA	C1A-C2A-CAA-CBA
15	a2	404	CLA	C1A-C2A-CAA-CBA
15	a3	413	CLA	C1A-C2A-CAA-CBA
15	a4	413	CLA	C1A-C2A-CAA-CBA
15	bA	803	CLA	C1A-C2A-CAA-CBA
15	bA	814	CLA	C1A-C2A-CAA-CBA
15	bA	824	CLA	C1A-C2A-CAA-CBA
15	bA	830	CLA	C1A-C2A-CAA-CBA
15	bB	816	CLA	C1A-C2A-CAA-CBA
15	bB	822	CLA	C1A-C2A-CAA-CBA
15	bB	828	CLA	C1A-C2A-CAA-CBA
15	bL	203	CLA	C1A-C2A-CAA-CBA
15	b1	404	CLA	C1A-C2A-CAA-CBA
15	b2	414	CLA	C1A-C2A-CAA-CBA
15	b3	404	CLA	C1A-C2A-CAA-CBA
15	b3	413	CLA	C1A-C2A-CAA-CBA
15	b4	404	CLA	C1A-C2A-CAA-CBA
15	cA	803	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	814	CLA	C1A-C2A-CAA-CBA
15	cA	824	CLA	C1A-C2A-CAA-CBA
15	cA	830	CLA	C1A-C2A-CAA-CBA
15	cB	816	CLA	C1A-C2A-CAA-CBA
15	cB	822	CLA	C1A-C2A-CAA-CBA
15	cB	828	CLA	C1A-C2A-CAA-CBA
15	cL	202	CLA	C1A-C2A-CAA-CBA
15	c2	414	CLA	C1A-C2A-CAA-CBA
15	c3	404	CLA	C1A-C2A-CAA-CBA
15	c3	413	CLA	C1A-C2A-CAA-CBA
15	c4	404	CLA	C1A-C2A-CAA-CBA
15	a2	406	CLA	C16-C17-C18-C19
15	a4	417	CLA	CAA-CBA-CGA-O1A
15	b5	417	CLA	CAA-CBA-CGA-O1A
15	c6	418	CLA	CAA-CBA-CGA-O1A
20	bB	851	LMG	C21-C22-C23-C24
20	cB	850	LMG	C21-C22-C23-C24
15	aB	832	CLA	C2-C1-O2A-CGA
15	bB	832	CLA	C2-C1-O2A-CGA
15	cB	832	CLA	C2-C1-O2A-CGA
20	aB	850	LMG	C21-C22-C23-C24
15	a1	409	CLA	C8-C10-C11-C12
15	a1	422	CLA	CAA-CBA-CGA-O1A
15	a2	418	CLA	CAA-CBA-CGA-O1A
15	a6	418	CLA	CAA-CBA-CGA-O1A
15	b1	417	CLA	CAA-CBA-CGA-O1A
15	b4	417	CLA	CAA-CBA-CGA-O1A
15	b6	418	CLA	CAA-CBA-CGA-O1A
15	c2	418	CLA	CAA-CBA-CGA-O1A
15	aB	813	CLA	CAA-CBA-CGA-O2A
15	bB	813	CLA	CAA-CBA-CGA-O2A
15	cB	813	CLA	CAA-CBA-CGA-O2A
15	aB	817	CLA	C2A-CAA-CBA-CGA
15	bB	817	CLA	C2A-CAA-CBA-CGA
15	cB	817	CLA	C2A-CAA-CBA-CGA
15	aB	821	CLA	CAA-CBA-CGA-O1A
15	a3	417	CLA	CAA-CBA-CGA-O1A
15	bB	821	CLA	CAA-CBA-CGA-O1A
15	b3	417	CLA	CAA-CBA-CGA-O1A
15	b6	422	CLA	CAA-CBA-CGA-O1A
15	cB	821	CLA	CAA-CBA-CGA-O1A
15	c1	417	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	417	CLA	CAA-CBA-CGA-O1A
15	bB	830	CLA	C15-C16-C17-C18
15	b5	410	CLA	C5-C6-C7-C8
15	c1	410	CLA	C8-C10-C11-C12
15	bF	201	CLA	CAA-CBA-CGA-O2A
15	b1	410	CLA	C8-C10-C11-C12
16	aA	846	PQN	C25-C26-C27-C28
15	a6	418	CLA	C3-C5-C6-C7
15	b3	417	CLA	C3-C5-C6-C7
15	c6	418	CLA	C3-C5-C6-C7
15	a1	416	CLA	CAA-CBA-CGA-O1A
15	aJ	201	CLA	CAA-CBA-CGA-O2A
15	cF	203	CLA	CAA-CBA-CGA-O2A
15	aB	830	CLA	C15-C16-C17-C18
15	cB	830	CLA	C15-C16-C17-C18
16	bA	846	PQN	C25-C26-C27-C28
16	cA	845	PQN	C25-C26-C27-C28
15	aA	829	CLA	CAA-CBA-CGA-O1A
15	bA	829	CLA	CAA-CBA-CGA-O1A
15	b2	418	CLA	CAA-CBA-CGA-O1A
15	cA	829	CLA	CAA-CBA-CGA-O1A
15	aA	817	CLA	O2A-C1-C2-C3
15	bA	817	CLA	O2A-C1-C2-C3
15	cA	817	CLA	O2A-C1-C2-C3
15	b2	422	CLA	CAA-CBA-CGA-O2A
15	b4	410	CLA	C13-C15-C16-C17
15	aX	102	CLA	CAA-CBA-CGA-O2A
15	bX	102	CLA	CAA-CBA-CGA-O2A
15	cX	102	CLA	CAA-CBA-CGA-O2A
18	aF	201	BCR	C5-C6-C7-C8
18	aF	202	BCR	C23-C24-C25-C26
18	aK	101	BCR	C23-C24-C25-C26
18	bA	848	BCR	C23-C24-C25-C26
18	bB	849	BCR	C5-C6-C7-C8
18	bF	202	BCR	C23-C24-C25-C26
18	b6	402	BCR	C5-C6-C7-C8
18	cF	202	BCR	C5-C6-C7-C8
18	cF	204	BCR	C23-C24-C25-C26
18	cK	101	BCR	C23-C24-C25-C26
15	aA	820	CLA	C15-C16-C17-C18
15	bA	820	CLA	C15-C16-C17-C18
15	b5	410	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	820	CLA	C15-C16-C17-C18
15	c4	410	CLA	C5-C6-C7-C8
15	aB	820	CLA	C8-C10-C11-C12
15	cB	820	CLA	C8-C10-C11-C12
15	c3	409	CLA	C16-C17-C18-C20
18	a3	418	BCR	C18-C19-C20-C21
18	a3	419	BCR	C18-C19-C20-C21
18	b2	420	BCR	C18-C19-C20-C21
18	b3	419	BCR	C18-C19-C20-C21
15	aA	809	CLA	CAA-CBA-CGA-O1A
15	bA	809	CLA	CAA-CBA-CGA-O1A
15	bB	817	CLA	O1D-CGD-O2D-CED
15	bB	820	CLA	C8-C10-C11-C12
15	a3	404	CLA	C10-C11-C12-C13
15	cA	809	CLA	CAA-CBA-CGA-O1A
15	aA	804	CLA	C13-C15-C16-C17
15	cA	804	CLA	C13-C15-C16-C17
15	aA	815	CLA	CAD-CBD-CGD-O1D
15	aA	828	CLA	CAD-CBD-CGD-O1D
15	aA	838	CLA	C2-C3-C5-C6
15	aB	815	CLA	CAD-CBD-CGD-O1D
15	aB	827	CLA	CAD-CBD-CGD-O1D
15	aB	834	CLA	CAD-CBD-CGD-O1D
15	aK	102	CLA	CAD-CBD-CGD-O1D
15	aL	203	CLA	CAD-CBD-CGD-O1D
15	a1	403	CLA	CAD-CBD-CGD-O1D
15	a1	414	CLA	CAD-CBD-CGD-O1D
15	a1	422	CLA	CAD-CBD-CGD-O1D
15	a2	404	CLA	CAD-CBD-CGD-O1D
15	a2	410	CLA	CAD-CBD-CGD-O1D
15	a2	416	CLA	CAD-CBD-CGD-O1D
15	a3	409	CLA	CAD-CBD-CGD-O1D
15	a3	415	CLA	CAD-CBD-CGD-O1D
15	a4	404	CLA	CAD-CBD-CGD-O1D
15	a4	415	CLA	CAD-CBD-CGD-O1D
15	a5	404	CLA	CAD-CBD-CGD-O1D
15	a6	405	CLA	CAD-CBD-CGD-O1D
15	a6	410	CLA	CAD-CBD-CGD-O1D
15	a6	416	CLA	CAD-CBD-CGD-O1D
15	a6	422	CLA	CAD-CBD-CGD-O1D
15	bA	815	CLA	CAD-CBD-CGD-O1D
15	bA	828	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	838	CLA	C2-C3-C5-C6
15	bB	815	CLA	CAD-CBD-CGD-O1D
15	bB	827	CLA	CAD-CBD-CGD-O1D
15	bB	834	CLA	CAD-CBD-CGD-O1D
15	bK	101	CLA	CAD-CBD-CGD-O1D
15	bL	204	CLA	CAD-CBD-CGD-O1D
15	b1	404	CLA	CAD-CBD-CGD-O1D
15	b1	415	CLA	CAD-CBD-CGD-O1D
15	b2	404	CLA	CAD-CBD-CGD-O1D
15	b2	410	CLA	CAD-CBD-CGD-O1D
15	b2	416	CLA	CAD-CBD-CGD-O1D
15	b3	404	CLA	CAD-CBD-CGD-O1D
15	b3	409	CLA	CAD-CBD-CGD-O1D
15	b3	415	CLA	CAD-CBD-CGD-O1D
15	b4	404	CLA	CAD-CBD-CGD-O1D
15	b4	415	CLA	CAD-CBD-CGD-O1D
15	b5	404	CLA	CAD-CBD-CGD-O1D
15	b6	405	CLA	CAD-CBD-CGD-O1D
15	b6	410	CLA	CAD-CBD-CGD-O1D
15	b6	416	CLA	CAD-CBD-CGD-O1D
15	b6	422	CLA	CAD-CBD-CGD-O1D
15	cA	828	CLA	CAD-CBD-CGD-O1D
15	cA	838	CLA	C2-C3-C5-C6
15	cB	815	CLA	CAD-CBD-CGD-O1D
15	cB	827	CLA	CAD-CBD-CGD-O1D
15	cB	834	CLA	CAD-CBD-CGD-O1D
15	cK	102	CLA	CAD-CBD-CGD-O1D
15	cL	203	CLA	CAD-CBD-CGD-O1D
15	c1	404	CLA	CAD-CBD-CGD-O1D
15	c1	415	CLA	CAD-CBD-CGD-O1D
15	c2	404	CLA	CAD-CBD-CGD-O1D
15	c2	410	CLA	CAD-CBD-CGD-O1D
15	c2	416	CLA	CAD-CBD-CGD-O1D
15	c3	409	CLA	CAD-CBD-CGD-O1D
15	c3	415	CLA	CAD-CBD-CGD-O1D
15	c4	404	CLA	CAD-CBD-CGD-O1D
15	c4	415	CLA	CAD-CBD-CGD-O1D
15	c5	404	CLA	CAD-CBD-CGD-O1D
15	c6	405	CLA	CAD-CBD-CGD-O1D
15	c6	410	CLA	CAD-CBD-CGD-O1D
15	c6	416	CLA	CAD-CBD-CGD-O1D
15	aA	843	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	842	CLA	CAA-CBA-CGA-O2A
15	aA	802	CLA	C14-C13-C15-C16
15	a1	409	CLA	C11-C10-C8-C9
15	a4	421	CLA	C14-C13-C15-C16
15	a6	422	CLA	C14-C13-C15-C16
15	bA	802	CLA	C14-C13-C15-C16
15	b4	421	CLA	C14-C13-C15-C16
15	b6	411	CLA	C11-C10-C8-C9
15	b6	422	CLA	C14-C13-C15-C16
15	cA	802	CLA	C14-C13-C15-C16
15	c1	410	CLA	C11-C10-C8-C9
15	aB	817	CLA	O1D-CGD-O2D-CED
15	a6	411	CLA	C5-C6-C7-C8
15	bA	804	CLA	C13-C15-C16-C17
15	c3	404	CLA	C10-C11-C12-C13
15	c5	410	CLA	C5-C6-C7-C8
15	aA	813	CLA	CAA-CBA-CGA-O2A
15	aB	801	CLA	CAA-CBA-CGA-O2A
15	a3	421	CLA	CAA-CBA-CGA-O2A
15	bA	813	CLA	CAA-CBA-CGA-O2A
15	bA	843	CLA	CAA-CBA-CGA-O2A
15	cB	801	CLA	CAA-CBA-CGA-O2A
15	c4	421	CLA	CAA-CBA-CGA-O2A
15	b3	404	CLA	C8-C10-C11-C12
15	c1	410	CLA	C13-C15-C16-C17
15	bA	824	CLA	CAA-CBA-CGA-O1A
15	a2	422	CLA	CAA-CBA-CGA-O2A
15	a4	421	CLA	CAA-CBA-CGA-O2A
15	b3	421	CLA	CAA-CBA-CGA-O2A
15	b4	421	CLA	CAA-CBA-CGA-O2A
15	b5	420	CLA	CAA-CBA-CGA-O2A
15	cA	813	CLA	CAA-CBA-CGA-O2A
15	c2	422	CLA	CAA-CBA-CGA-O2A
15	c3	421	CLA	CAA-CBA-CGA-O2A
15	c5	420	CLA	CAA-CBA-CGA-O2A
19	aA	854	LHG	O7-C7-C8-C9
15	a1	403	CLA	C8-C10-C11-C12
15	a2	411	CLA	C5-C6-C7-C8
15	aL	201	CLA	C4-C3-C5-C6
15	bL	202	CLA	C4-C3-C5-C6
15	cL	201	CLA	C4-C3-C5-C6
15	aB	814	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	422	CLA	C13-C15-C16-C17
15	bB	814	CLA	C15-C16-C17-C18
15	cB	814	CLA	C15-C16-C17-C18
15	aA	806	CLA	C11-C10-C8-C7
15	aA	814	CLA	C3A-C2A-CAA-CBA
15	aB	807	CLA	C11-C10-C8-C7
15	aB	808	CLA	C11-C12-C13-C15
15	aB	811	CLA	C11-C10-C8-C7
15	aL	201	CLA	C11-C10-C8-C7
15	a1	409	CLA	C11-C10-C8-C7
15	a3	421	CLA	C12-C13-C15-C16
15	a4	421	CLA	C12-C13-C15-C16
15	bA	806	CLA	C11-C10-C8-C7
15	bA	814	CLA	C3A-C2A-CAA-CBA
15	bB	807	CLA	C11-C10-C8-C7
15	bB	808	CLA	C11-C12-C13-C15
15	bB	811	CLA	C11-C10-C8-C7
15	bL	202	CLA	C11-C10-C8-C7
15	b1	410	CLA	C11-C10-C8-C7
15	b4	421	CLA	C12-C13-C15-C16
15	cA	806	CLA	C11-C10-C8-C7
15	cA	814	CLA	C3A-C2A-CAA-CBA
15	cB	807	CLA	C11-C10-C8-C7
15	cB	808	CLA	C11-C12-C13-C15
15	cB	811	CLA	C11-C10-C8-C7
15	cL	201	CLA	C11-C10-C8-C7
15	c1	410	CLA	C11-C10-C8-C7
15	c3	421	CLA	C12-C13-C15-C16
15	c4	421	CLA	C12-C13-C15-C16
16	aB	843	PQN	C16-C17-C18-C20
16	bB	843	PQN	C16-C17-C18-C20
16	cB	843	PQN	C16-C17-C18-C20
15	aA	824	CLA	CAA-CBA-CGA-O1A
15	aB	823	CLA	CAA-CBA-CGA-O1A
15	bB	823	CLA	CAA-CBA-CGA-O1A
15	cA	824	CLA	CAA-CBA-CGA-O1A
15	cB	823	CLA	CAA-CBA-CGA-O1A
15	a5	420	CLA	CAA-CBA-CGA-O2A
15	bB	801	CLA	CAA-CBA-CGA-O2A
19	bA	855	LHG	O7-C7-C8-C9
19	cA	853	LHG	O7-C7-C8-C9
15	b2	411	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	832	CLA	O2A-C1-C2-C3
15	bB	832	CLA	O2A-C1-C2-C3
15	cB	832	CLA	O2A-C1-C2-C3
15	c5	417	CLA	C3-C5-C6-C7
15	b1	404	CLA	C10-C11-C12-C13
18	aK	101	BCR	C21-C22-C23-C24
18	bA	848	BCR	C21-C22-C23-C24
18	cK	101	BCR	C21-C22-C23-C24
15	bF	201	CLA	CAA-CBA-CGA-O1A
18	a6	402	BCR	C15-C16-C17-C18
18	b5	401	BCR	C15-C16-C17-C18
18	b6	402	BCR	C15-C16-C17-C18
15	cB	817	CLA	O1D-CGD-O2D-CED
15	a6	411	CLA	C13-C15-C16-C17
15	b6	411	CLA	C13-C15-C16-C17
15	c1	404	CLA	C8-C10-C11-C12
15	c3	404	CLA	C8-C10-C11-C12
15	aJ	201	CLA	CAA-CBA-CGA-O1A
15	cF	203	CLA	CAA-CBA-CGA-O1A
15	aA	810	CLA	CAA-CBA-CGA-O2A
15	aB	810	CLA	CAA-CBA-CGA-O2A
15	bA	810	CLA	CAA-CBA-CGA-O2A
15	bB	810	CLA	CAA-CBA-CGA-O2A
15	cA	810	CLA	CAA-CBA-CGA-O2A
15	cB	810	CLA	CAA-CBA-CGA-O2A
15	cB	818	CLA	CAA-CBA-CGA-O2A
15	b1	417	CLA	C5-C6-C7-C8
15	aB	834	CLA	CAA-CBA-CGA-O1A
15	bB	834	CLA	CAA-CBA-CGA-O1A
15	cB	834	CLA	CAA-CBA-CGA-O1A
15	a1	416	CLA	C2A-CAA-CBA-CGA
15	b1	417	CLA	C2A-CAA-CBA-CGA
15	aA	826	CLA	C13-C15-C16-C17
15	a3	417	CLA	C5-C6-C7-C8
15	b1	410	CLA	C13-C15-C16-C17
15	cA	826	CLA	C13-C15-C16-C17
15	b5	417	CLA	C3-C5-C6-C7
15	a6	422	CLA	CAA-CBA-CGA-O1A
15	aB	818	CLA	CAA-CBA-CGA-O2A
15	aB	829	CLA	CAA-CBA-CGA-O2A
15	bA	840	CLA	CAA-CBA-CGA-O2A
15	bB	818	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

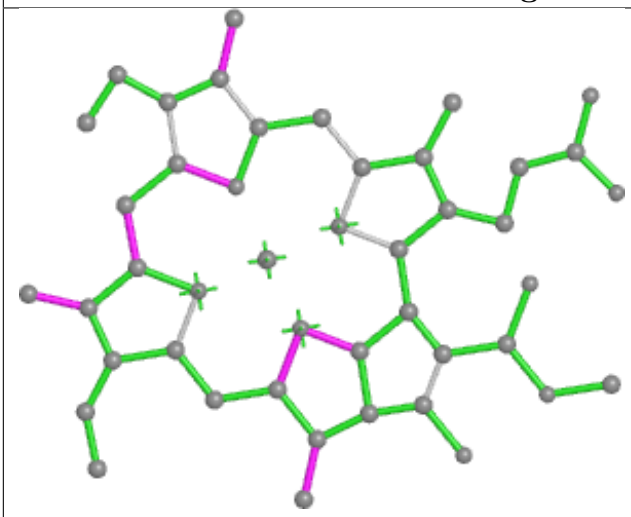
Mol	Chain	Res	Type	Atoms
15	bB	829	CLA	CAA-CBA-CGA-O2A
15	cA	840	CLA	CAA-CBA-CGA-O2A
15	cB	829	CLA	CAA-CBA-CGA-O2A
15	bA	826	CLA	C13-C15-C16-C17

There are no ring outliers.

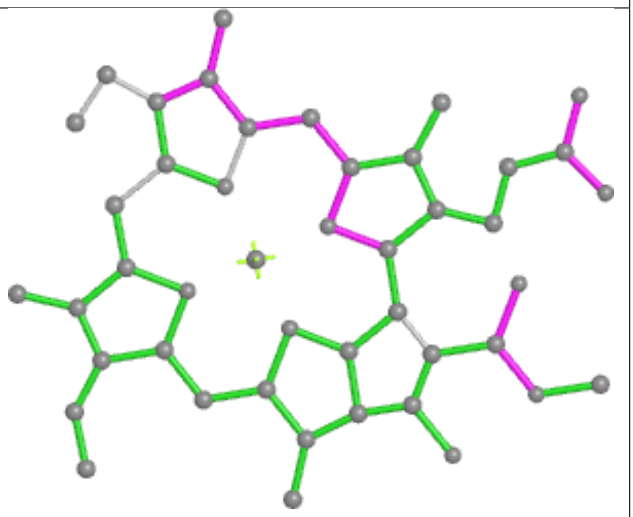
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

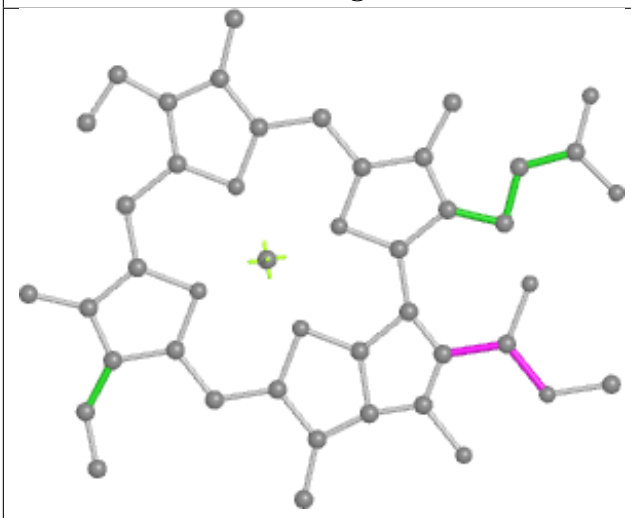
Ligand CLA c6 407



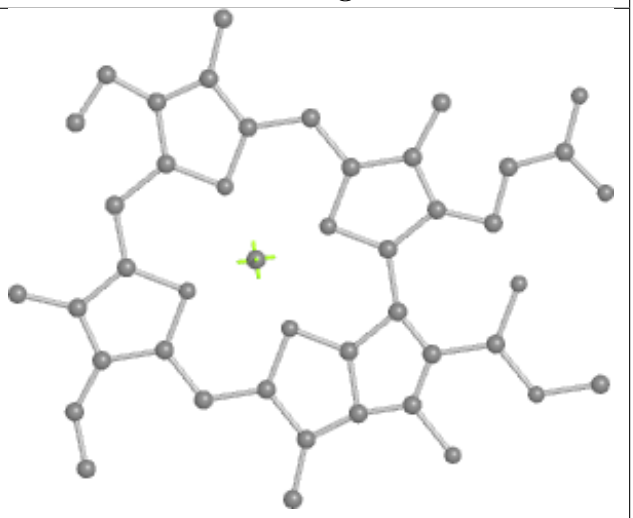
Bond lengths



Bond angles

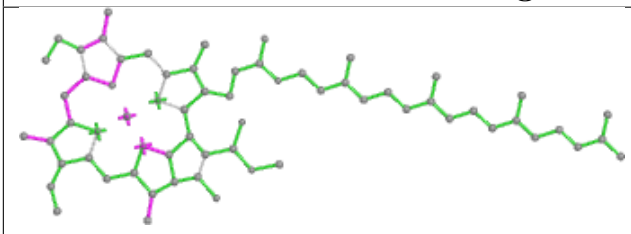


Torsions

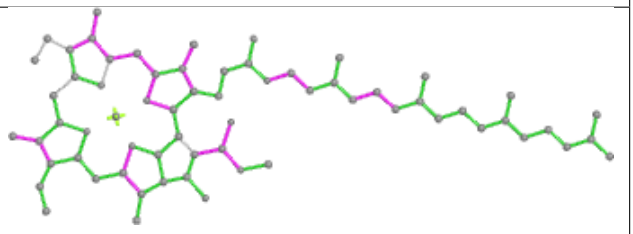


Rings

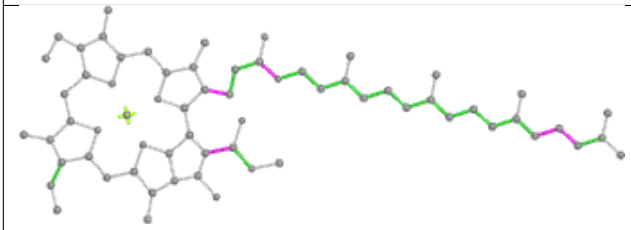
Ligand CLA cB 830



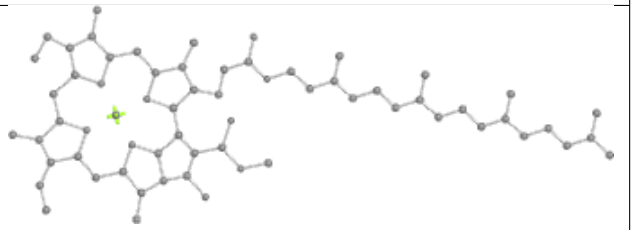
Bond lengths



Bond angles

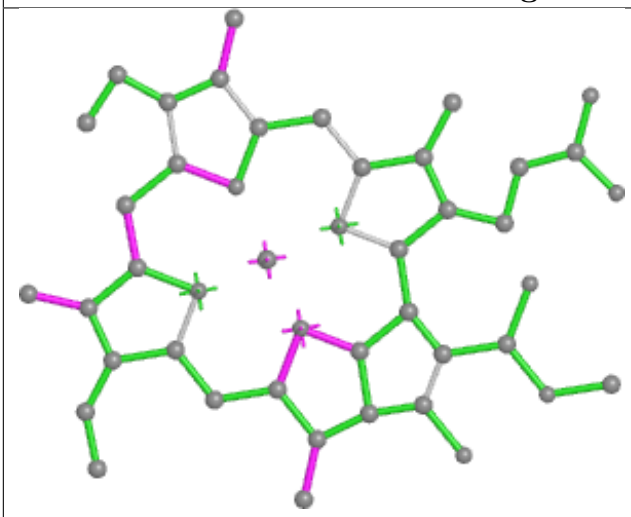


Torsions

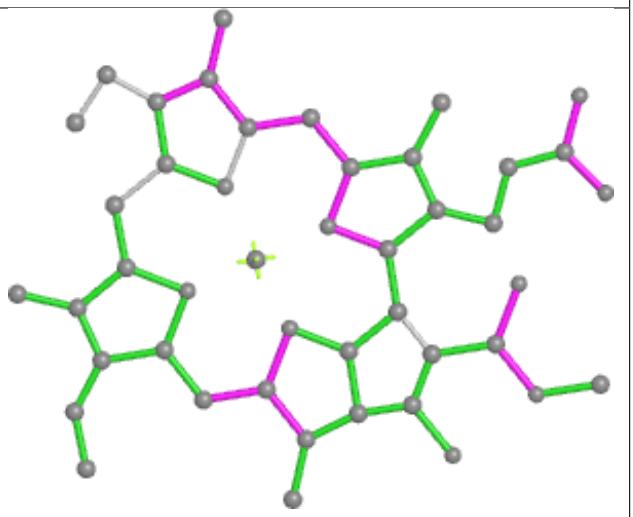


Rings

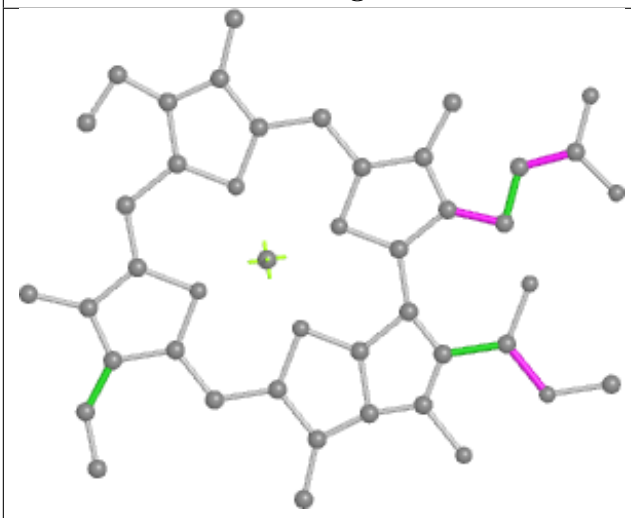
Ligand CLA c2 409



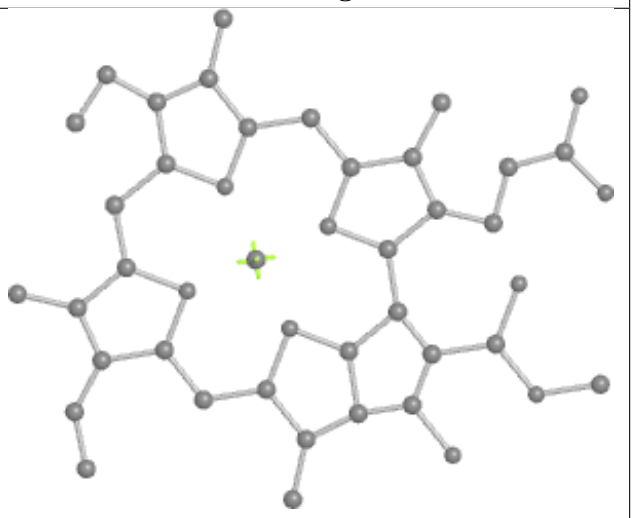
Bond lengths



Bond angles

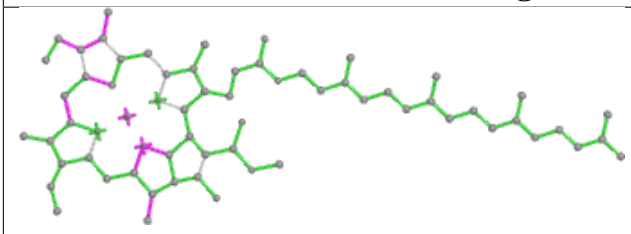


Torsions

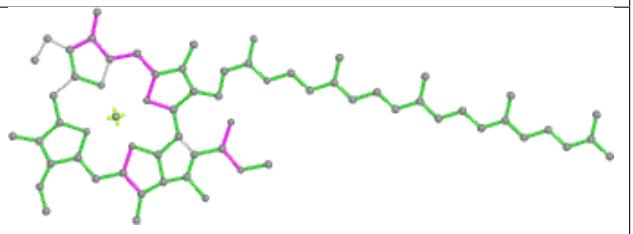


Rings

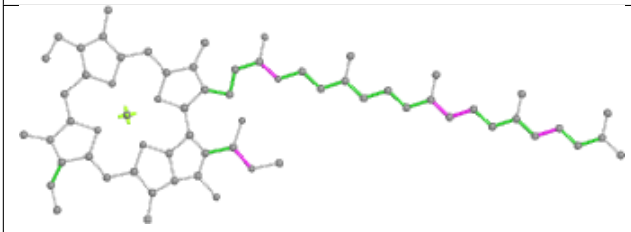
Ligand CLA aB 820



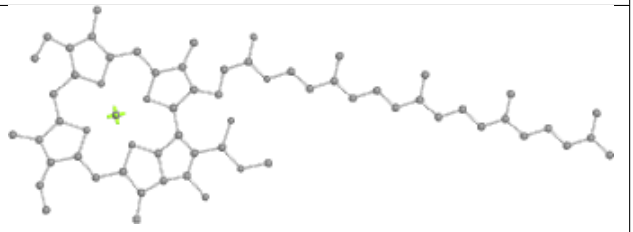
Bond lengths



Bond angles

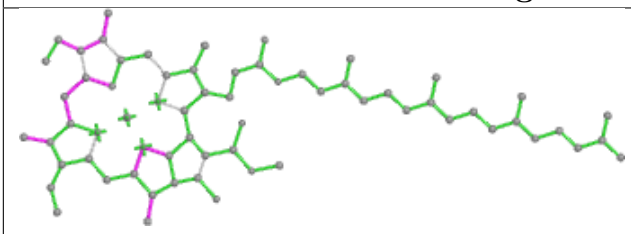


Torsions

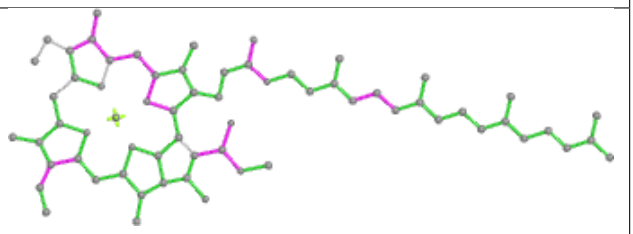


Rings

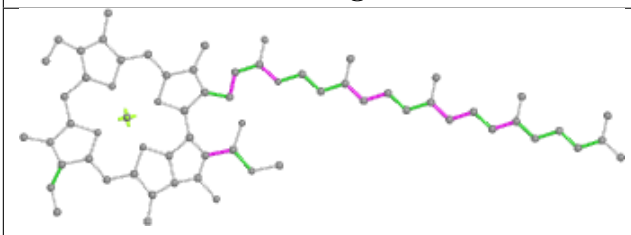
Ligand CLA aB 808



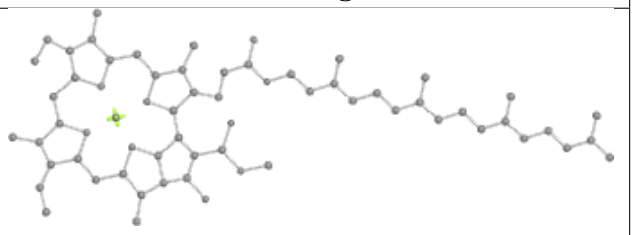
Bond lengths



Bond angles

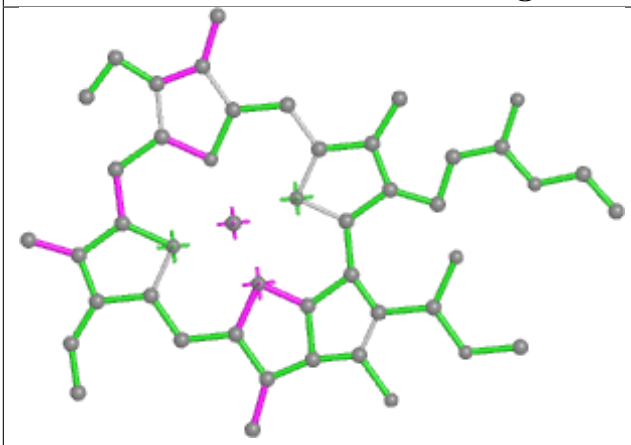


Torsions

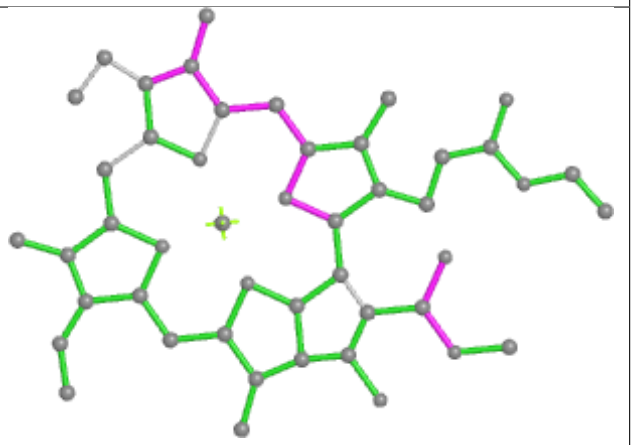


Rings

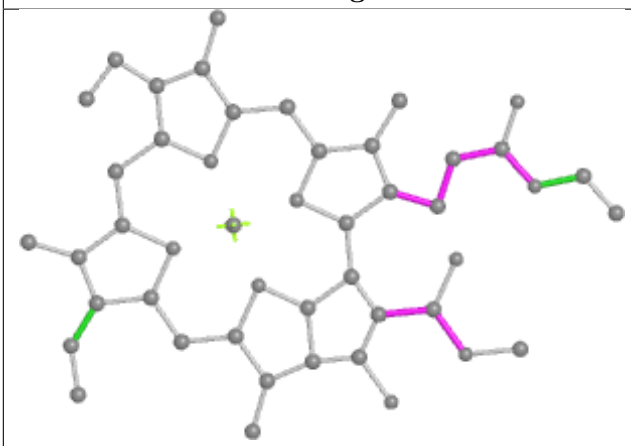
Ligand CLA cB 821



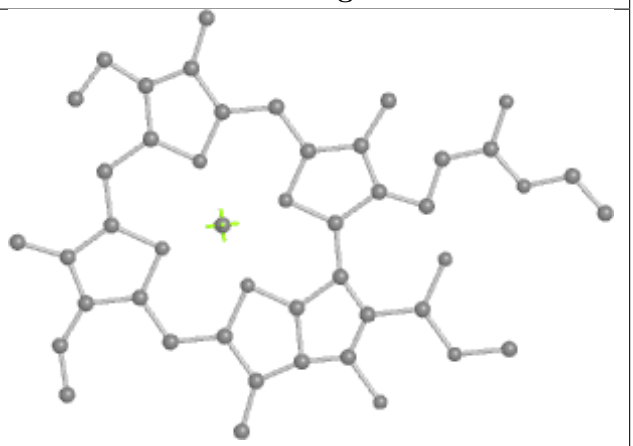
Bond lengths



Bond angles

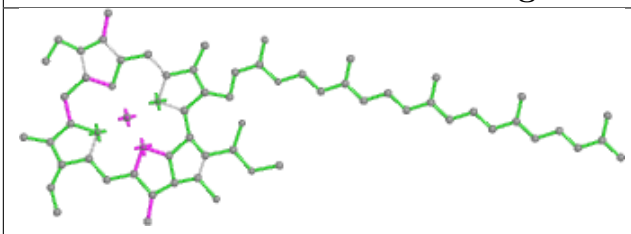


Torsions

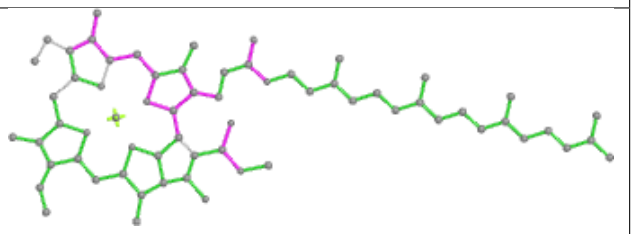


Rings

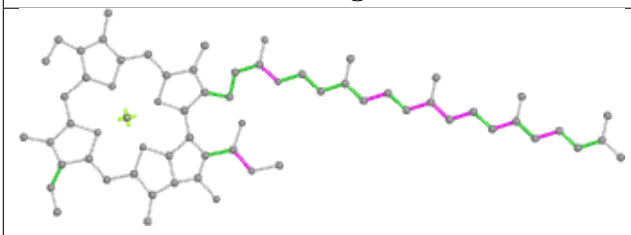
Ligand CLA b3 403



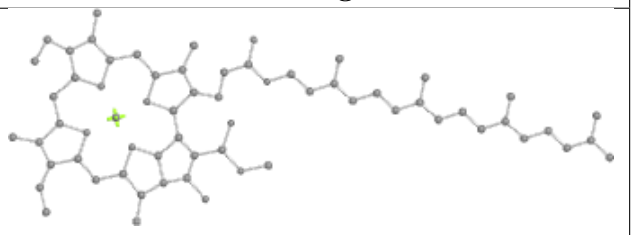
Bond lengths



Bond angles

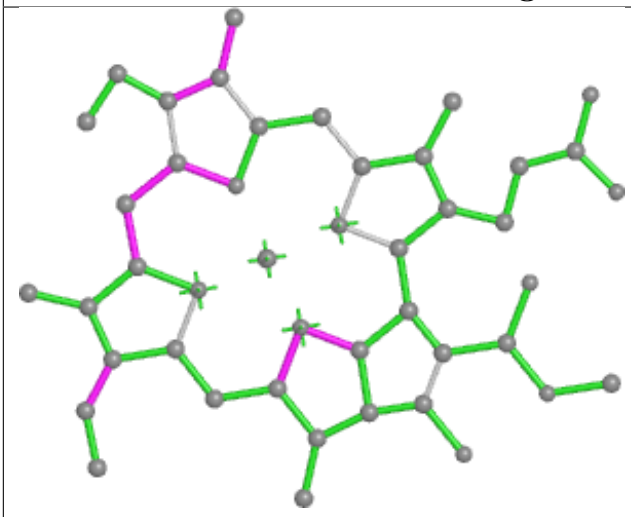


Torsions

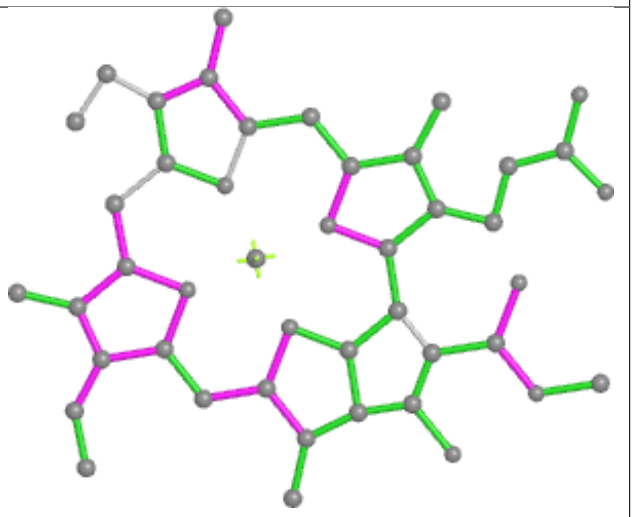


Rings

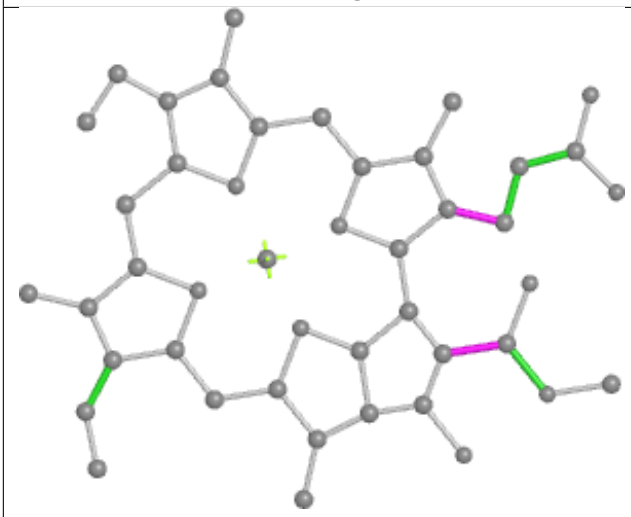
Ligand CLA b6 414



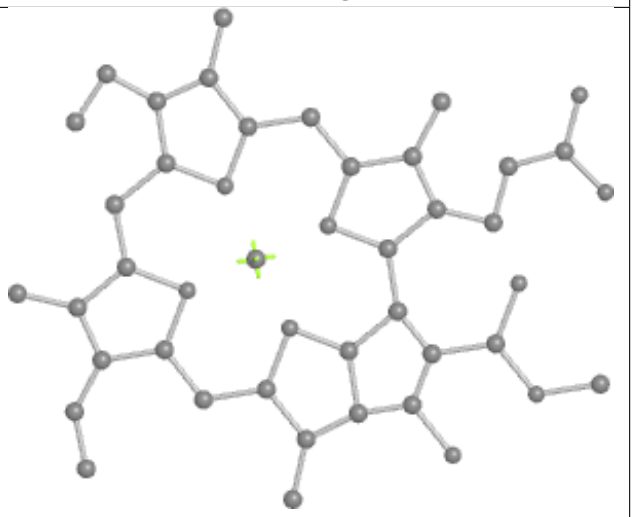
Bond lengths



Bond angles

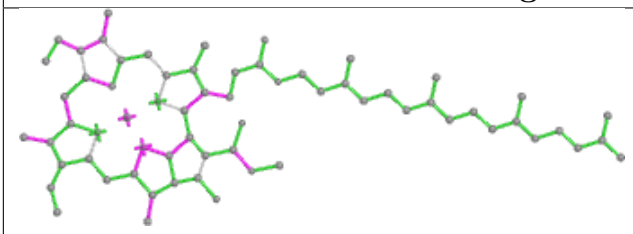


Torsions

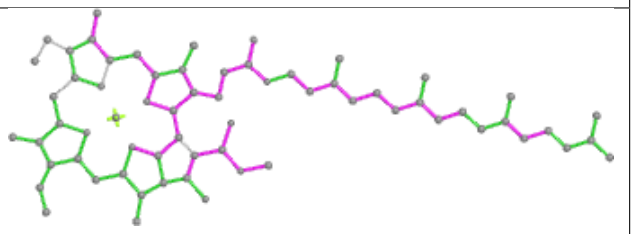


Rings

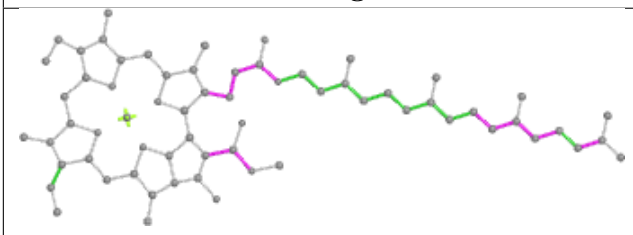
Ligand CLA a6 422



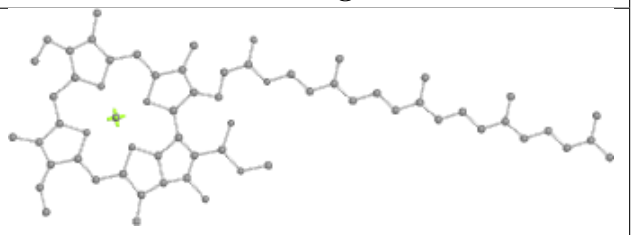
Bond lengths



Bond angles

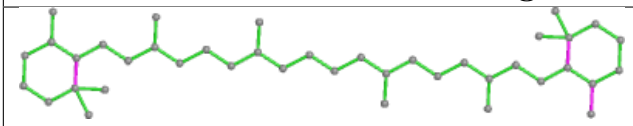


Torsions

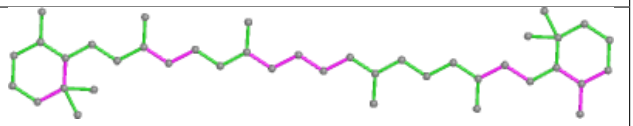


Rings

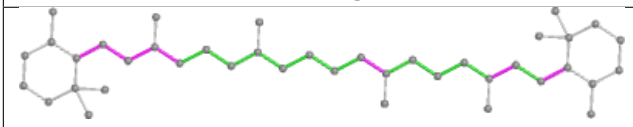
Ligand BCR cJ 104



Bond lengths



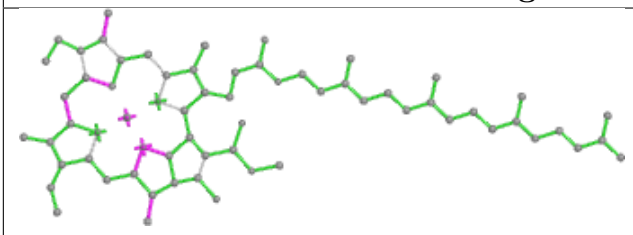
Bond angles



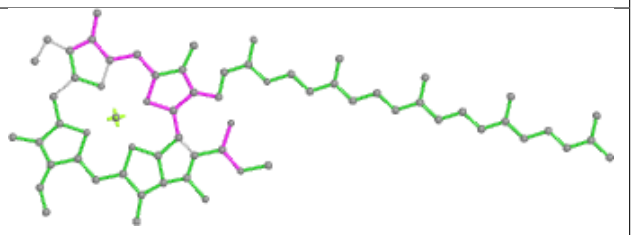
Torsions

Rings

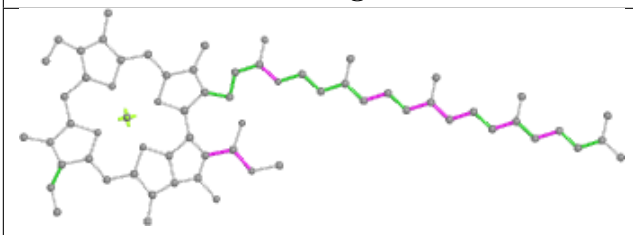
Ligand CLA b2 403



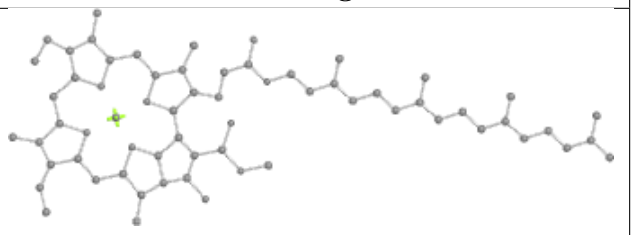
Bond lengths



Bond angles

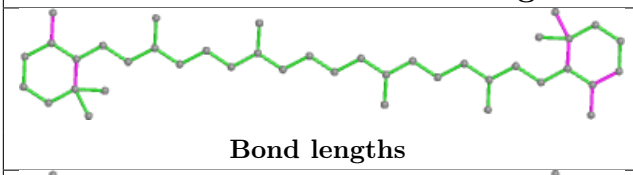


Torsions

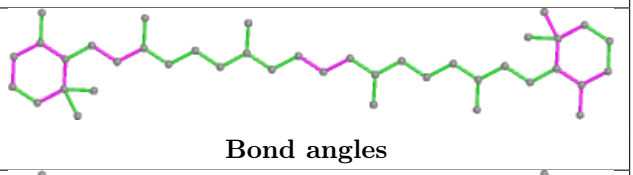


Rings

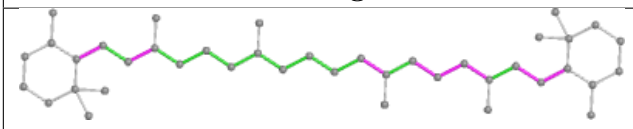
Ligand BCR a5 418



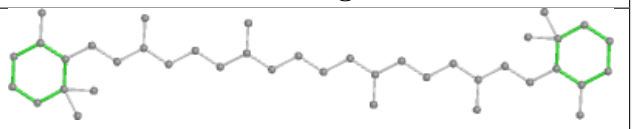
Bond lengths



Bond angles

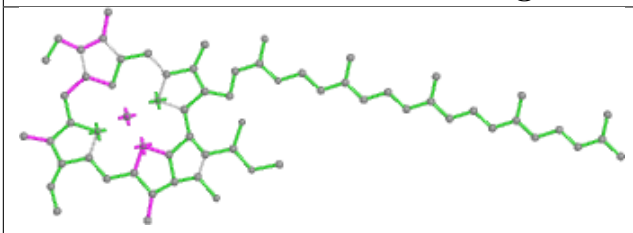


Torsions

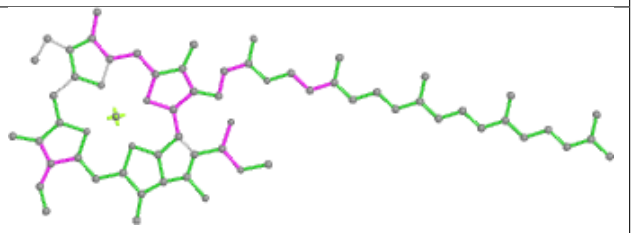


Rings

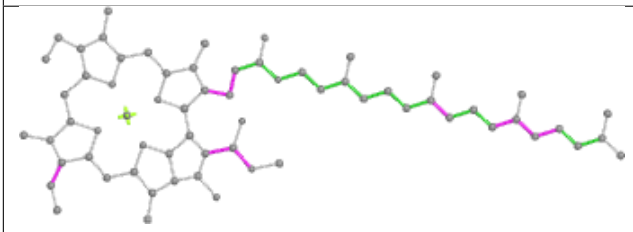
Ligand CLA aB 840



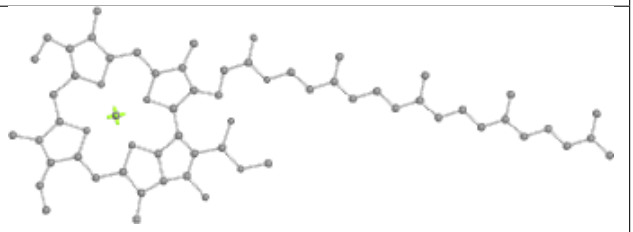
Bond lengths



Bond angles

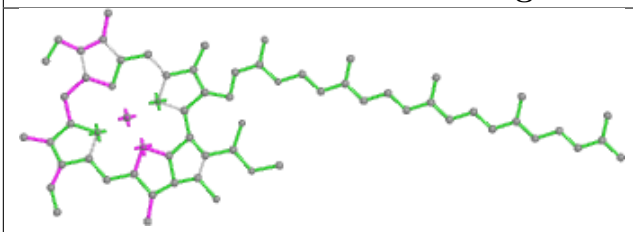


Torsions

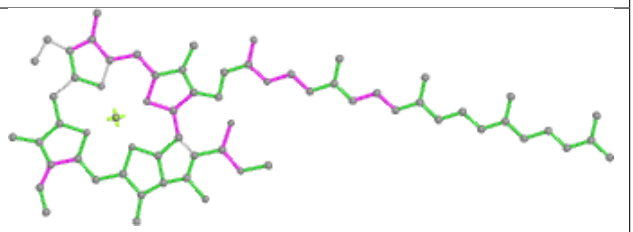


Rings

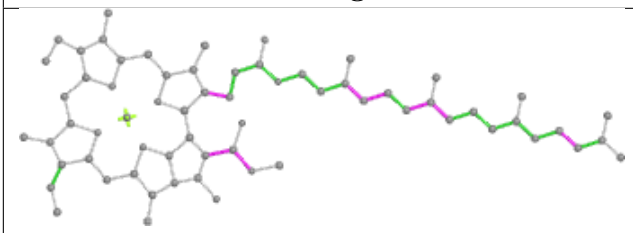
Ligand CLA aB 811



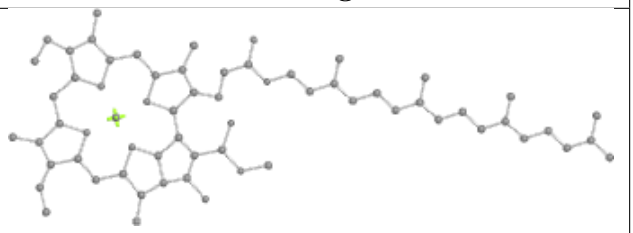
Bond lengths



Bond angles

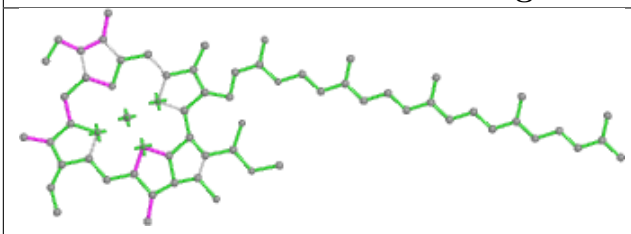


Torsions

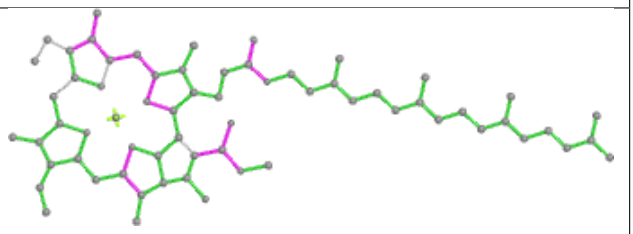


Rings

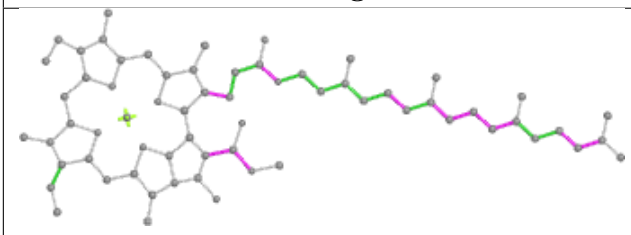
Ligand CLA aB 815



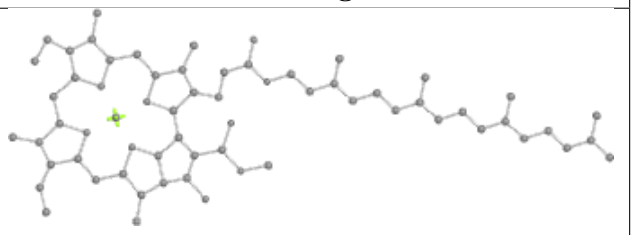
Bond lengths



Bond angles

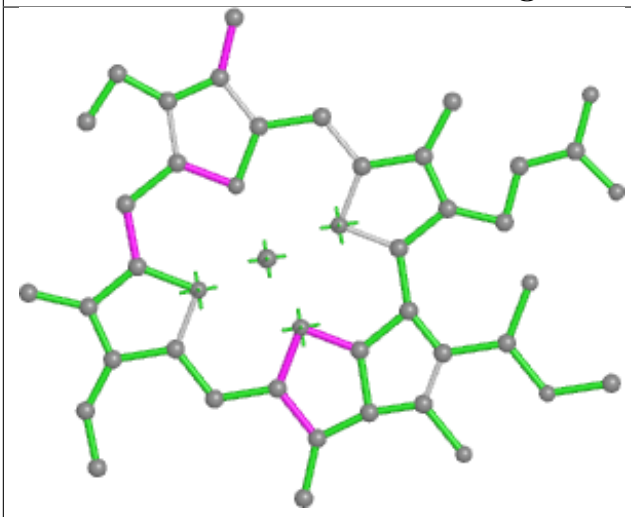


Torsions

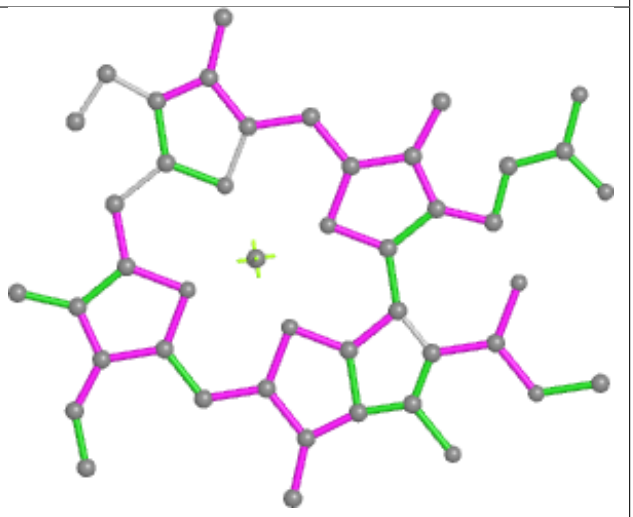


Rings

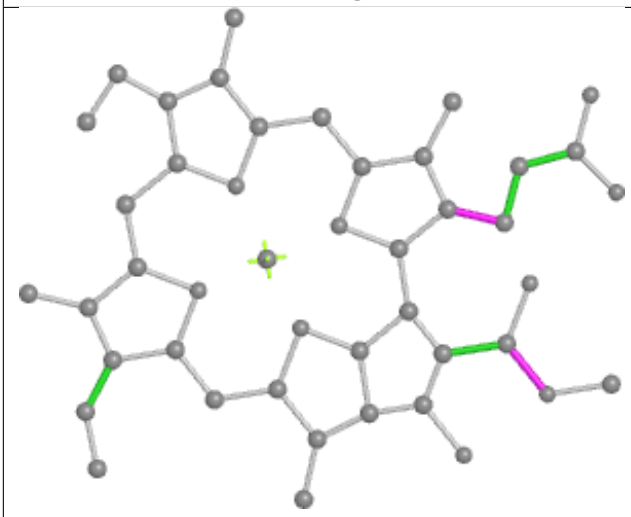
Ligand CLA b1 405



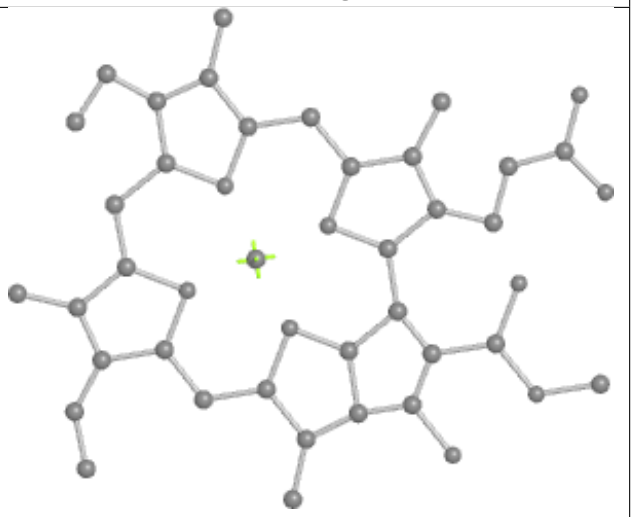
Bond lengths



Bond angles

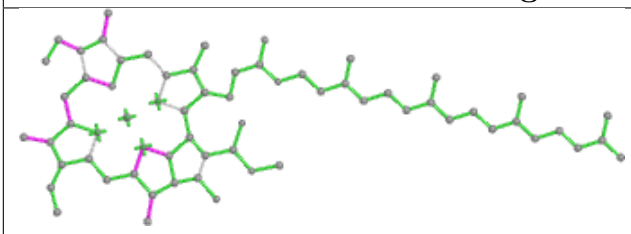


Torsions

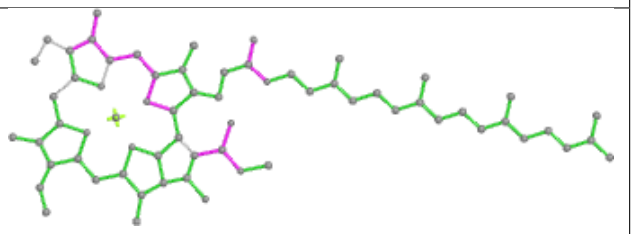


Rings

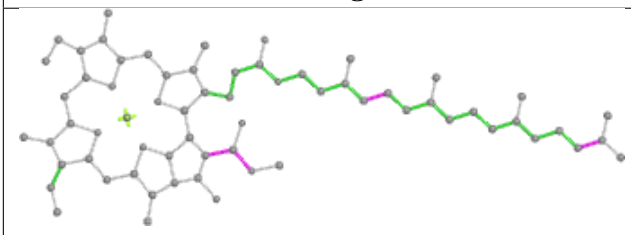
Ligand CLA c3 409



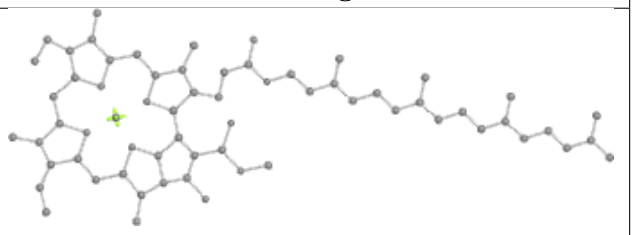
Bond lengths



Bond angles

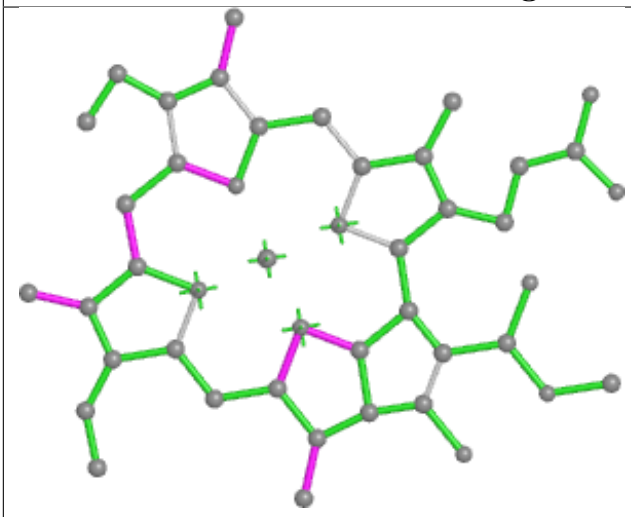


Torsions

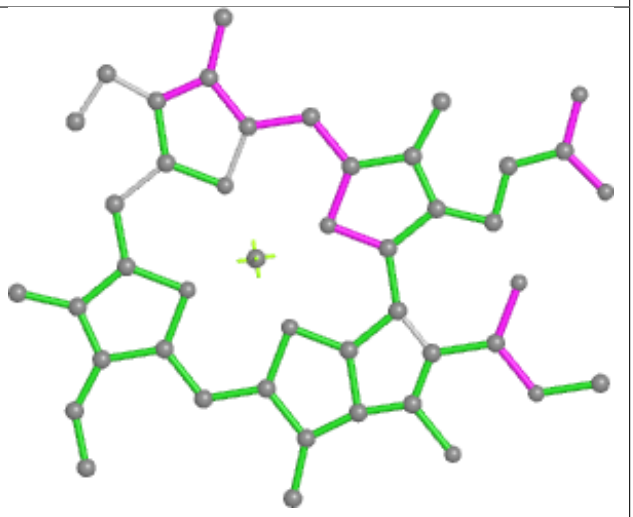


Rings

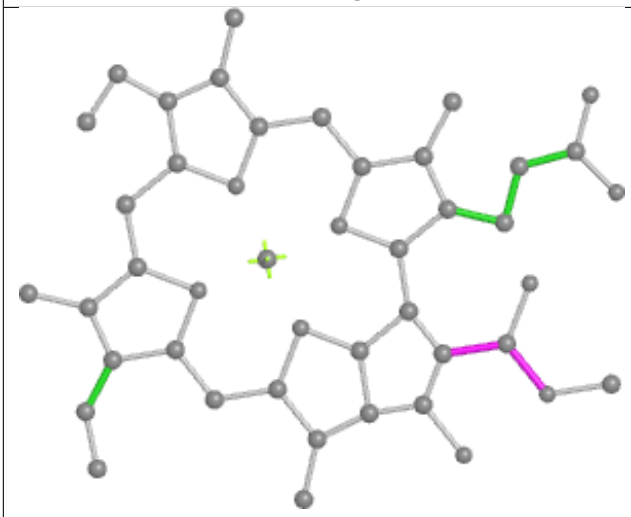
Ligand CLA c5 406



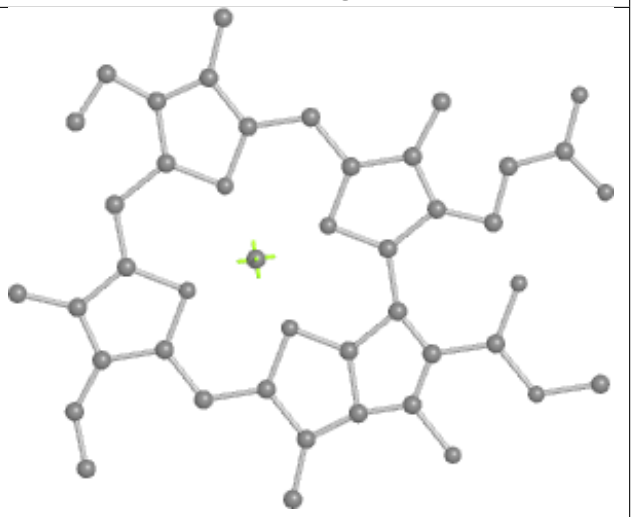
Bond lengths



Bond angles

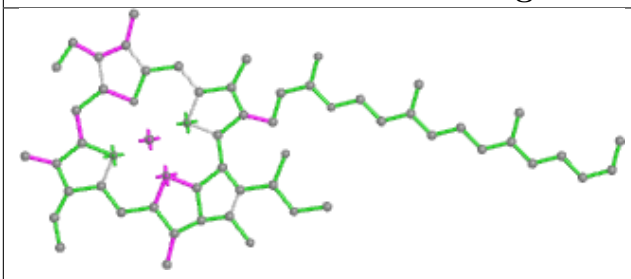


Torsions

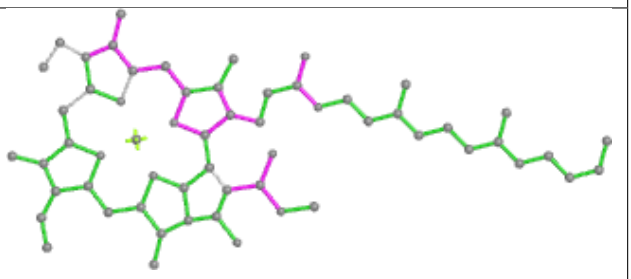


Rings

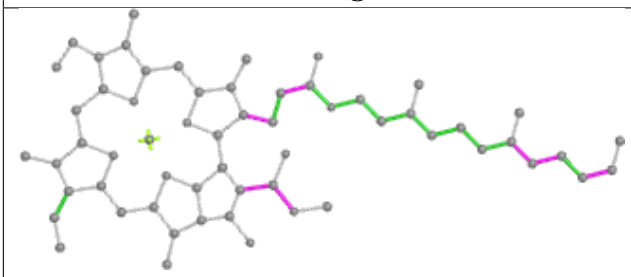
Ligand CLA cA 805



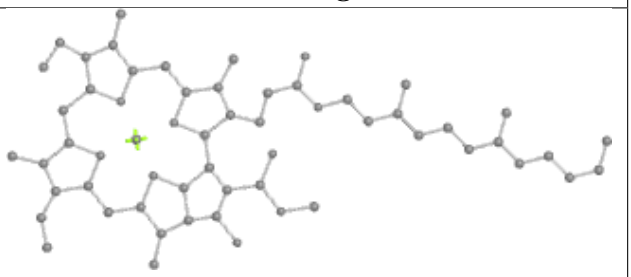
Bond lengths



Bond angles

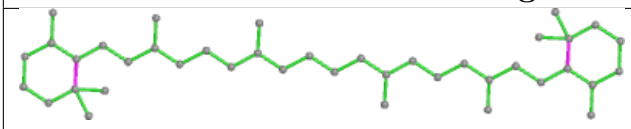


Torsions

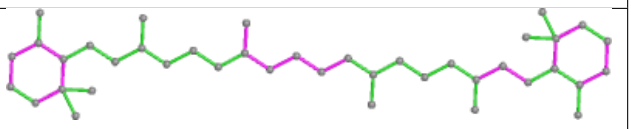


Rings

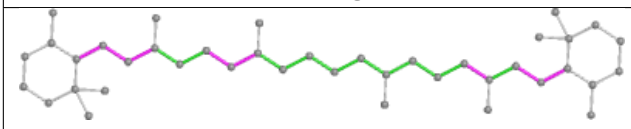
Ligand BCR c2 421



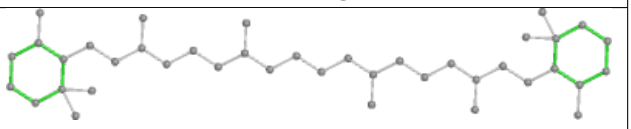
Bond lengths



Bond angles

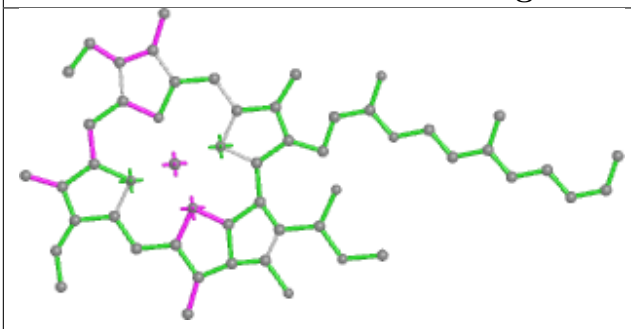


Torsions

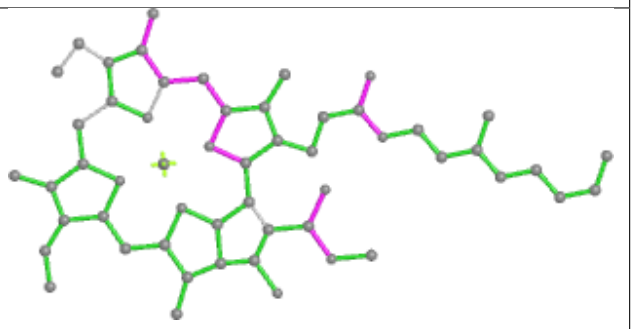


Rings

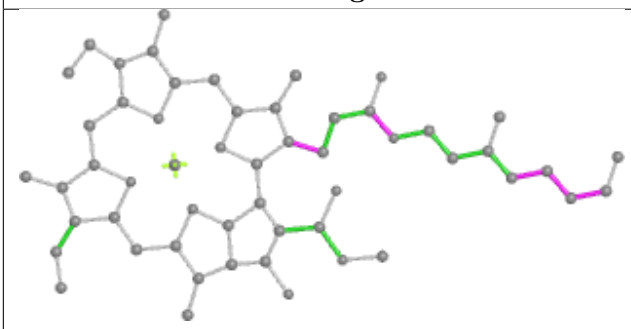
Ligand CLA cA 836



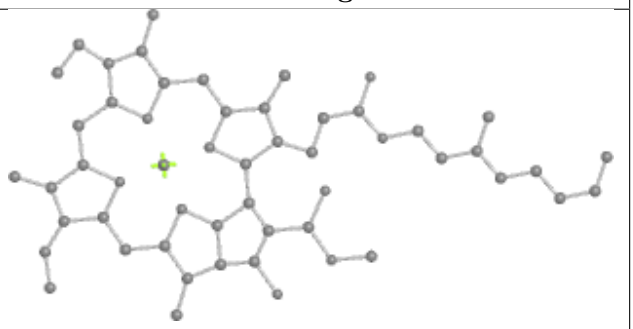
Bond lengths



Bond angles

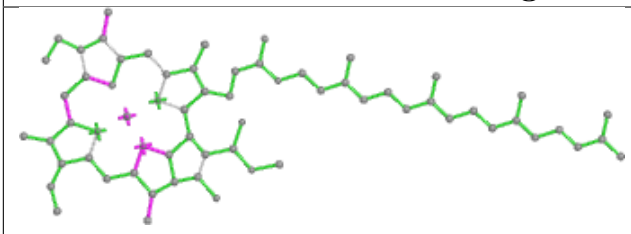


Torsions

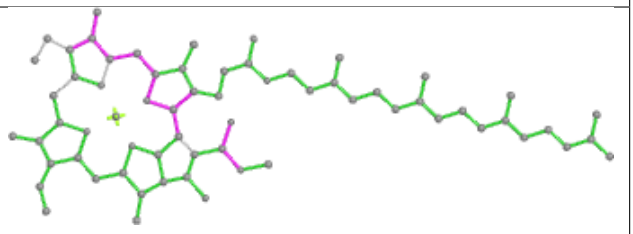


Rings

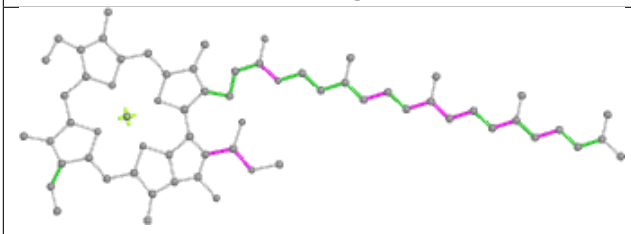
Ligand CLA c4 403



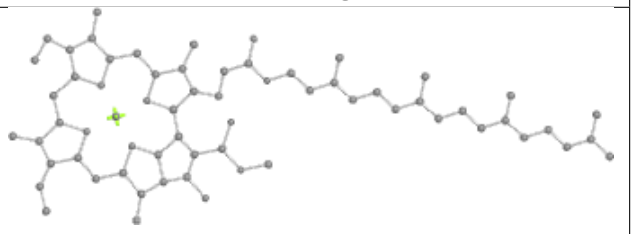
Bond lengths



Bond angles

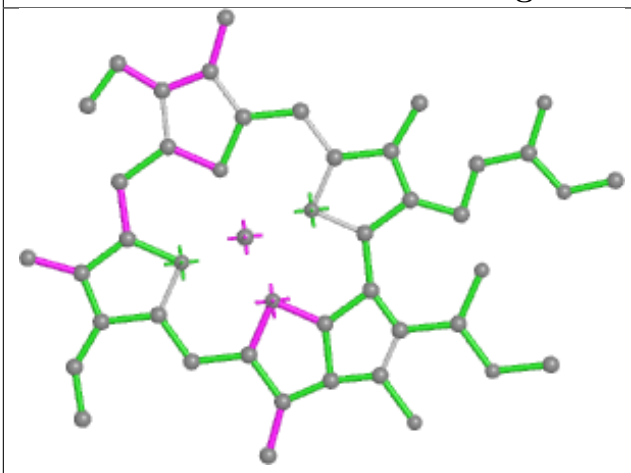


Torsions

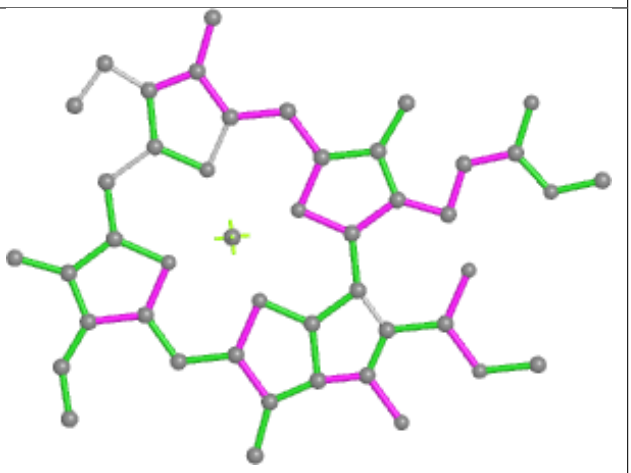


Rings

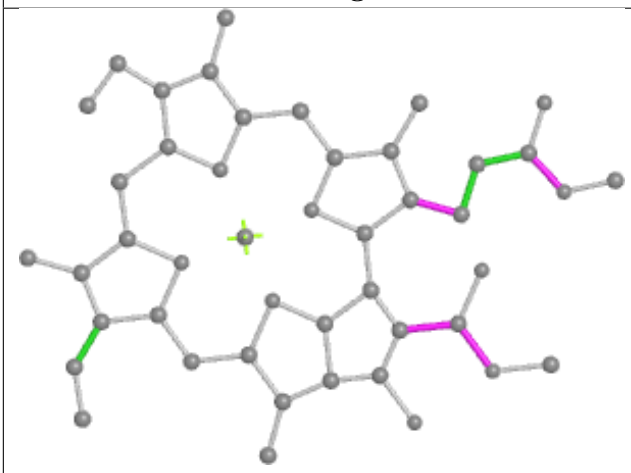
Ligand CLA aB 826



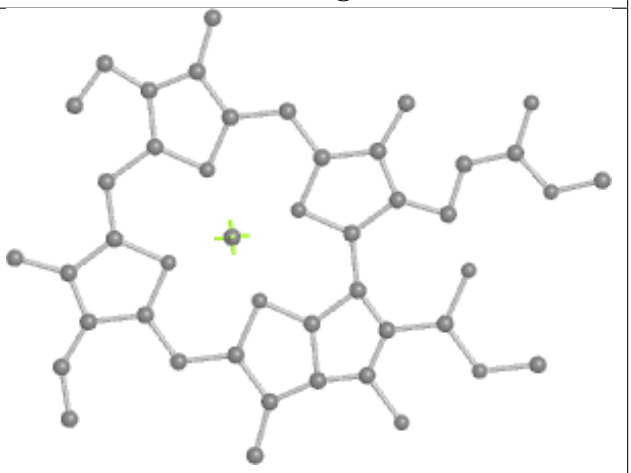
Bond lengths



Bond angles

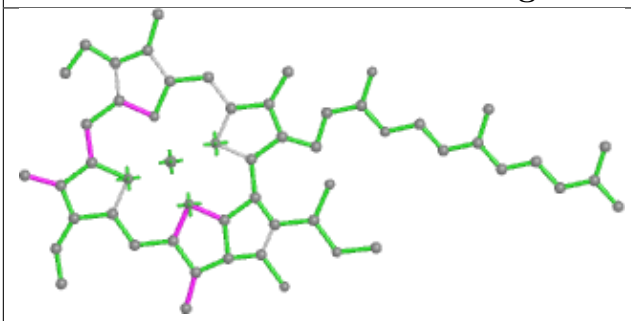


Torsions

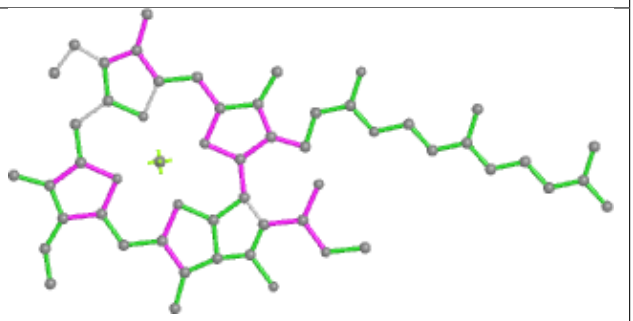


Rings

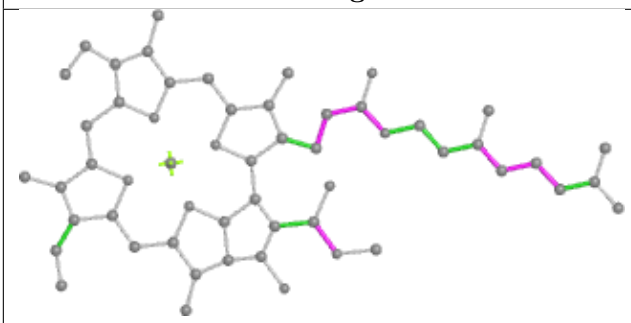
Ligand CLA b1 417



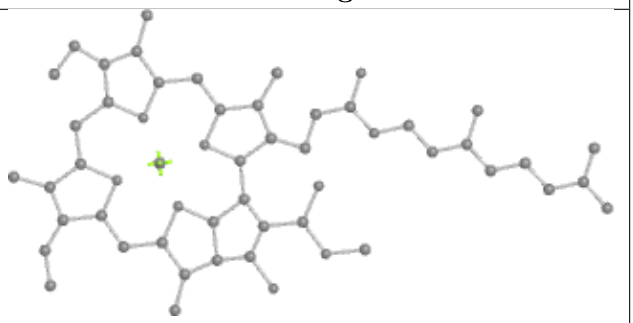
Bond lengths



Bond angles

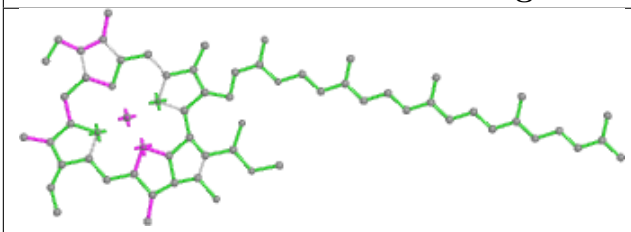


Torsions

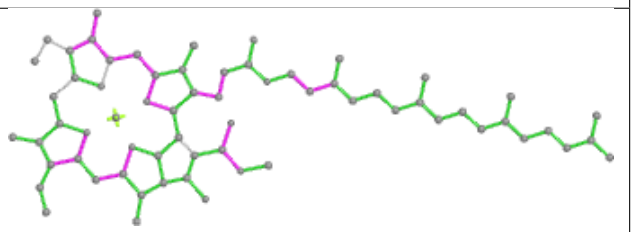


Rings

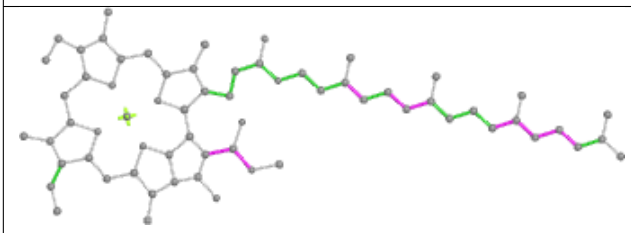
Ligand CLA aB 837



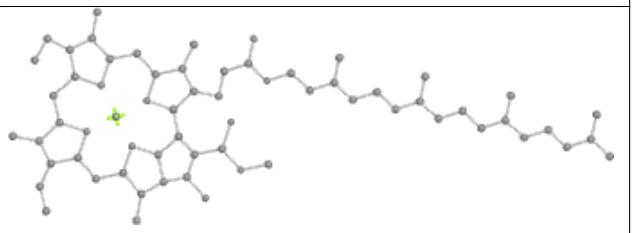
Bond lengths



Bond angles

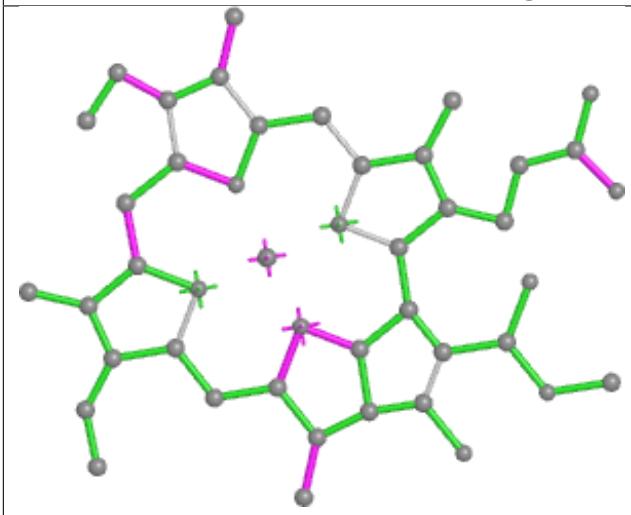


Torsions

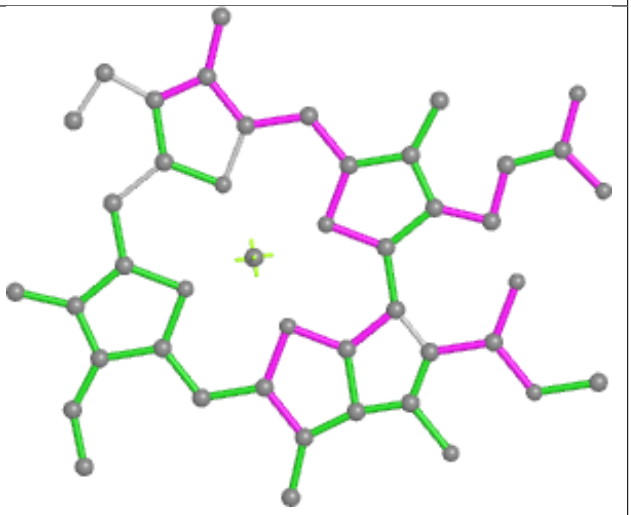


Rings

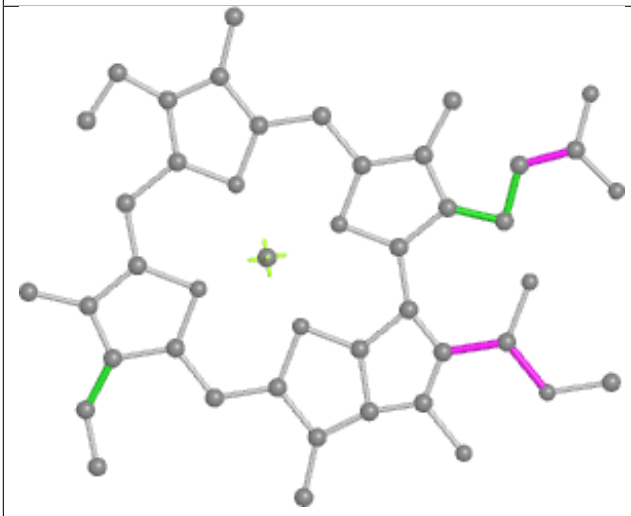
Ligand CLA c5 415



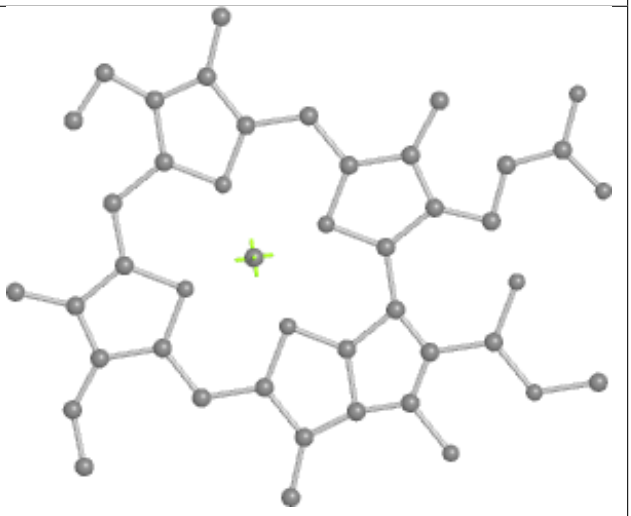
Bond lengths



Bond angles

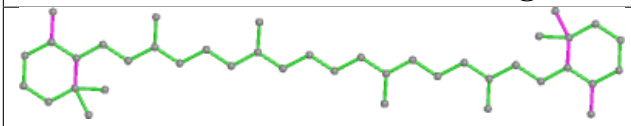


Torsions

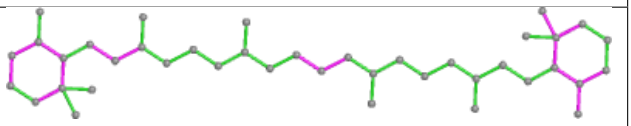


Rings

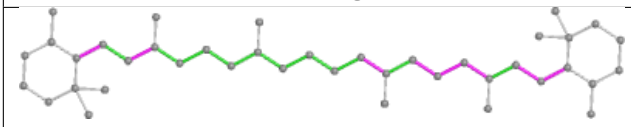
Ligand BCR c5 418



Bond lengths



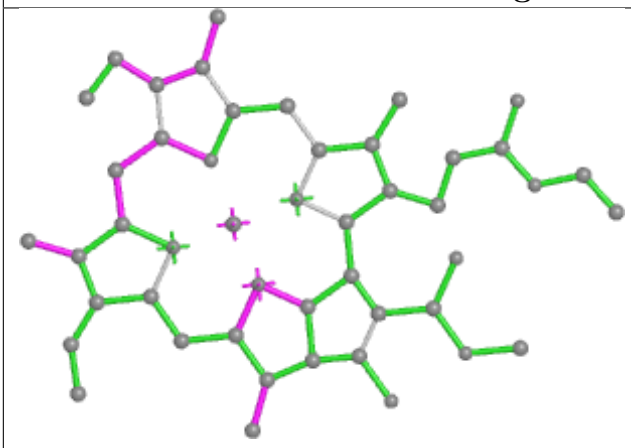
Bond angles



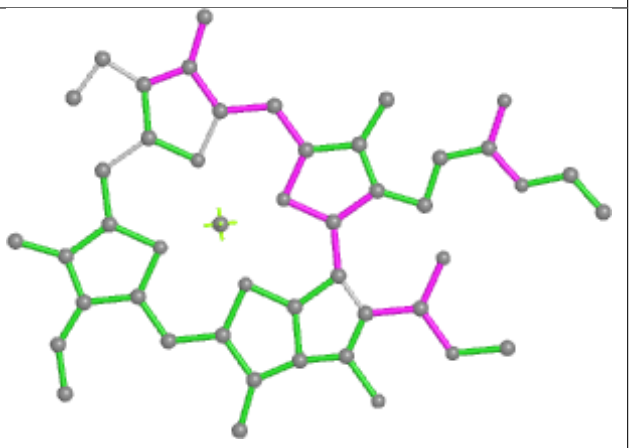
Torsions

Rings

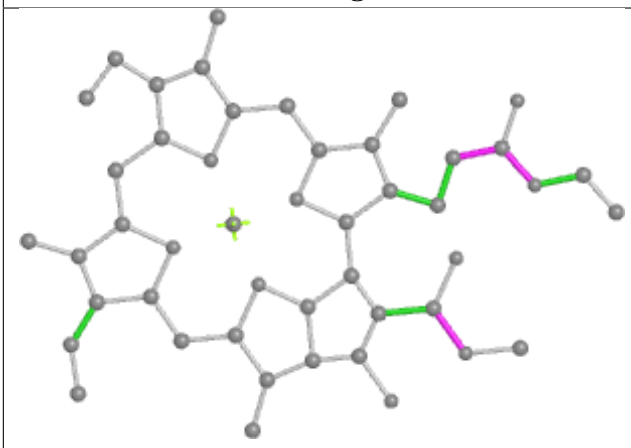
Ligand CLA bA 840



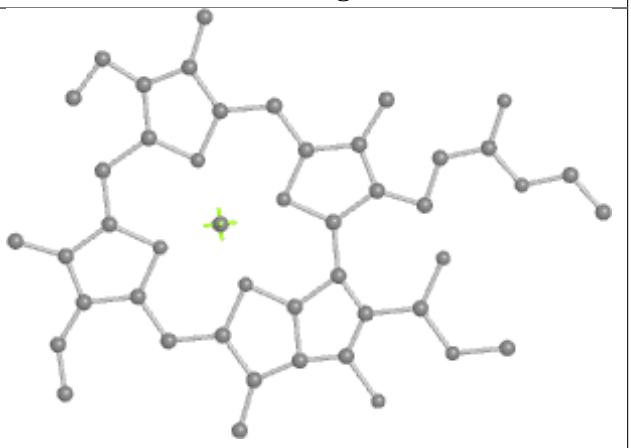
Bond lengths



Bond angles

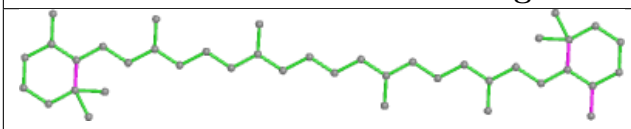


Torsions

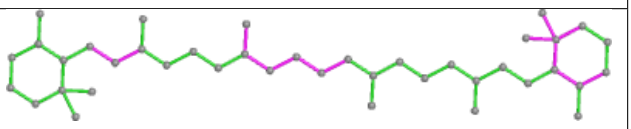


Rings

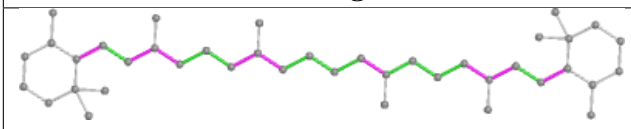
Ligand BCR aB 846



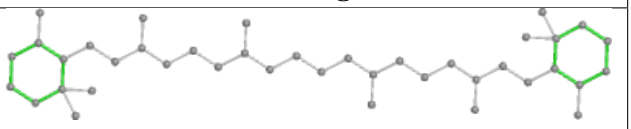
Bond lengths



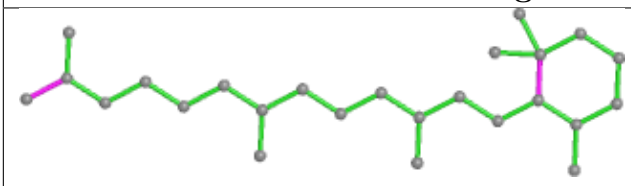
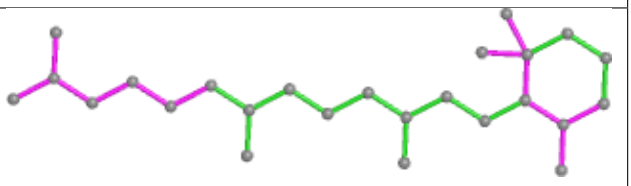
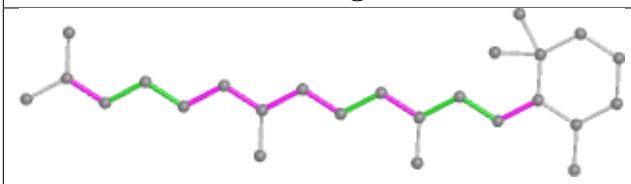
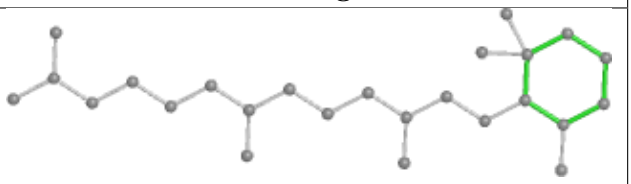
Bond angles

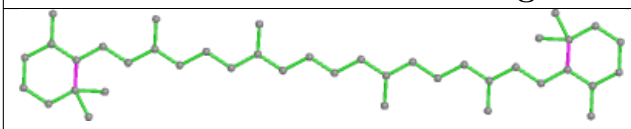
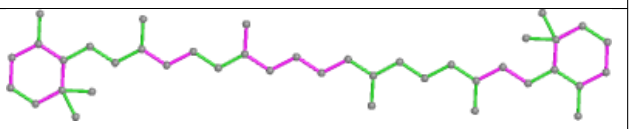
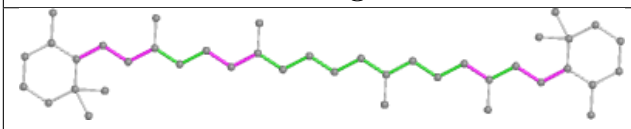
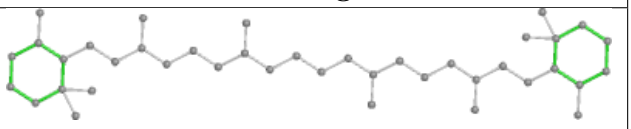


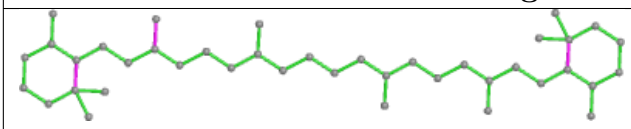
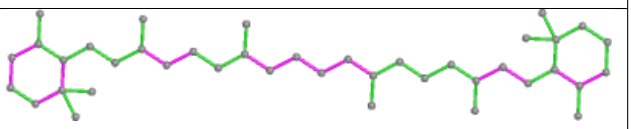
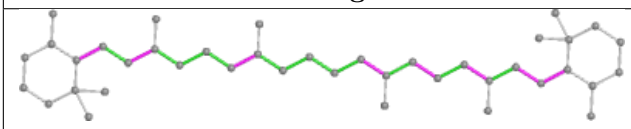
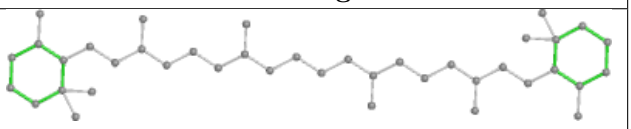
Torsions



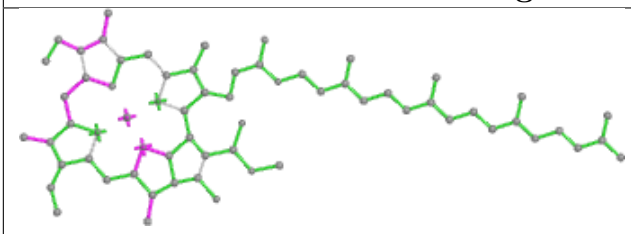
Rings

Ligand BCR cB 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

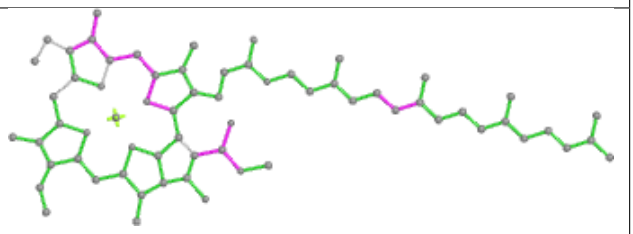
Ligand BCR a5 419	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR cI 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

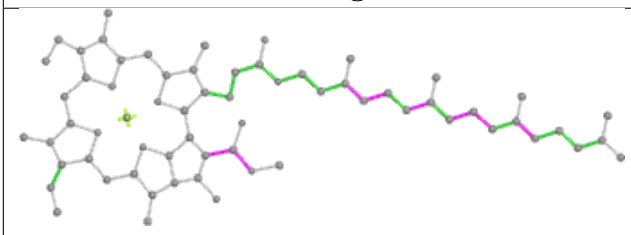
Ligand CLA cA 839



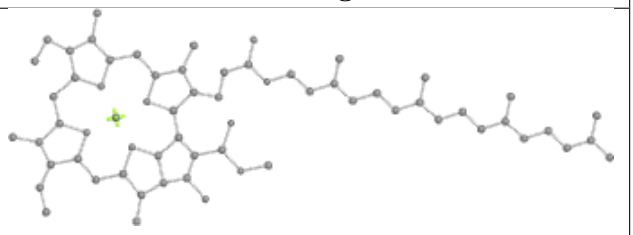
Bond lengths



Bond angles

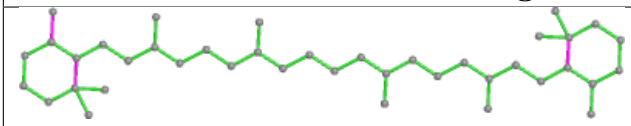


Torsions

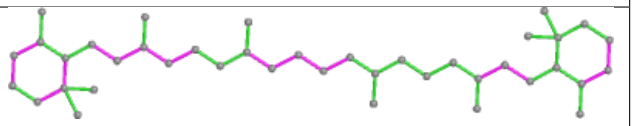


Rings

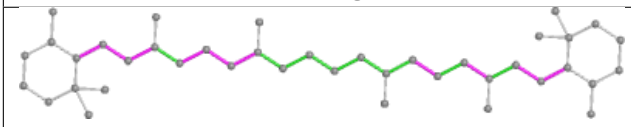
Ligand BCR b6 421



Bond lengths



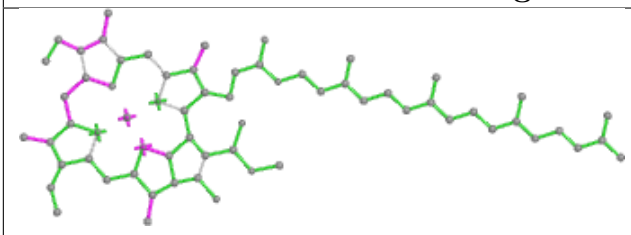
Bond angles



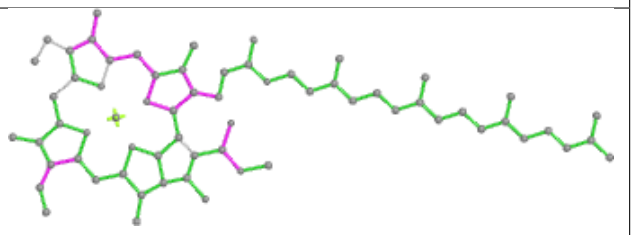
Torsions

Rings

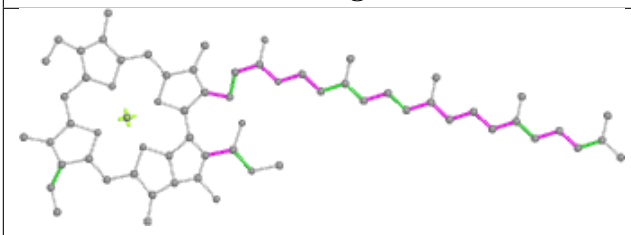
Ligand CLA bA 806



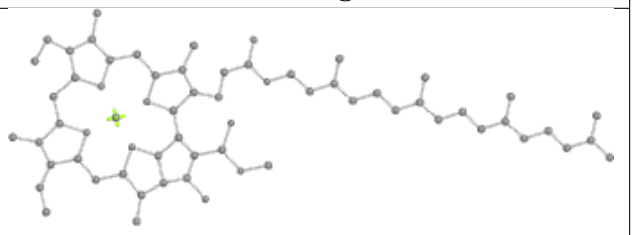
Bond lengths



Bond angles

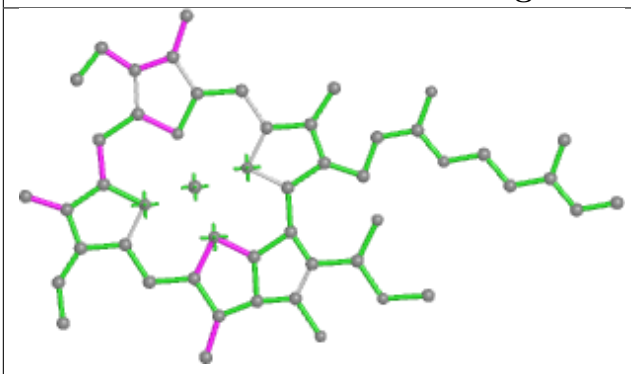


Torsions

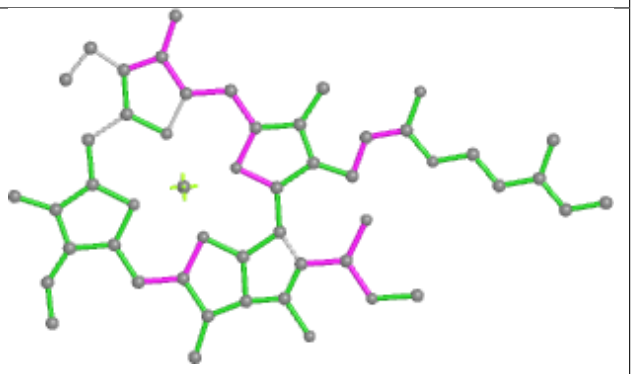


Rings

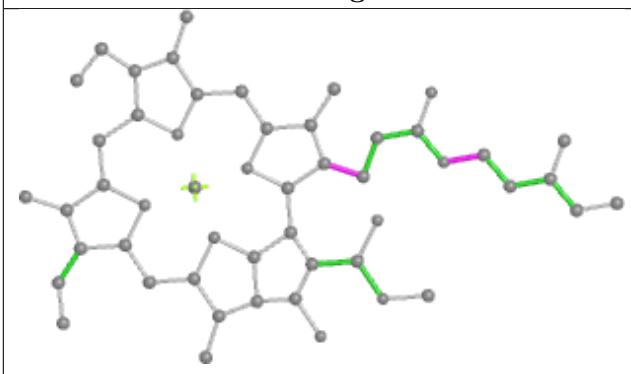
Ligand CLA aA 808



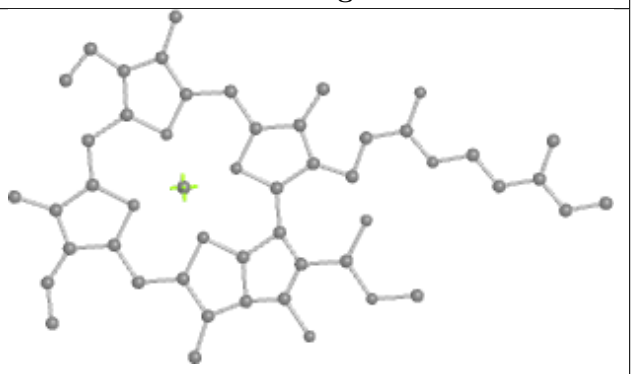
Bond lengths



Bond angles

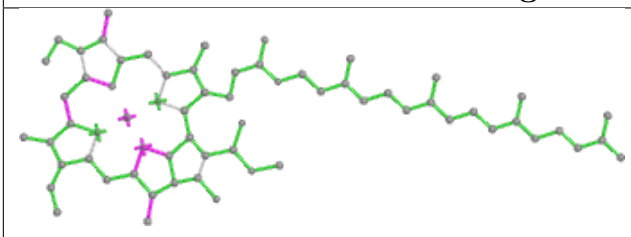


Torsions

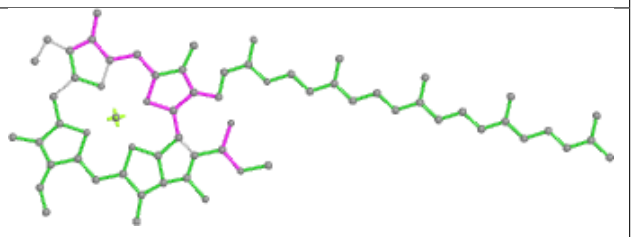


Rings

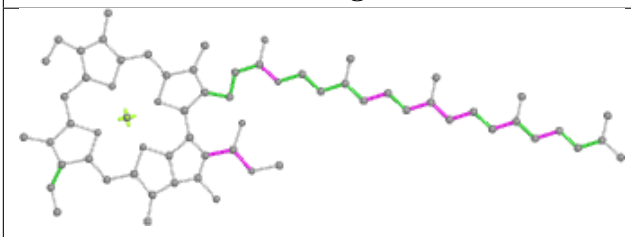
Ligand CLA a1 402



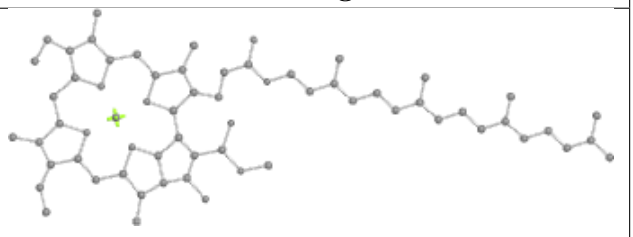
Bond lengths



Bond angles

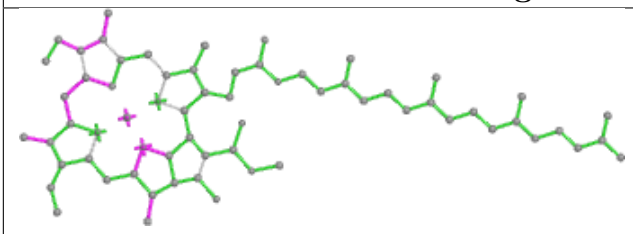


Torsions

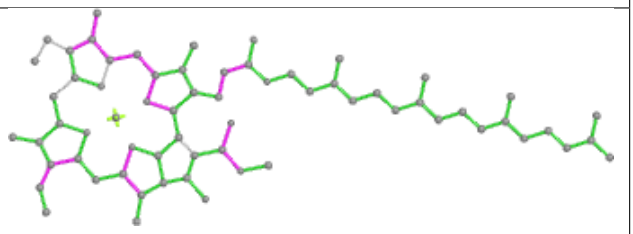


Rings

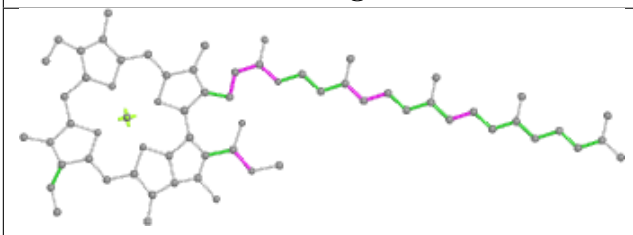
Ligand CLA bB 801



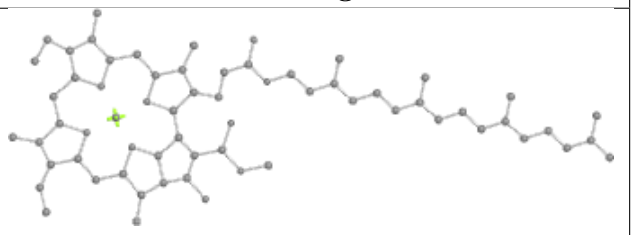
Bond lengths



Bond angles

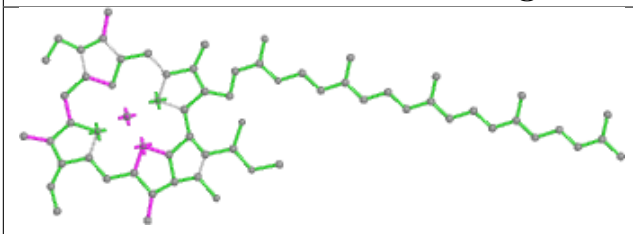


Torsions

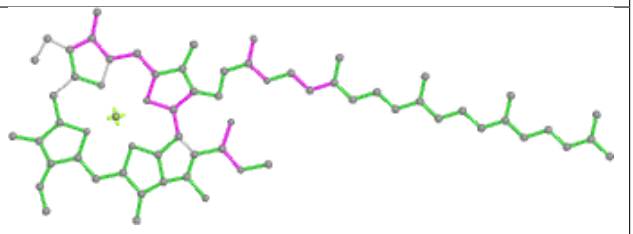


Rings

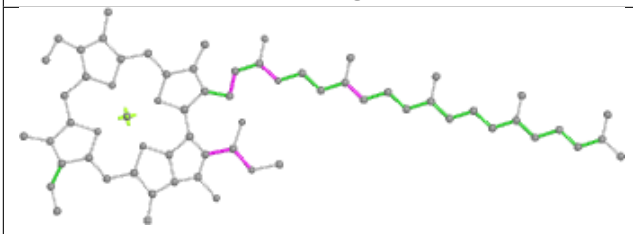
Ligand CLA b6 405



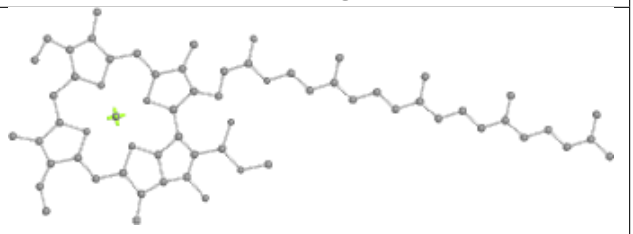
Bond lengths



Bond angles

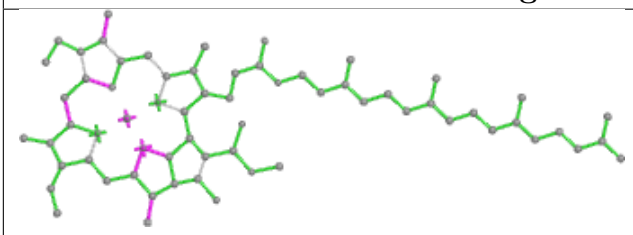


Torsions

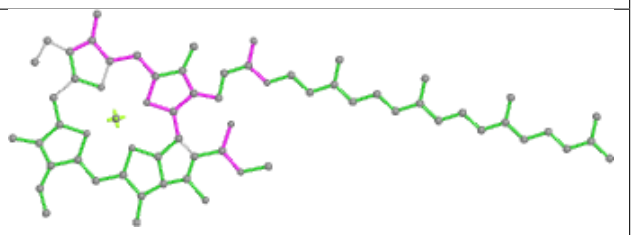


Rings

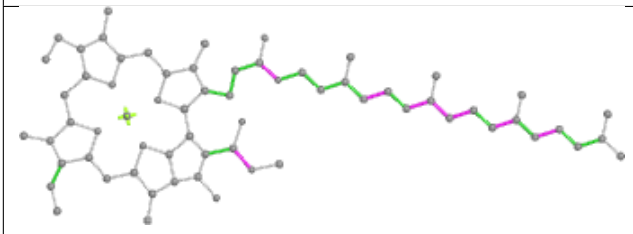
Ligand CLA a3 403



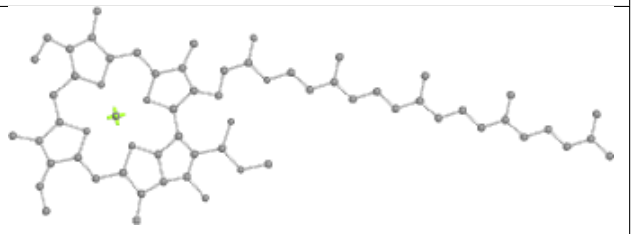
Bond lengths



Bond angles

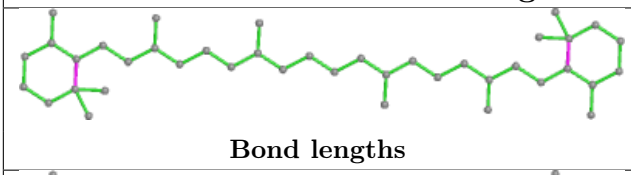


Torsions

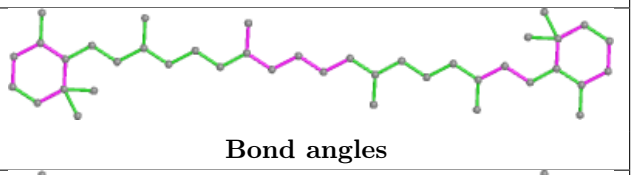


Rings

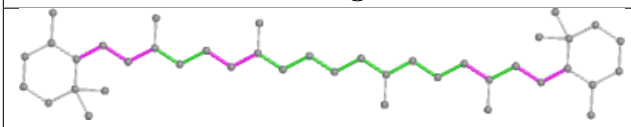
Ligand BCR c3 420



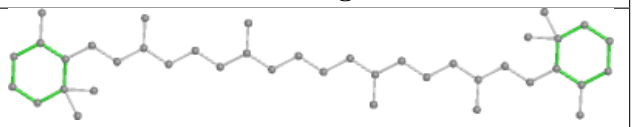
Bond lengths



Bond angles

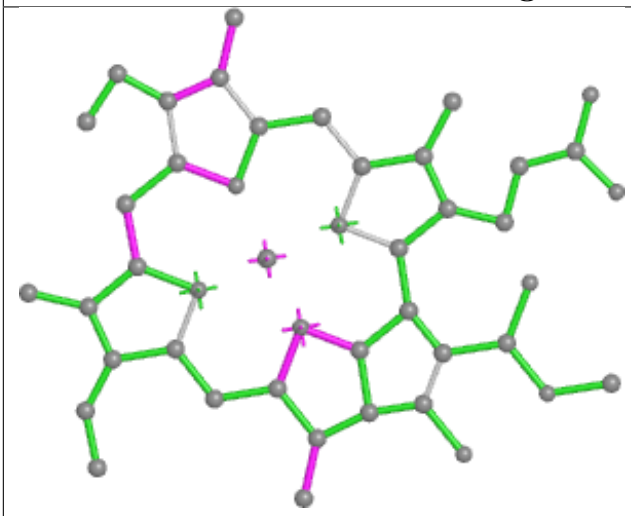


Torsions

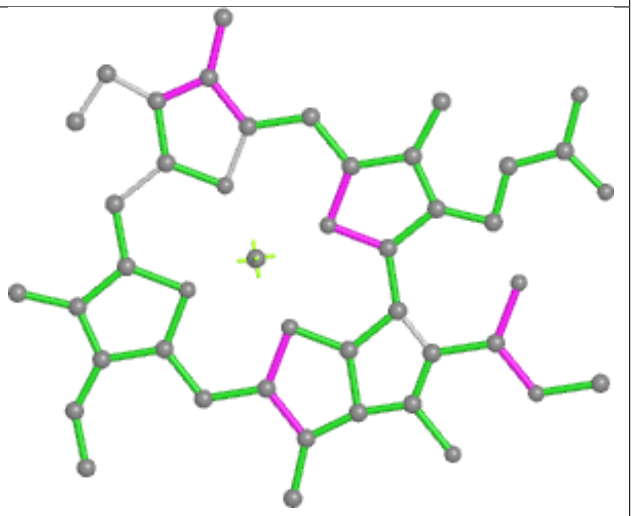


Rings

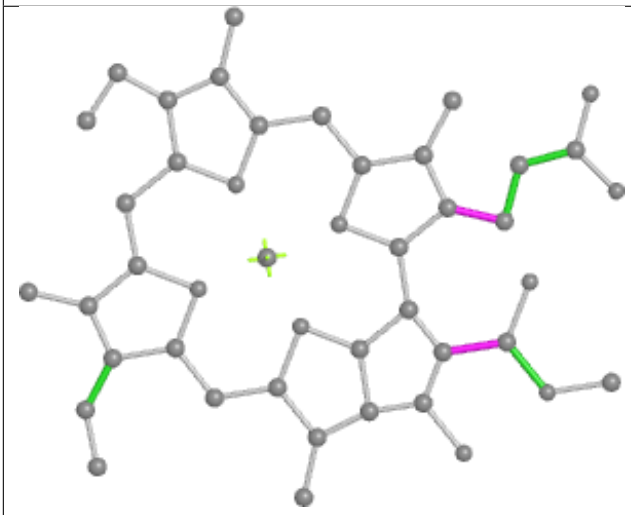
Ligand CLA b1 413



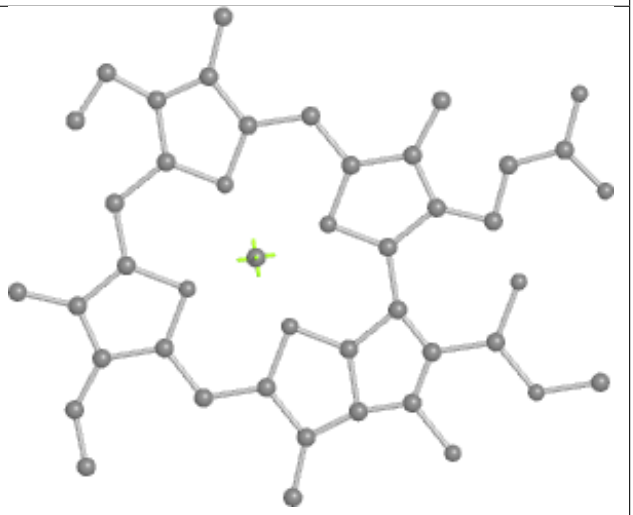
Bond lengths



Bond angles

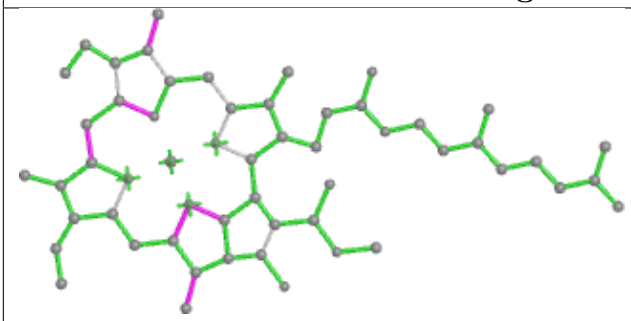


Torsions

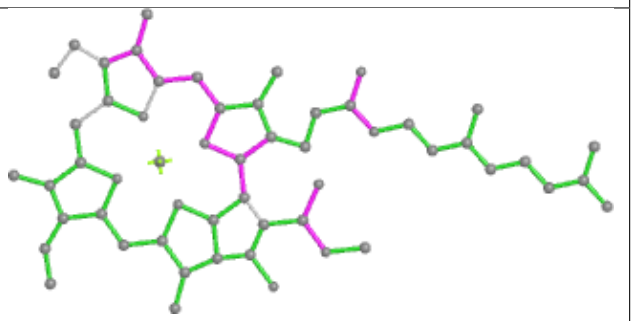


Rings

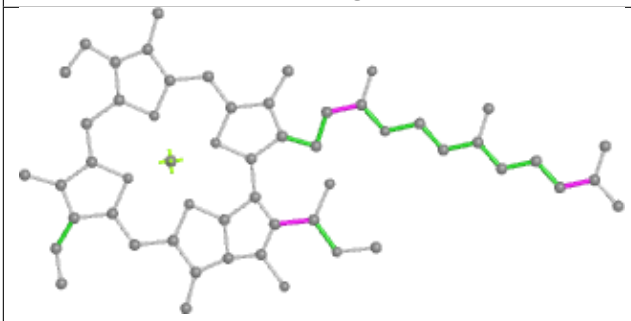
Ligand CLA cB 823



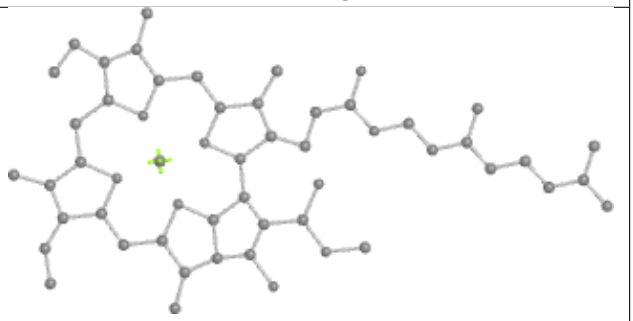
Bond lengths



Bond angles

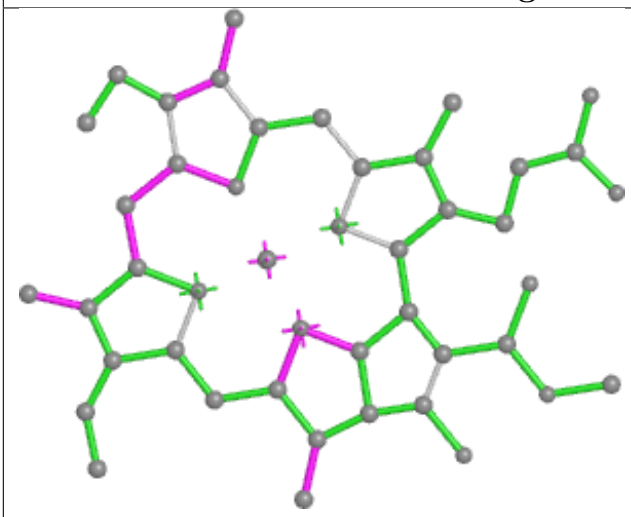


Torsions

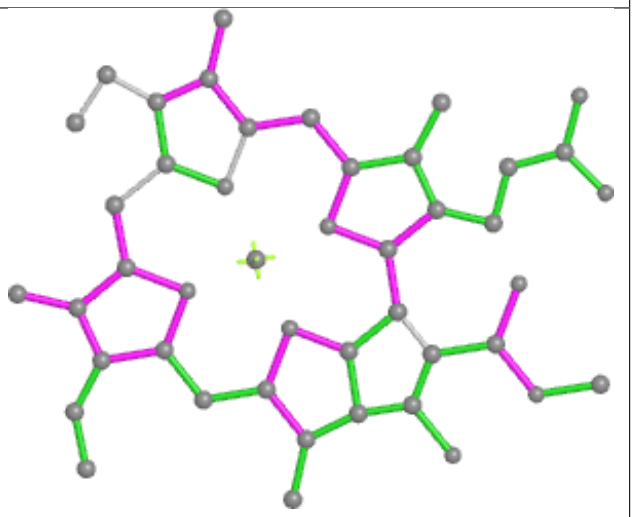


Rings

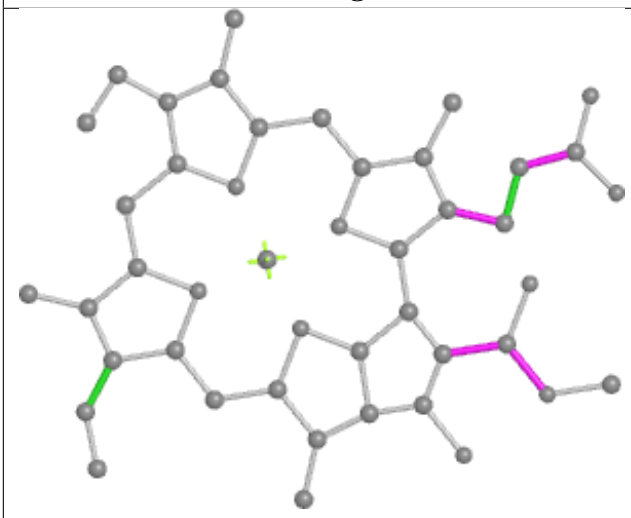
Ligand CLA b3 412



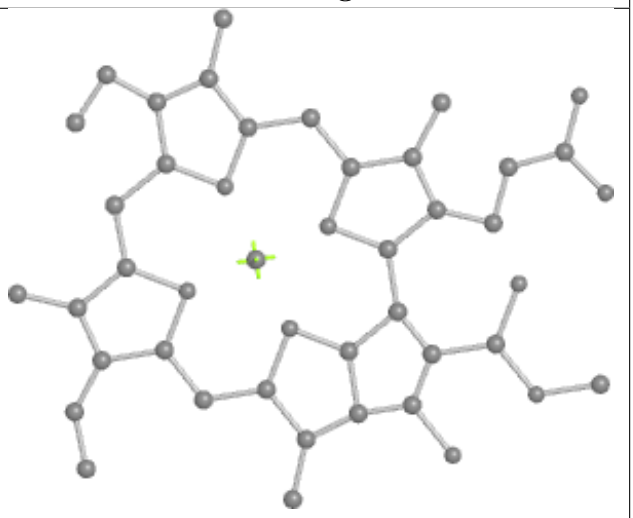
Bond lengths



Bond angles

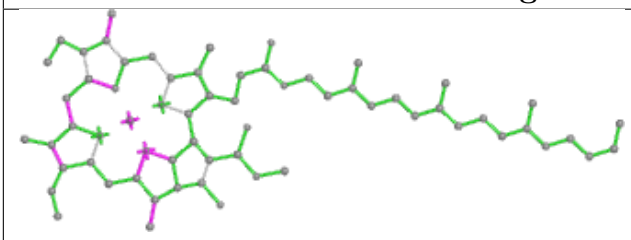


Torsions

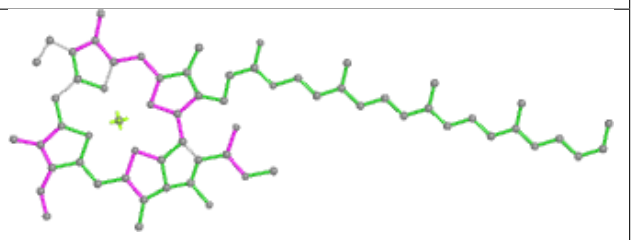


Rings

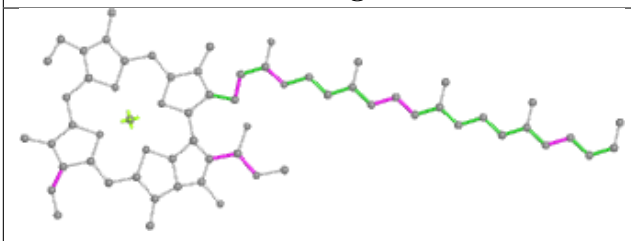
Ligand CLA a2 411



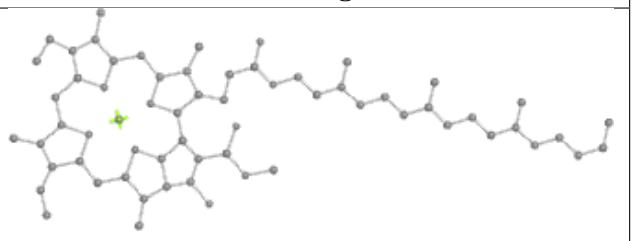
Bond lengths



Bond angles

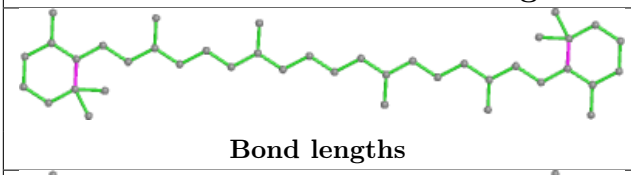


Torsions

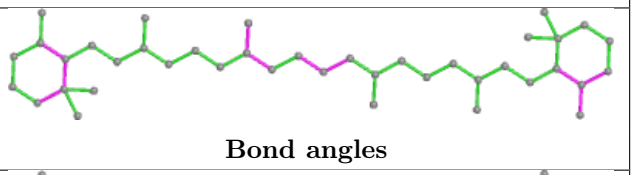


Rings

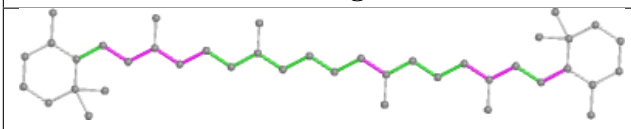
Ligand BCR aI 101



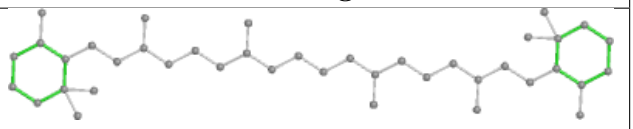
Bond lengths



Bond angles

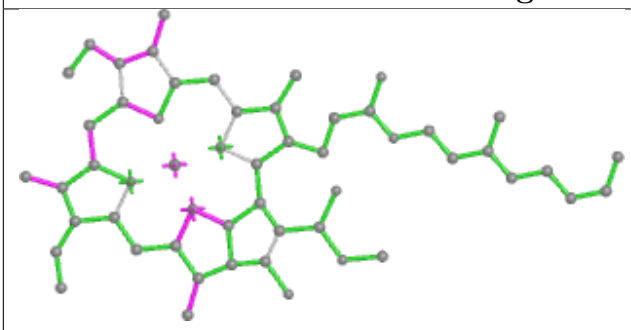


Torsions

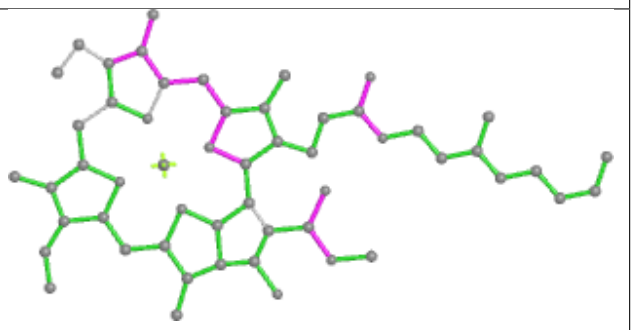


Rings

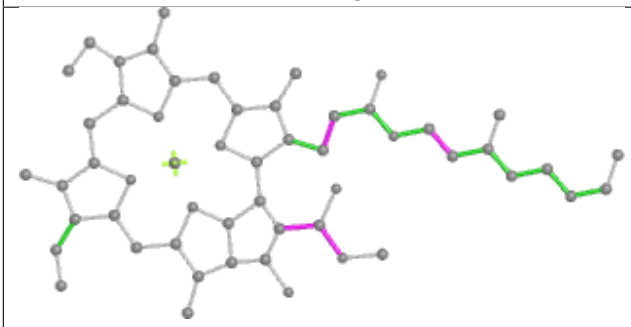
Ligand CLA cB 805



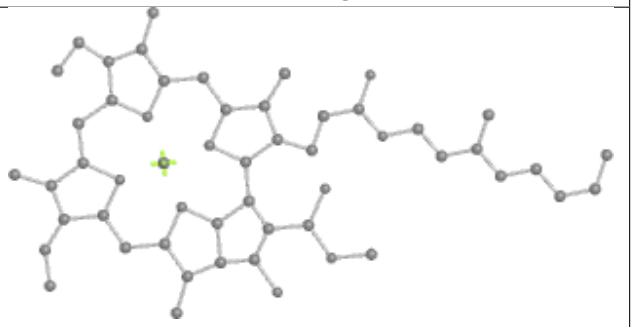
Bond lengths



Bond angles

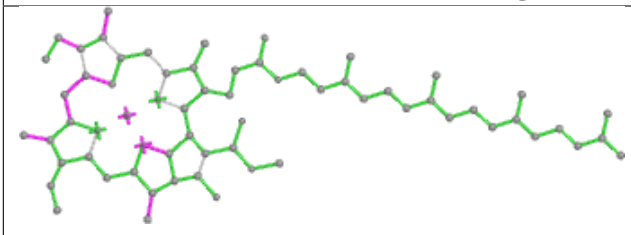


Torsions

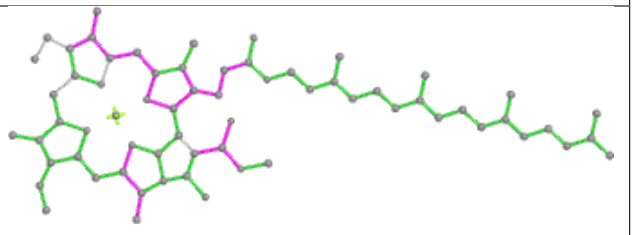


Rings

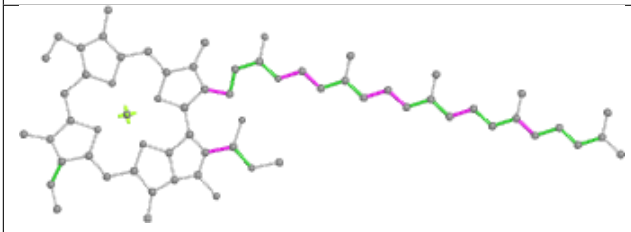
Ligand CLA bA 827



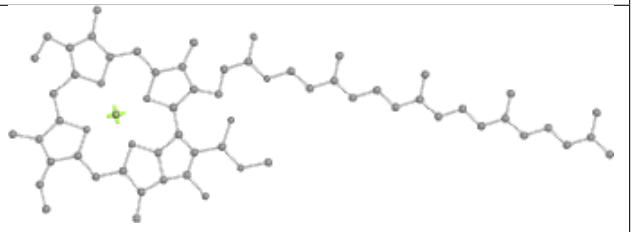
Bond lengths



Bond angles

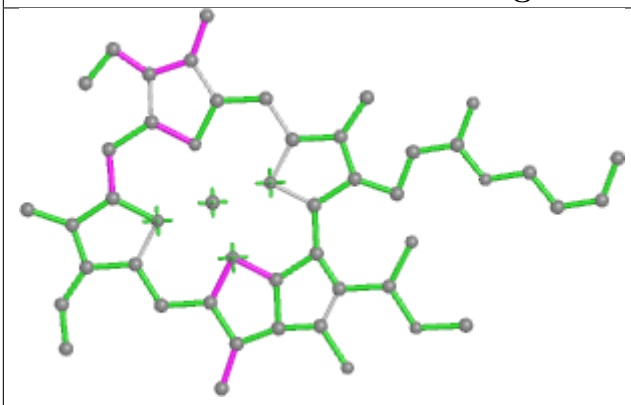


Torsions

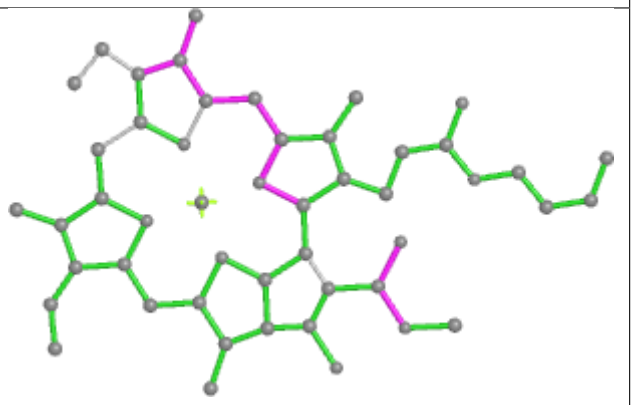


Rings

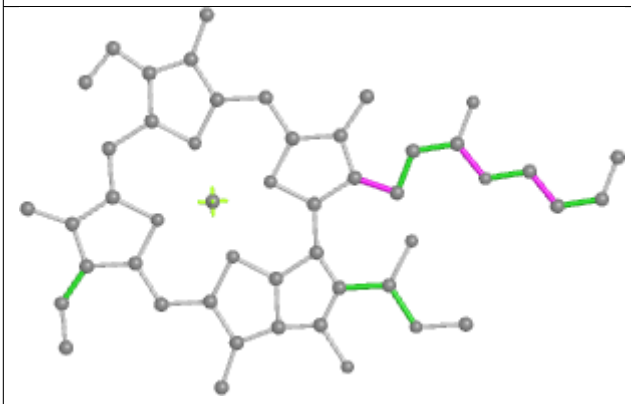
Ligand CLA bA 817



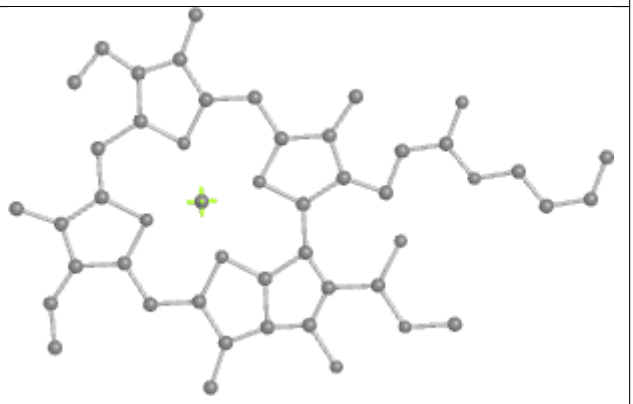
Bond lengths



Bond angles

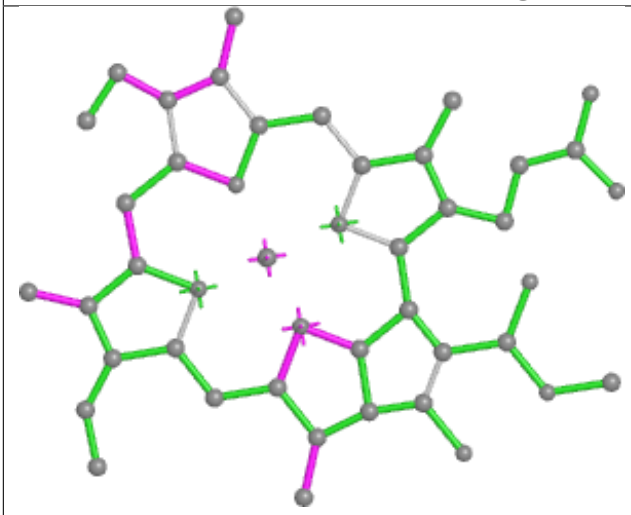


Torsions

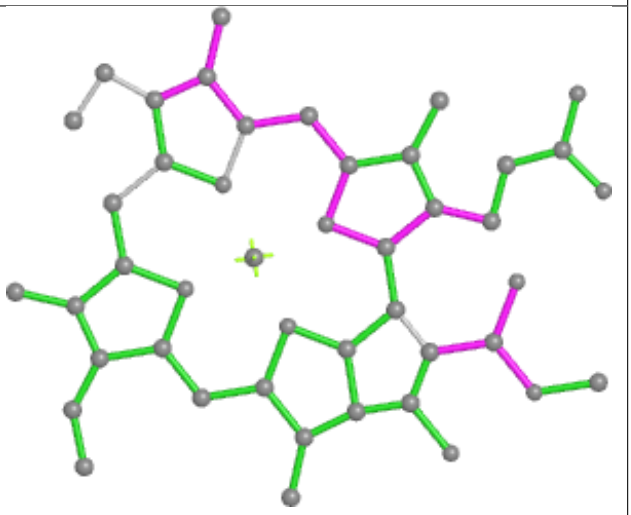


Rings

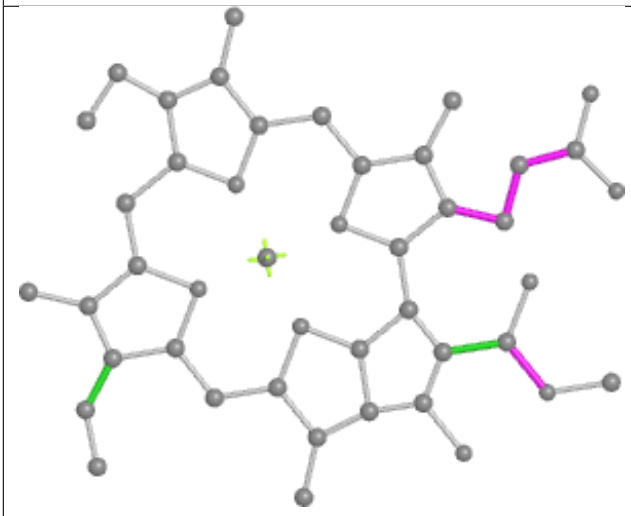
Ligand CLA bB 835



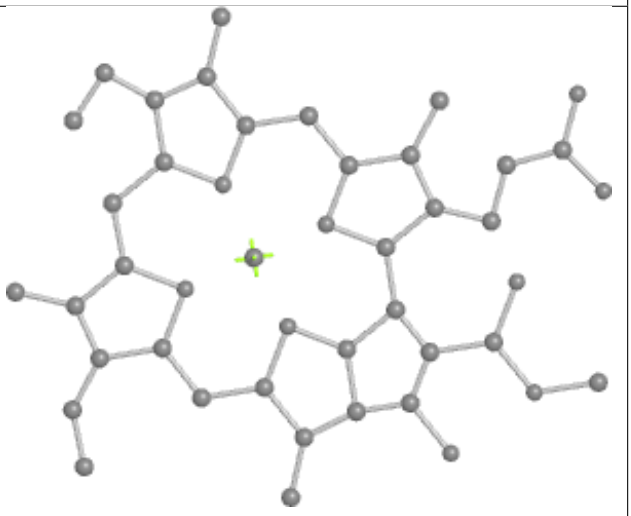
Bond lengths



Bond angles

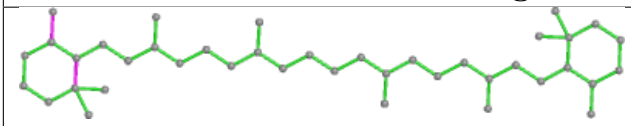


Torsions

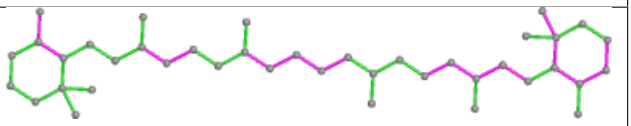


Rings

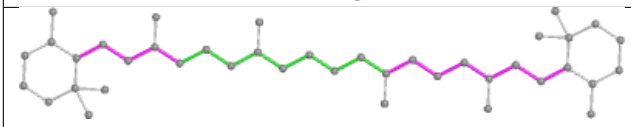
Ligand BCR bA 851



Bond lengths



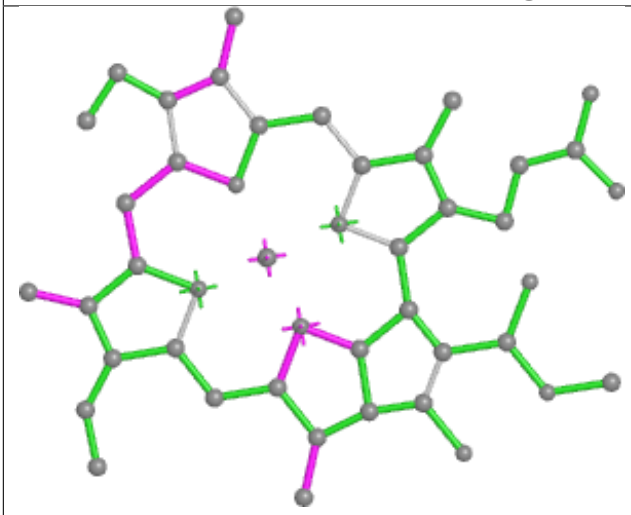
Bond angles



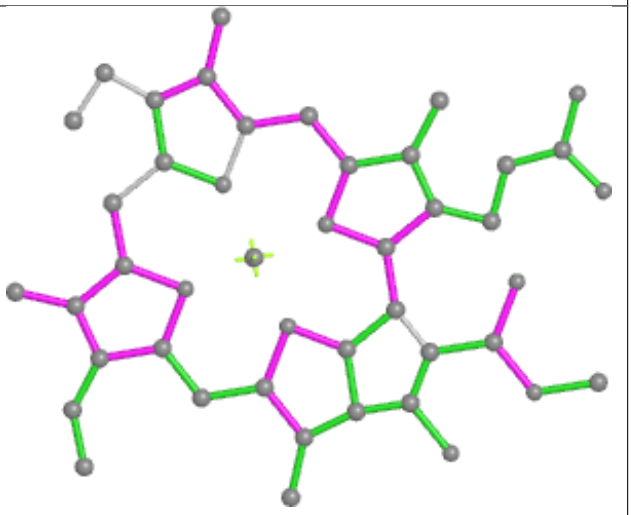
Torsions

Rings

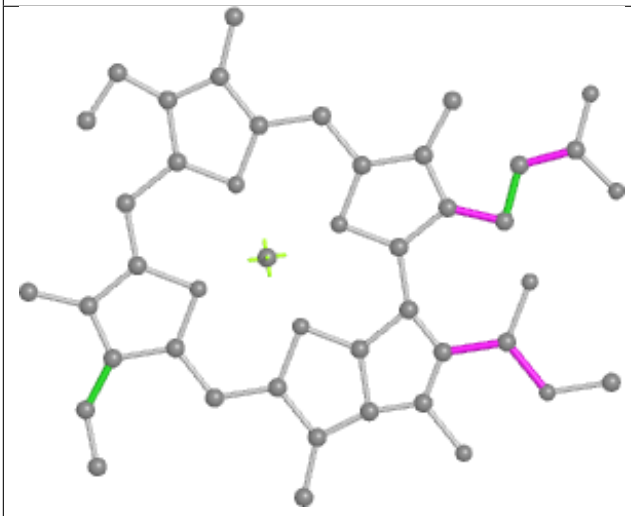
Ligand CLA c4 412



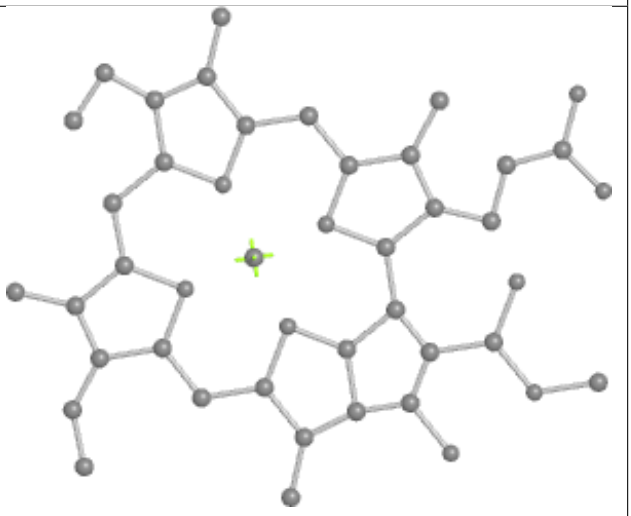
Bond lengths



Bond angles

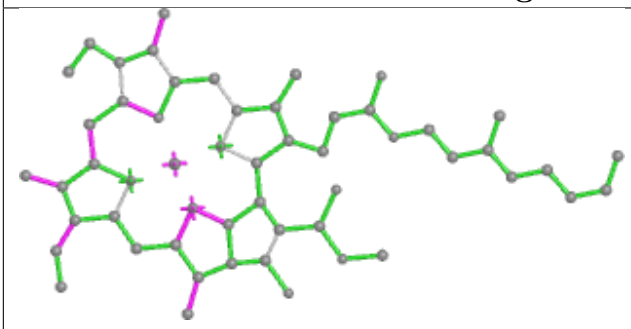


Torsions

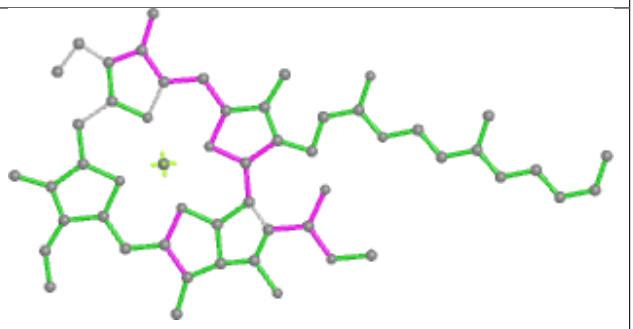


Rings

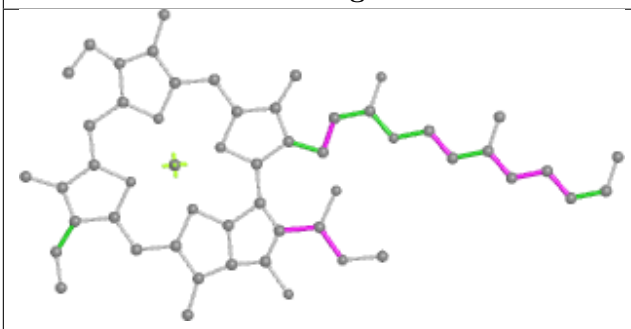
Ligand CLA aB 825



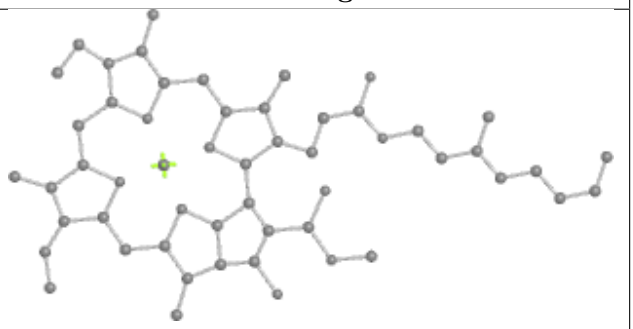
Bond lengths



Bond angles

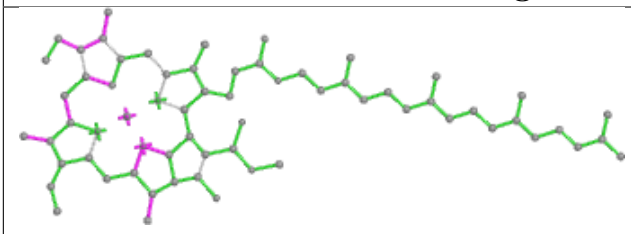


Torsions

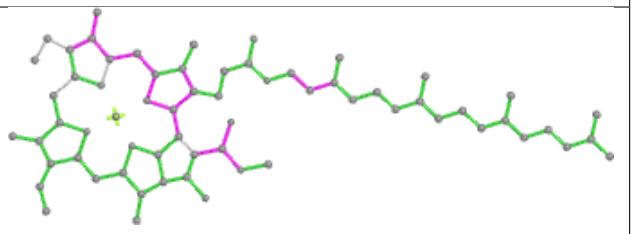


Rings

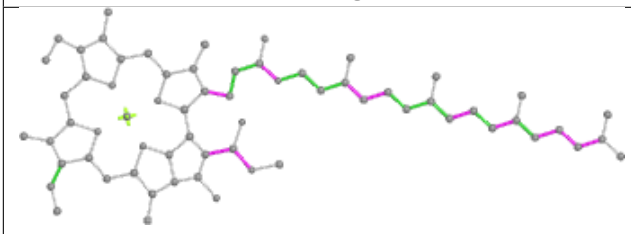
Ligand CLA bA 820



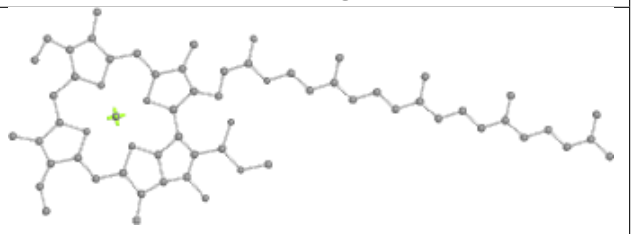
Bond lengths



Bond angles

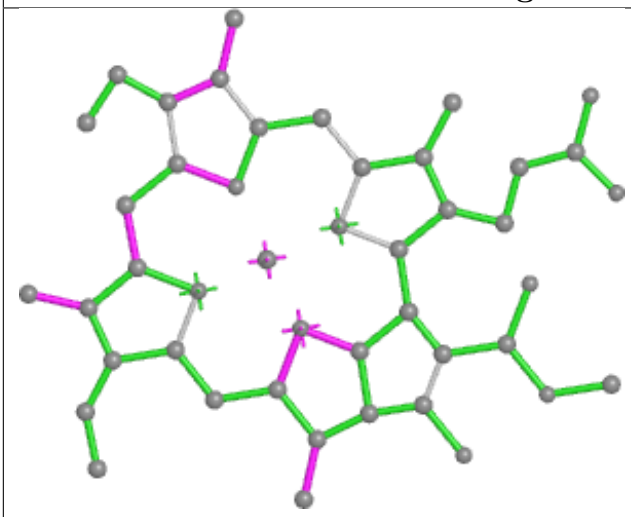


Torsions

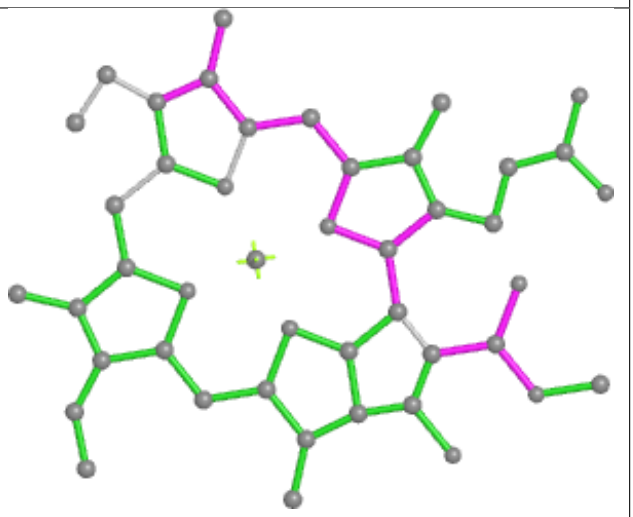


Rings

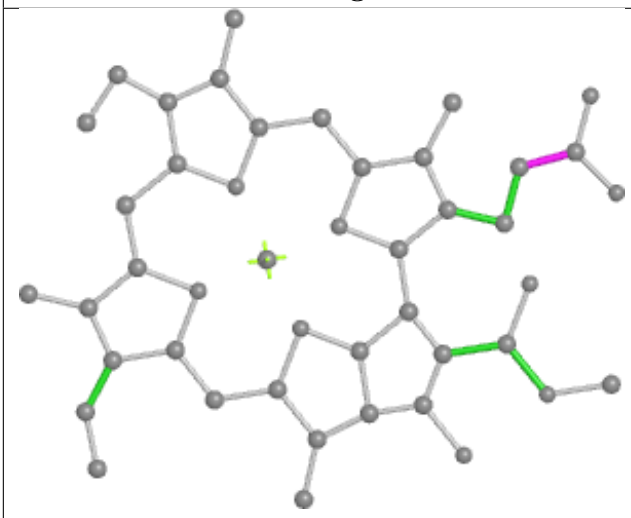
Ligand CLA cB 841



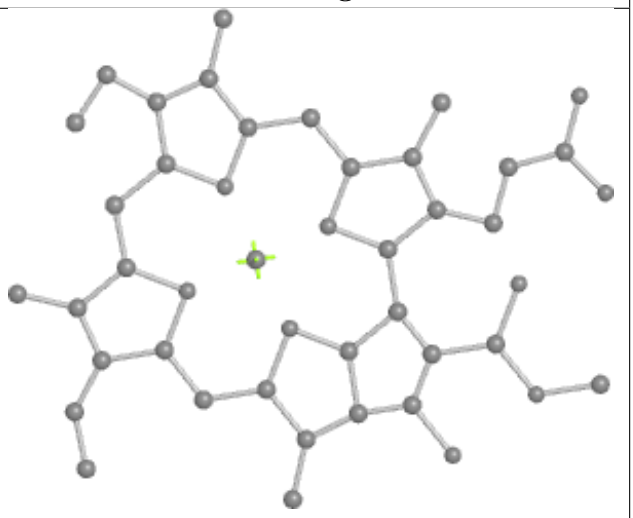
Bond lengths



Bond angles

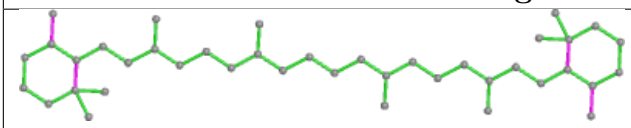


Torsions

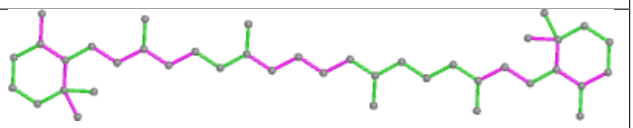


Rings

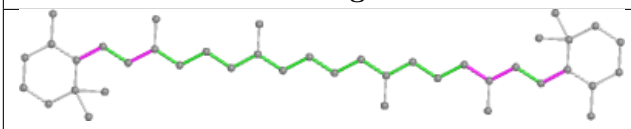
Ligand BCR bL 205



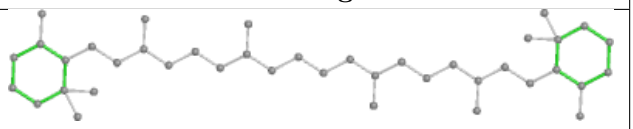
Bond lengths



Bond angles

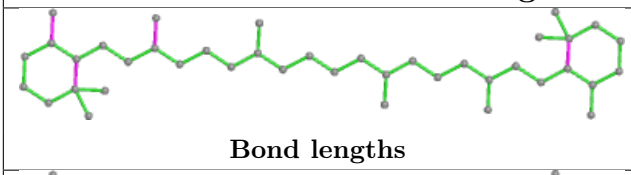


Torsions

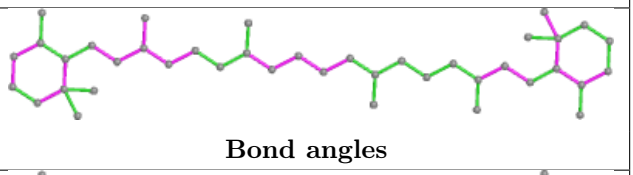


Rings

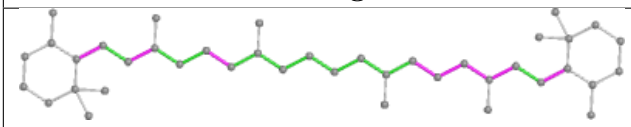
Ligand BCR c1 419



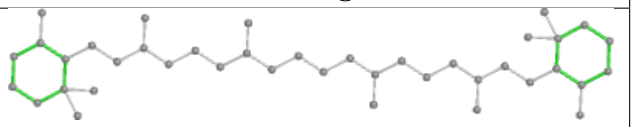
Bond lengths



Bond angles

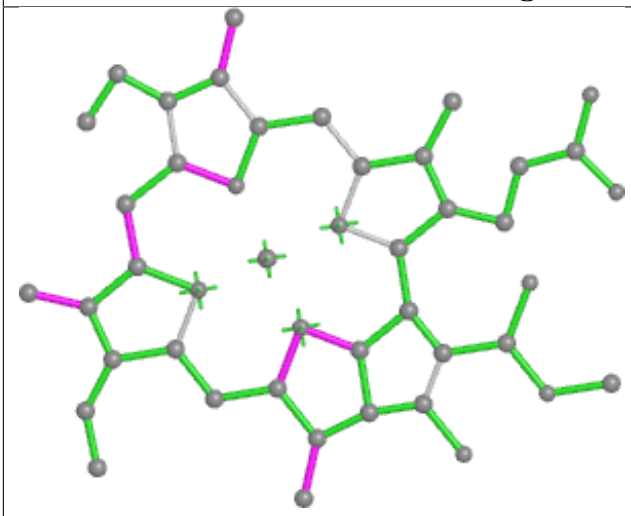


Torsions

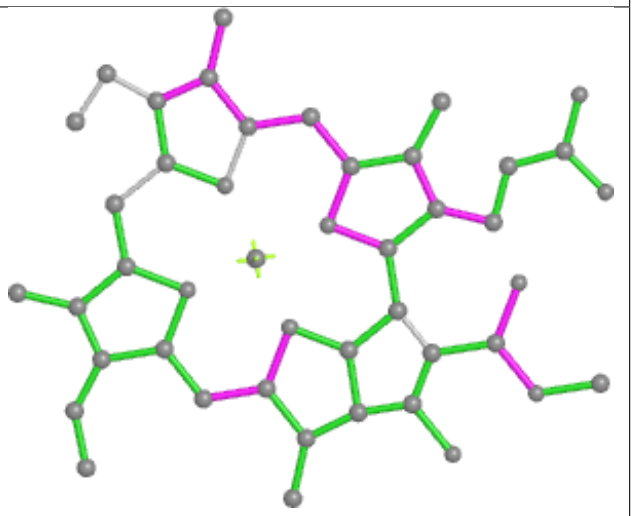


Rings

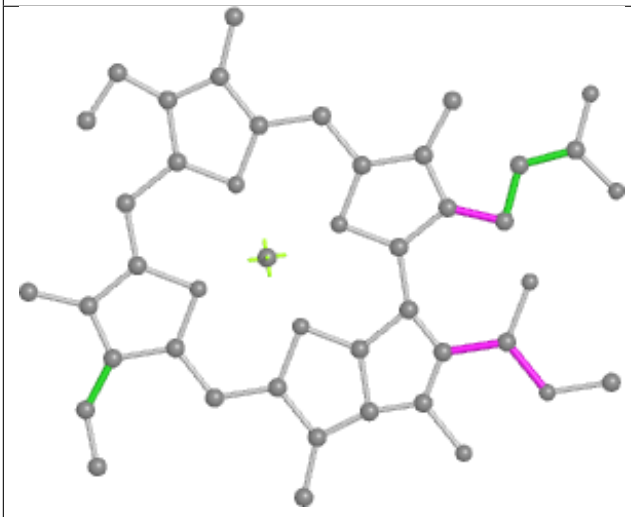
Ligand CLA b4 411



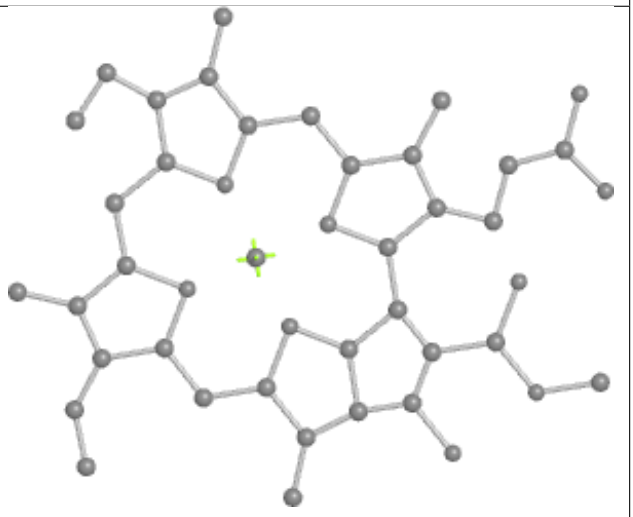
Bond lengths



Bond angles

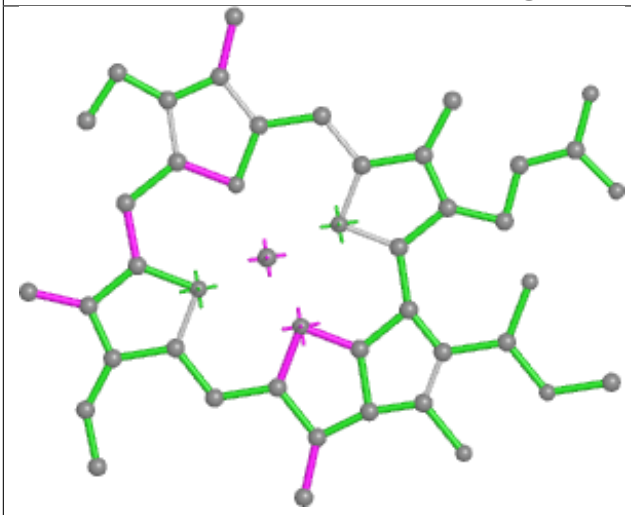


Torsions

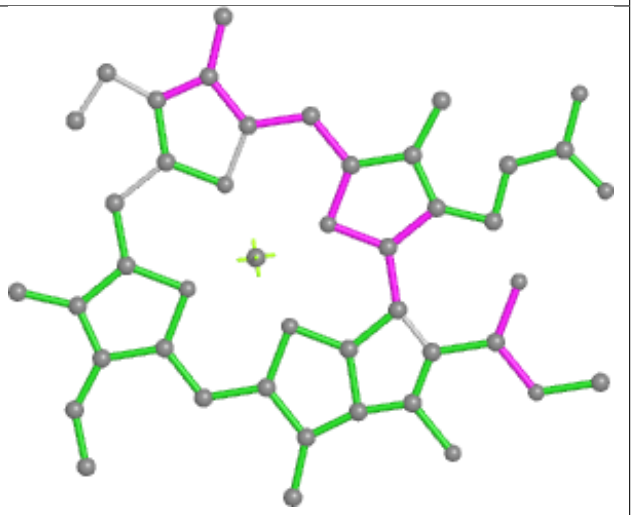


Rings

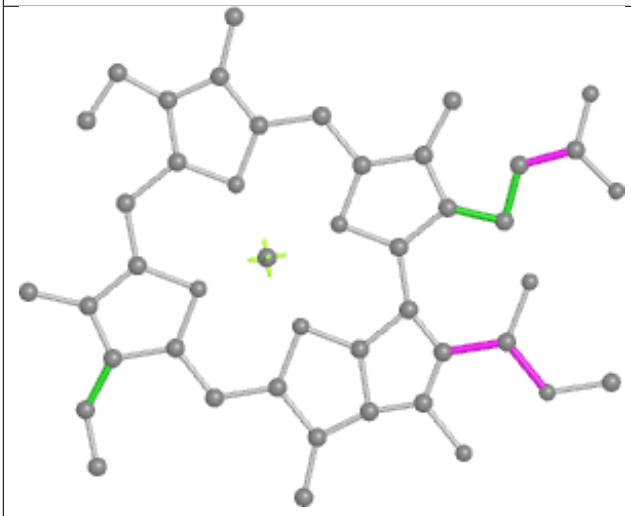
Ligand CLA c3 407



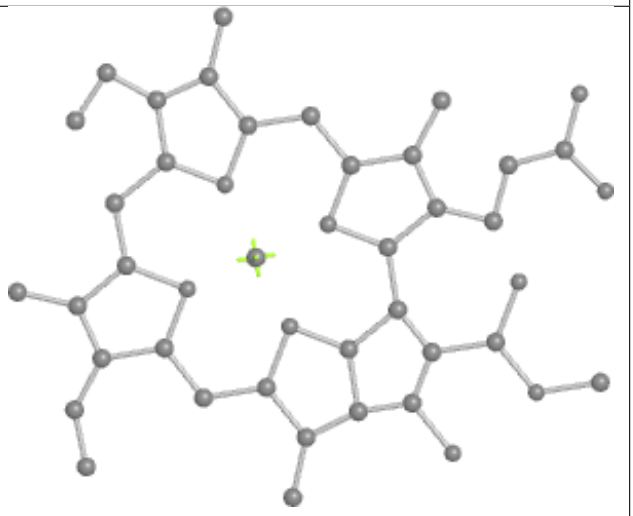
Bond lengths



Bond angles

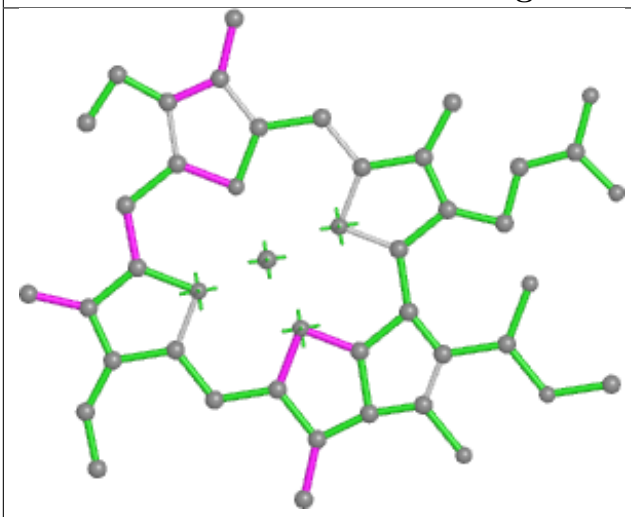


Torsions

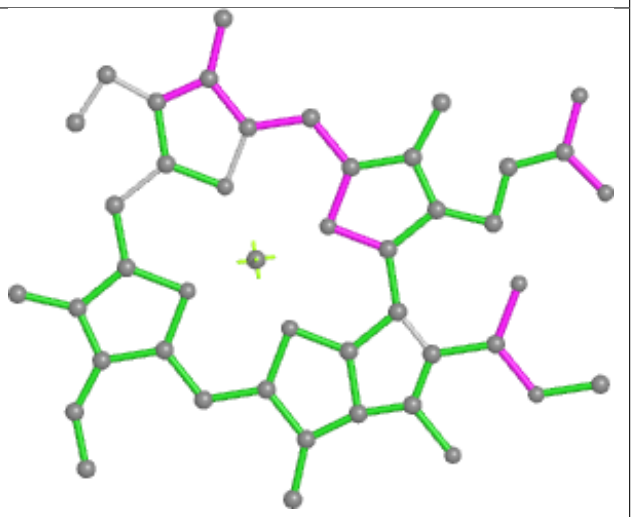


Rings

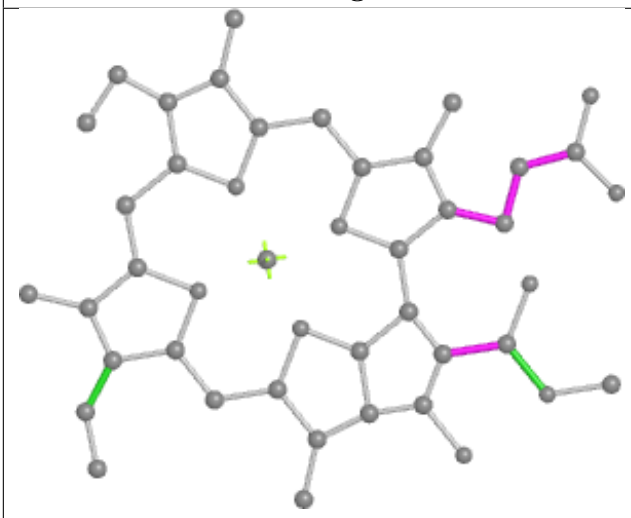
Ligand CLA cA 837



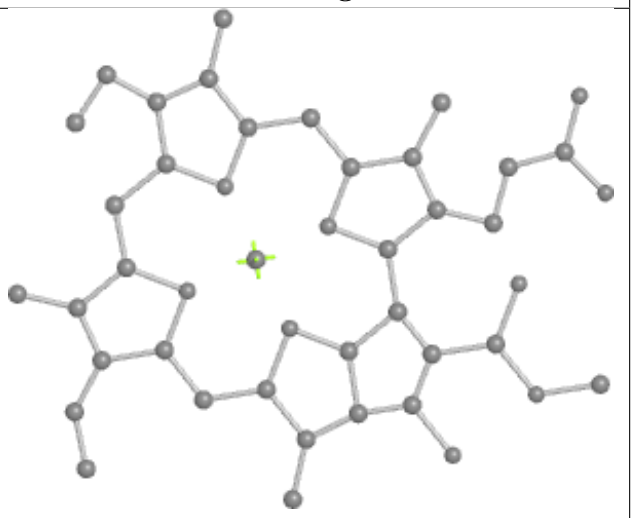
Bond lengths



Bond angles

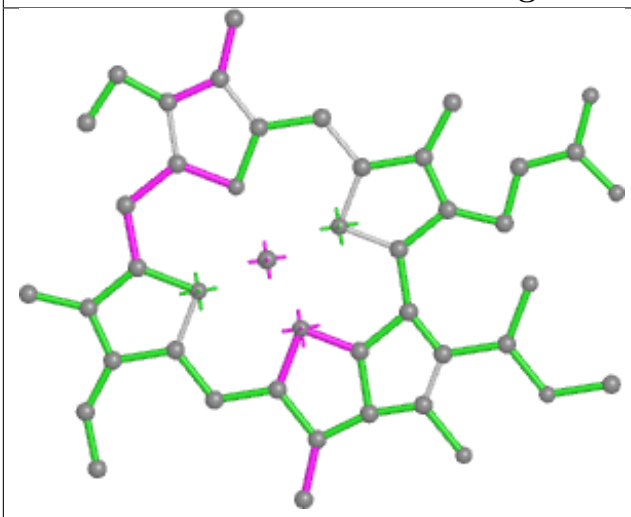


Torsions

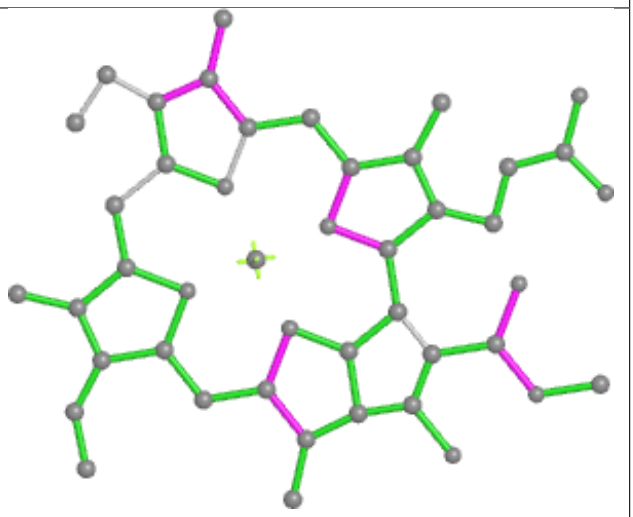


Rings

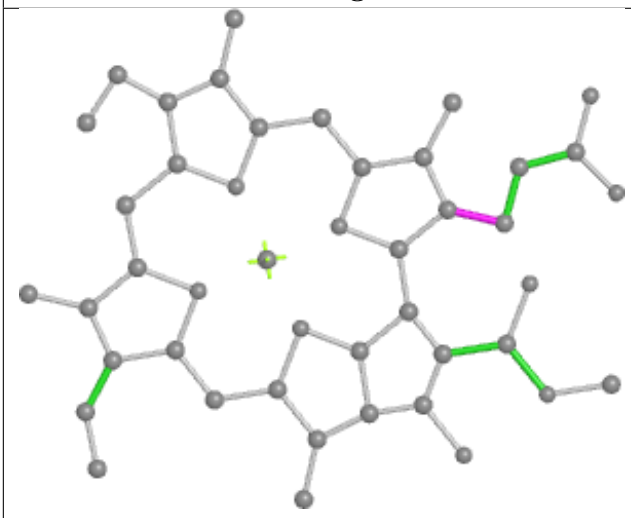
Ligand CLA b3 413



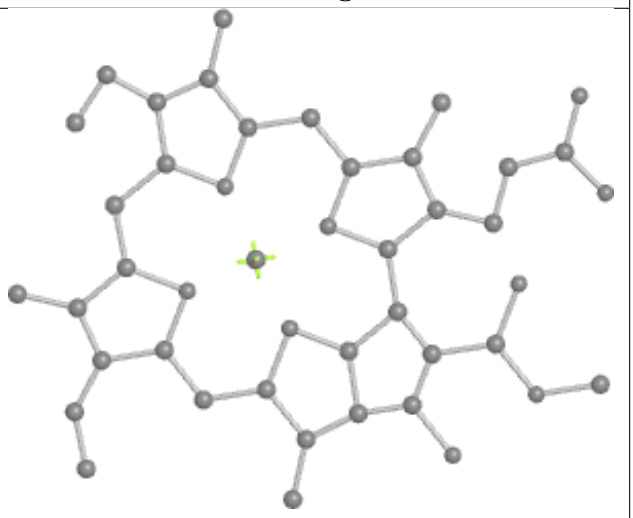
Bond lengths



Bond angles

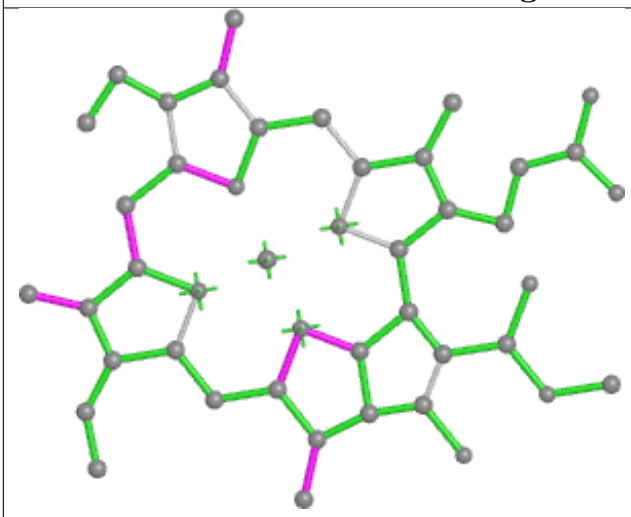


Torsions

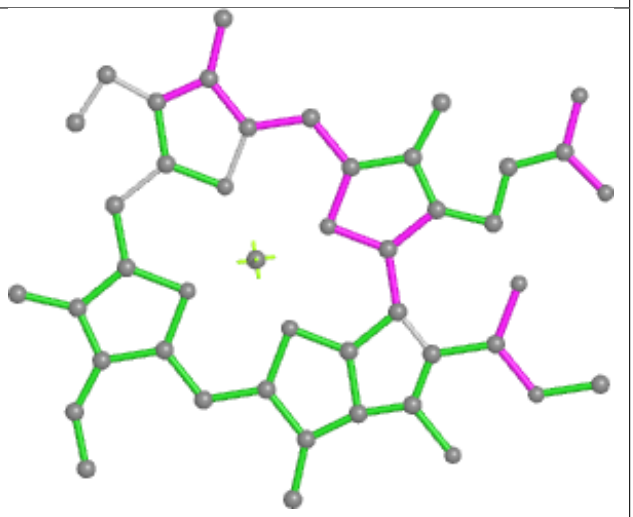


Rings

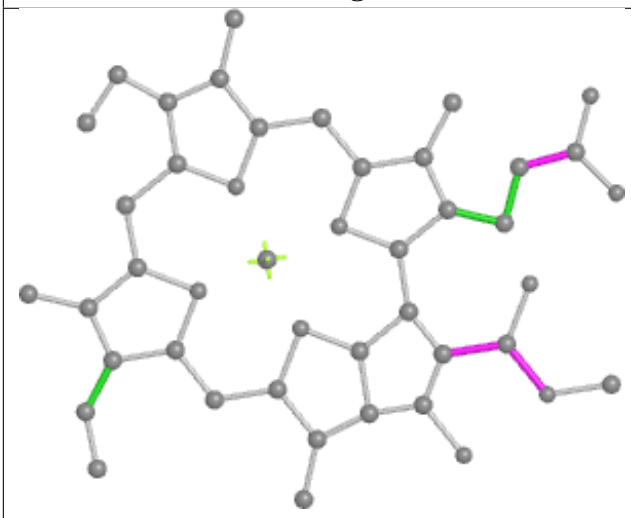
Ligand CLA a1 406



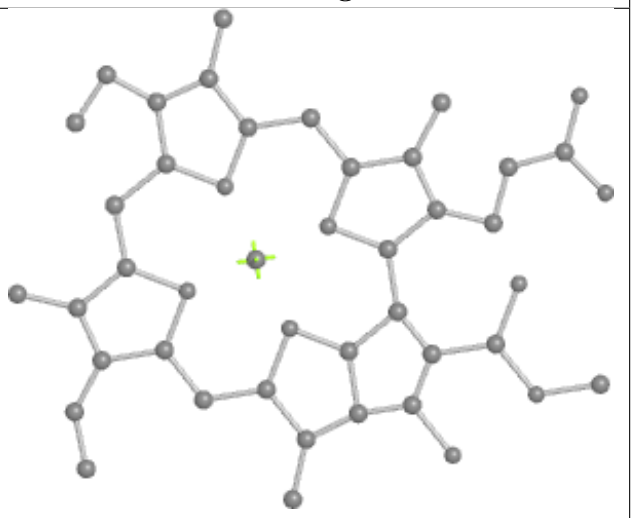
Bond lengths



Bond angles

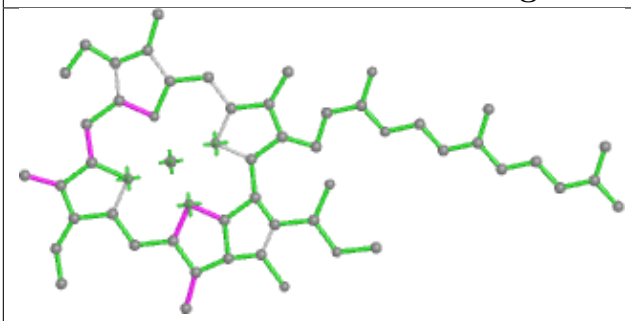


Torsions

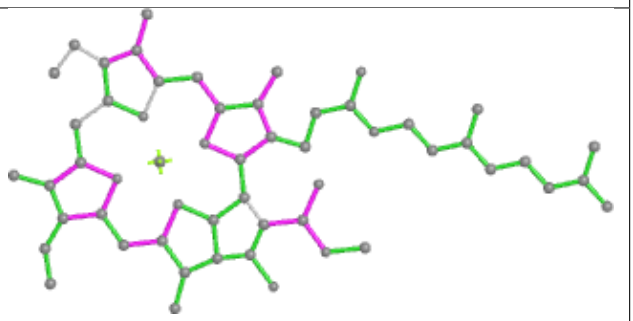


Rings

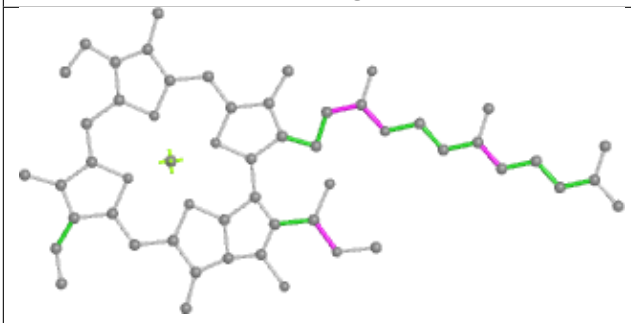
Ligand CLA a5 417



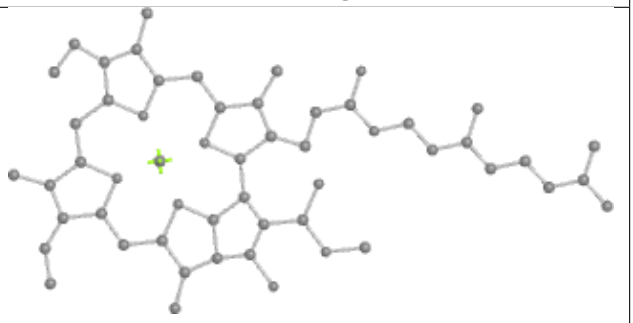
Bond lengths



Bond angles

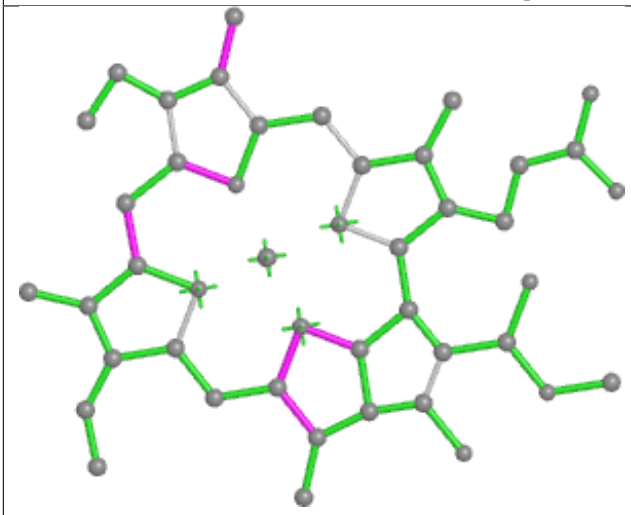


Torsions

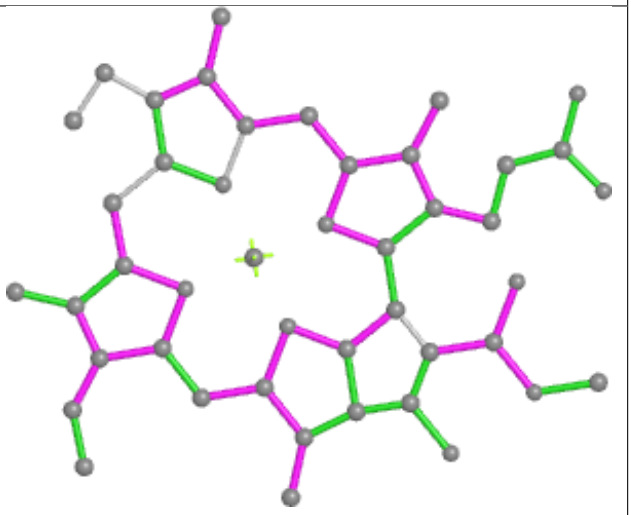


Rings

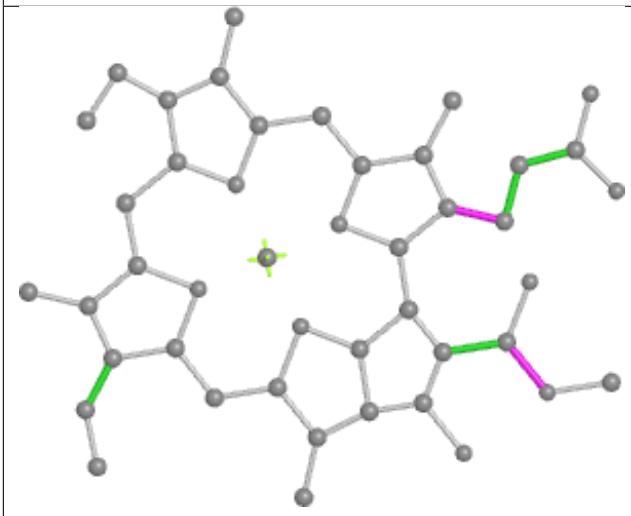
Ligand CLA b6 406



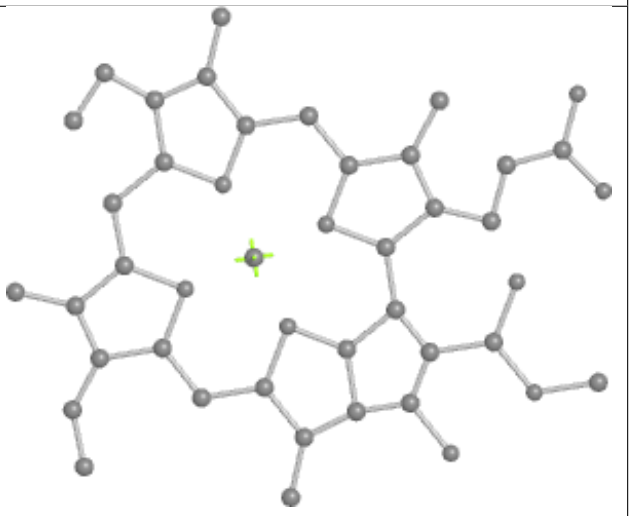
Bond lengths



Bond angles

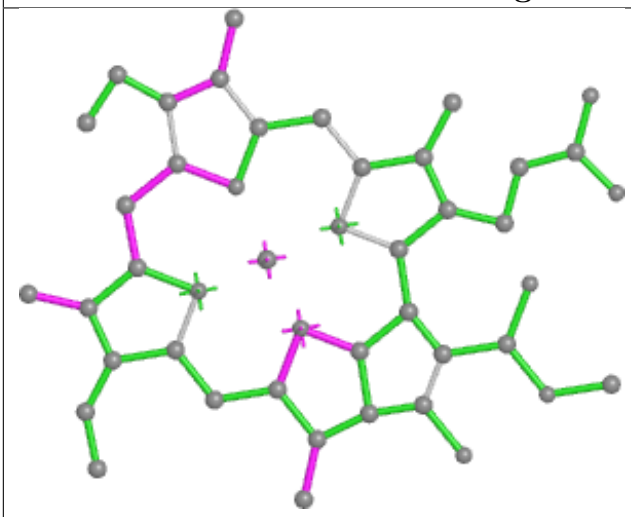


Torsions

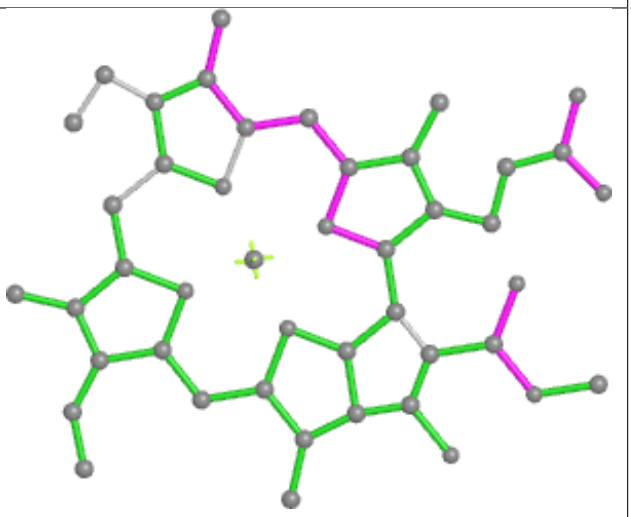


Rings

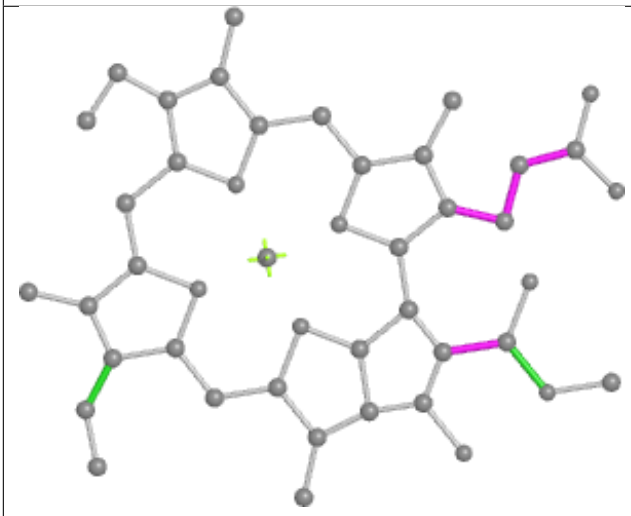
Ligand CLA bB 831



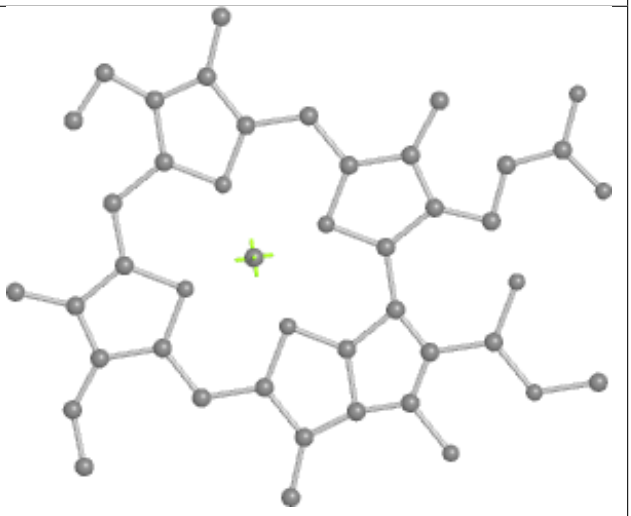
Bond lengths



Bond angles

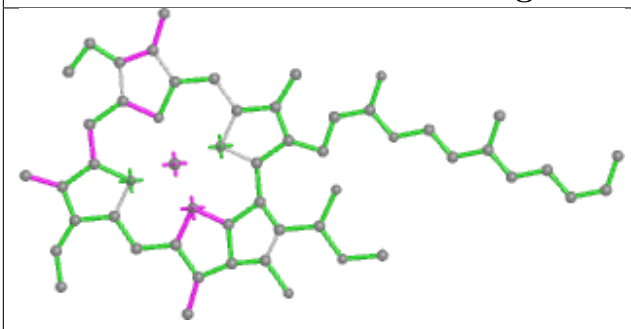


Torsions

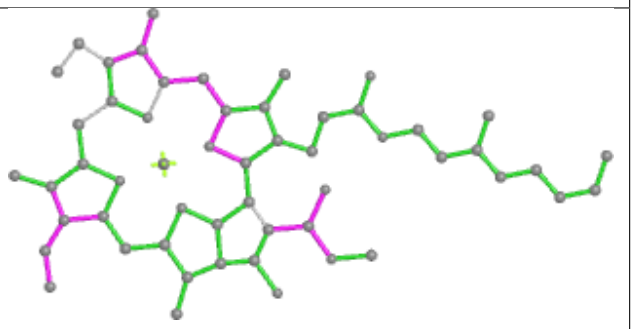


Rings

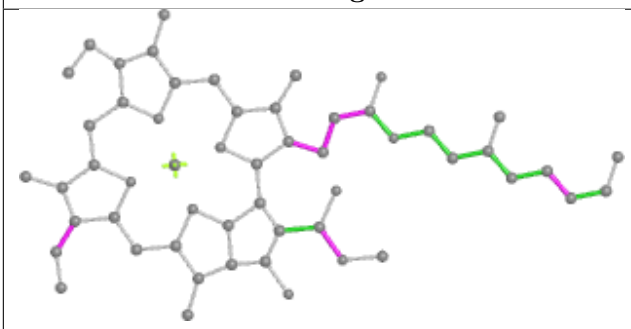
Ligand CLA cA 819



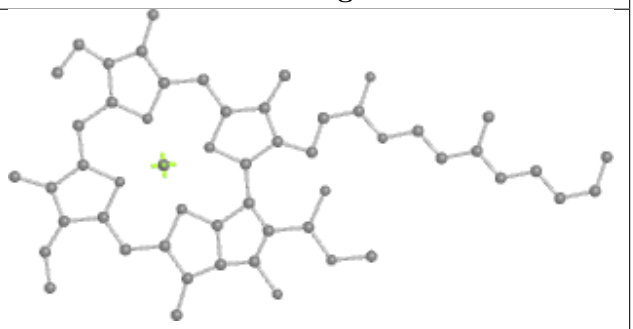
Bond lengths



Bond angles

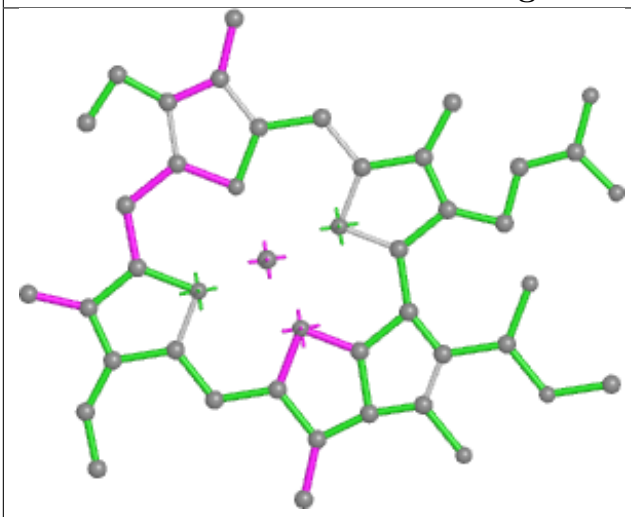


Torsions

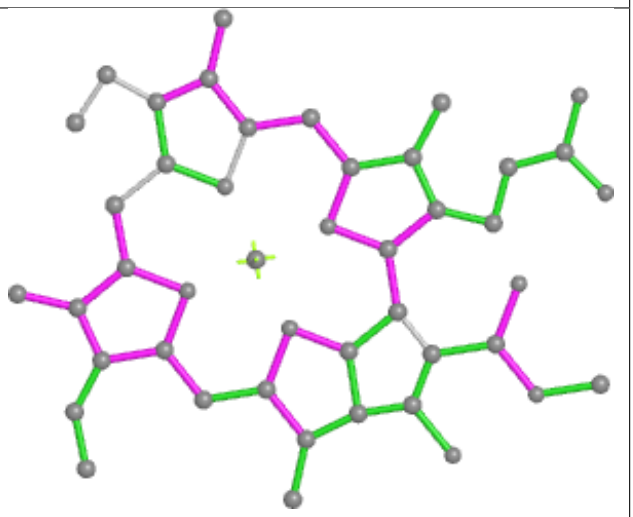


Rings

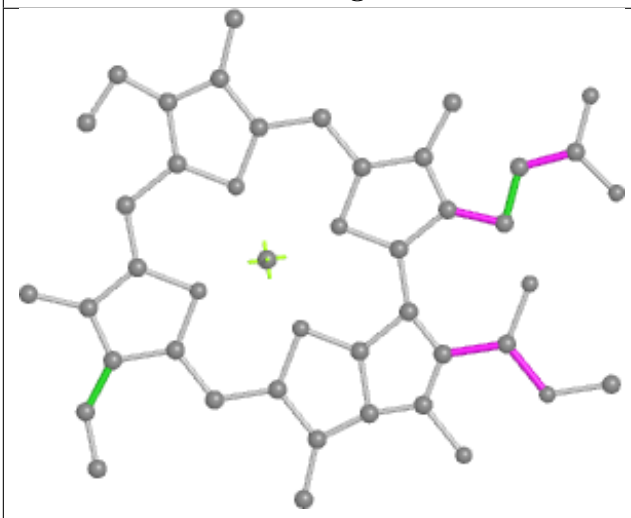
Ligand CLA b2 413



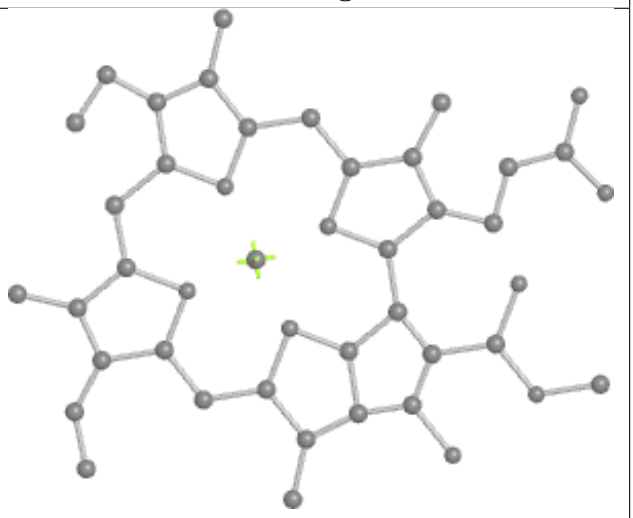
Bond lengths



Bond angles

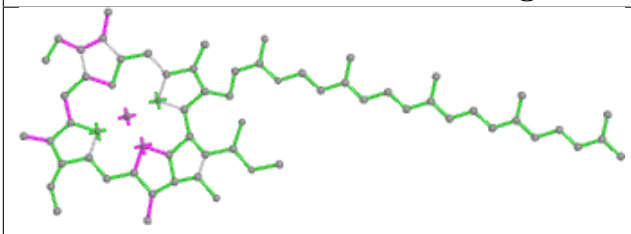


Torsions

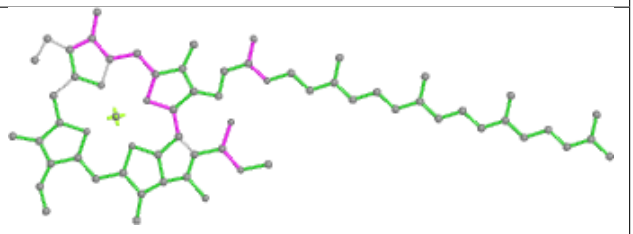


Rings

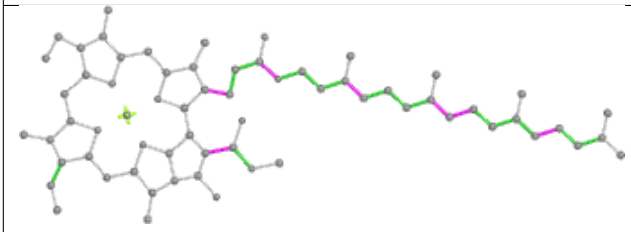
Ligand CLA cL 201



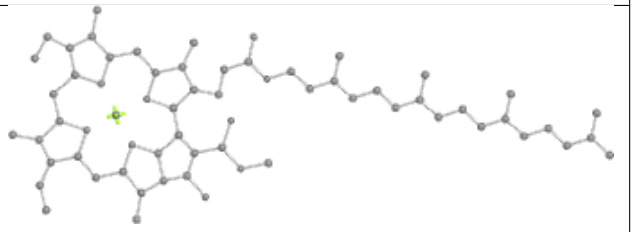
Bond lengths



Bond angles

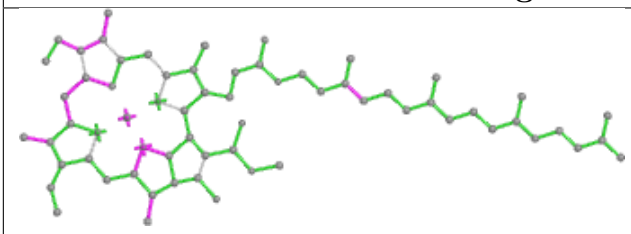


Torsions

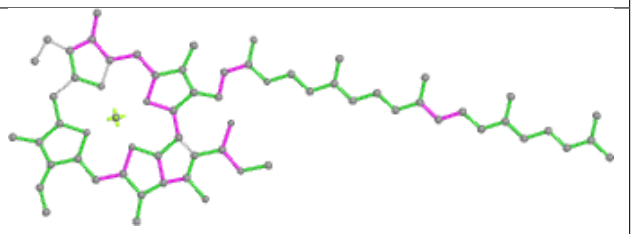


Rings

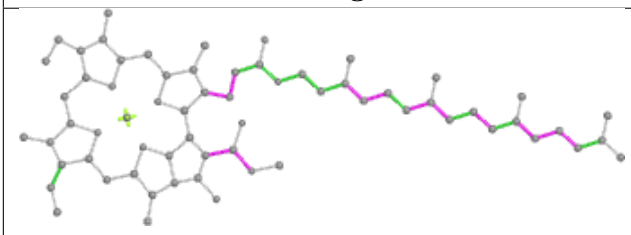
Ligand CLA cA 802



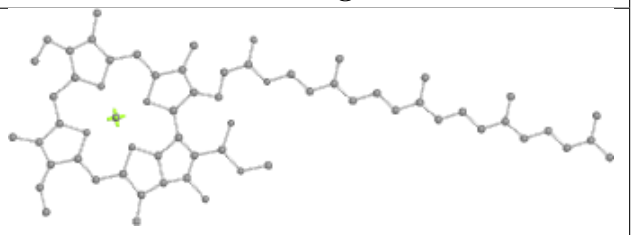
Bond lengths



Bond angles

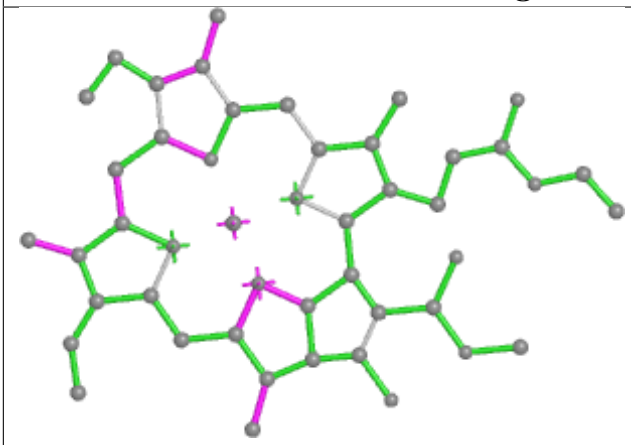


Torsions

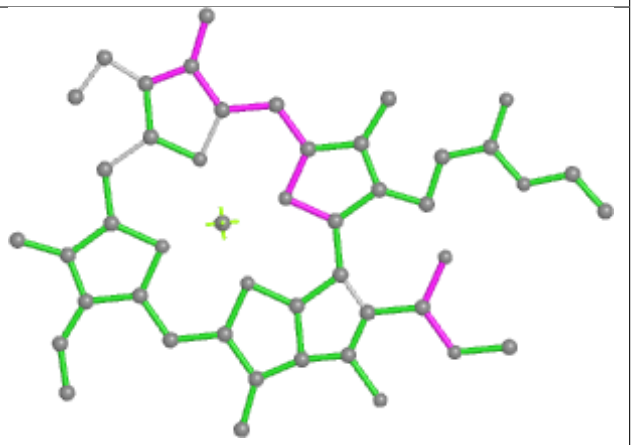


Rings

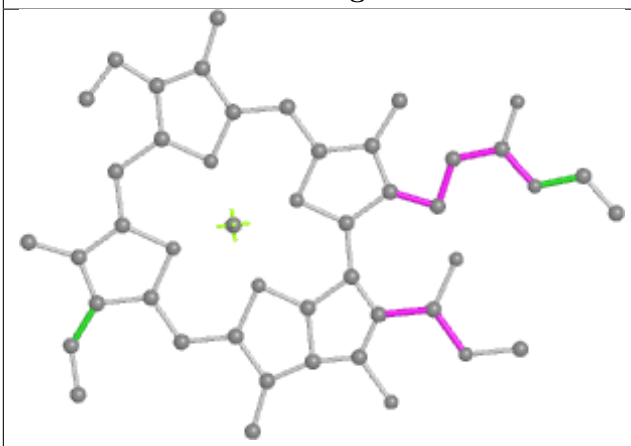
Ligand CLA bB 821



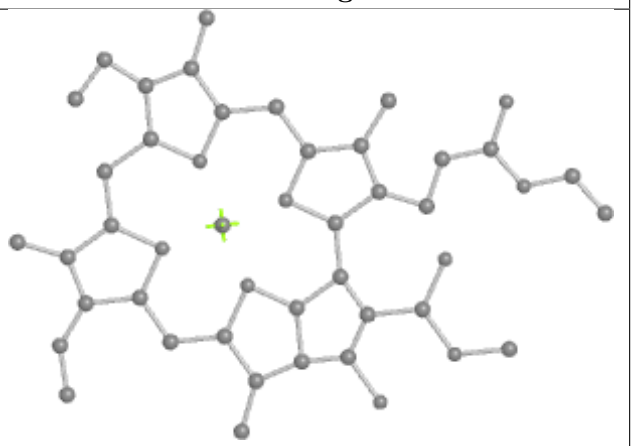
Bond lengths



Bond angles

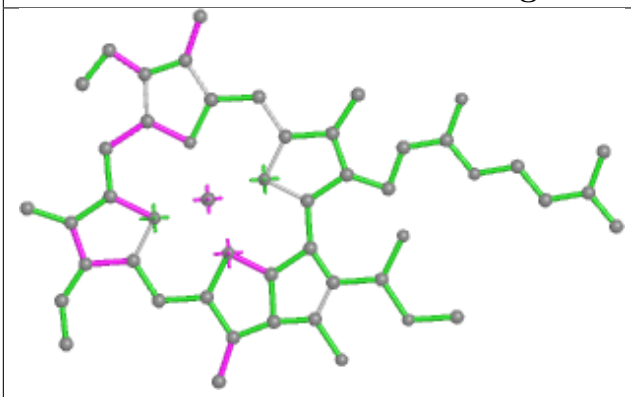


Torsions

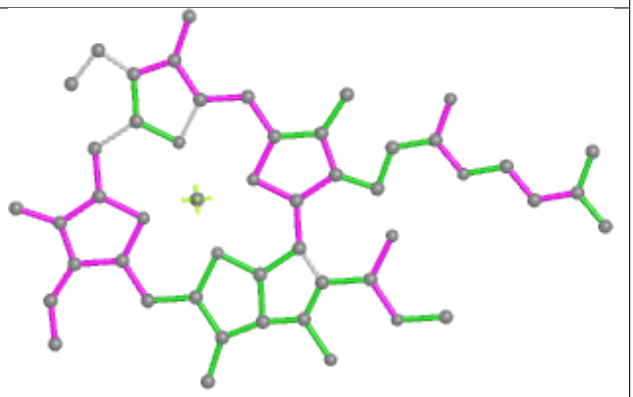


Rings

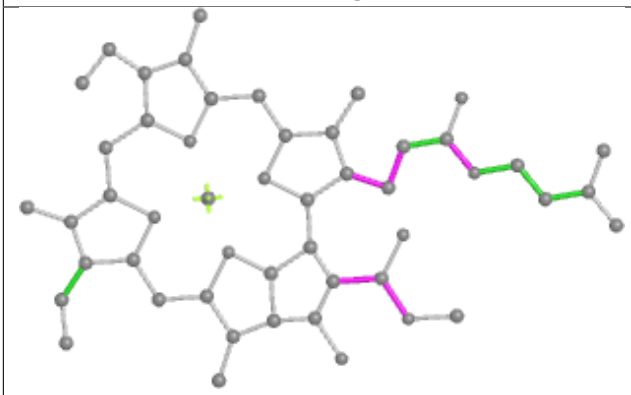
Ligand CLA a3 416



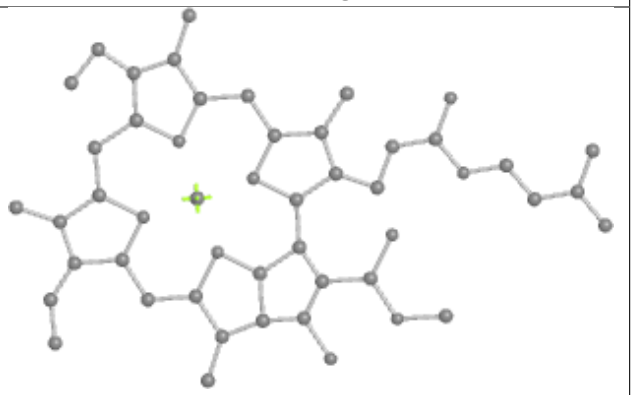
Bond lengths



Bond angles

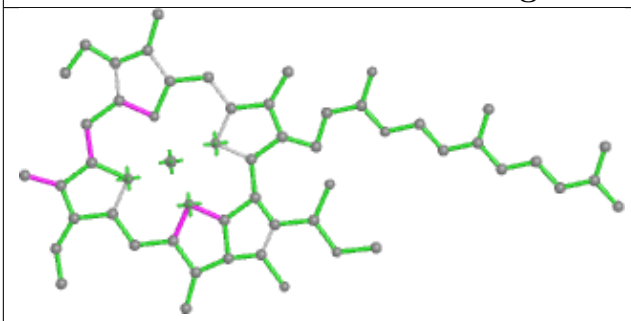


Torsions

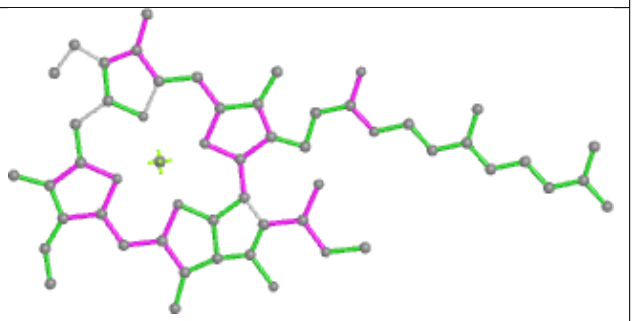


Rings

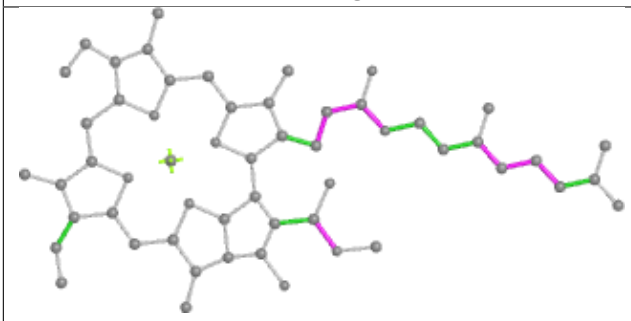
Ligand CLA a3 417



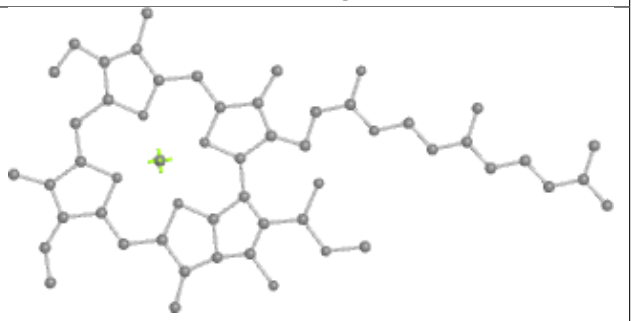
Bond lengths



Bond angles

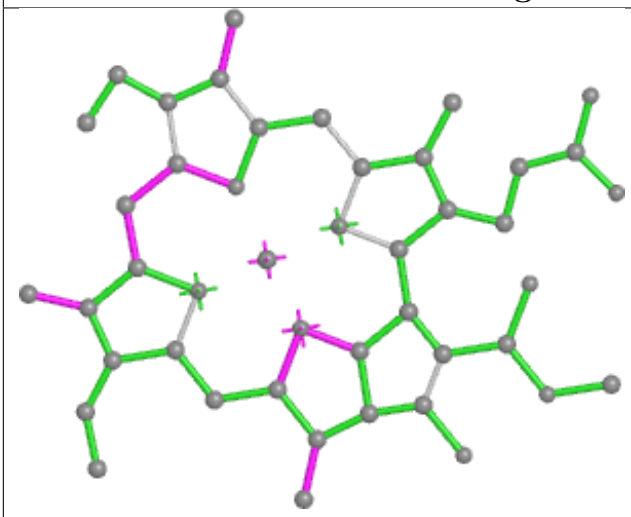


Torsions

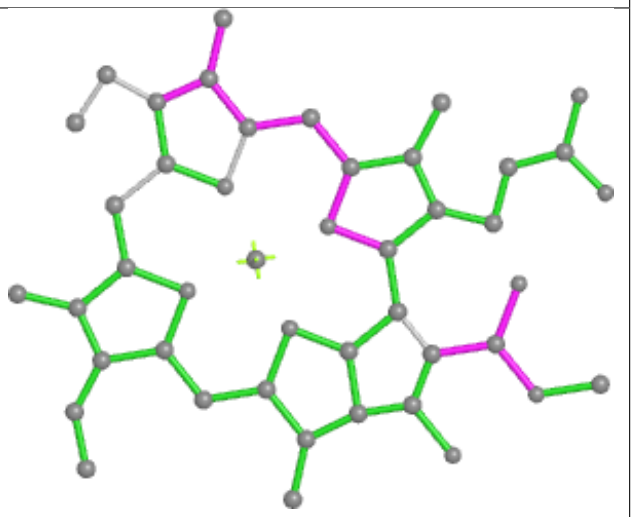


Rings

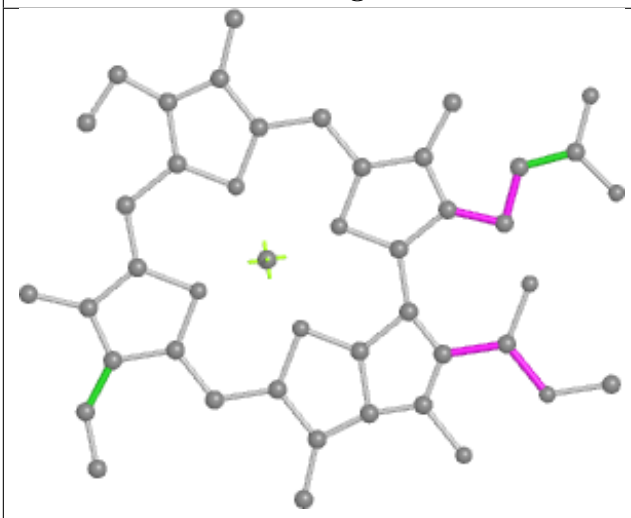
Ligand CLA bB 816



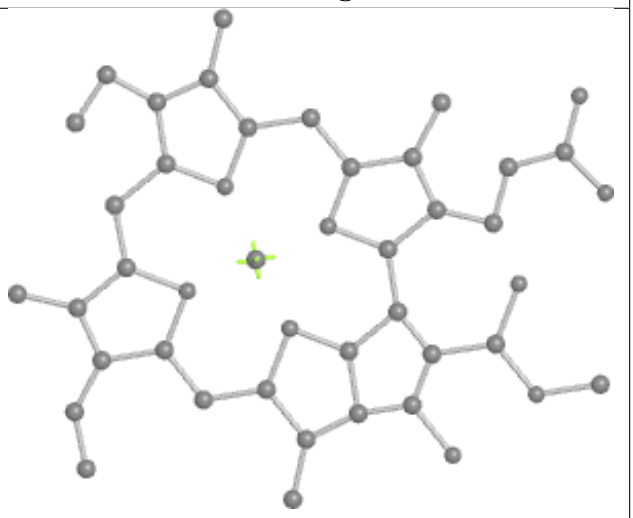
Bond lengths



Bond angles

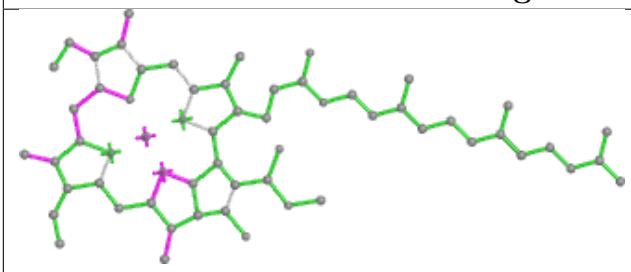


Torsions

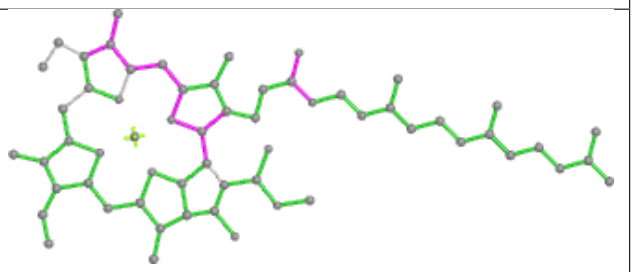


Rings

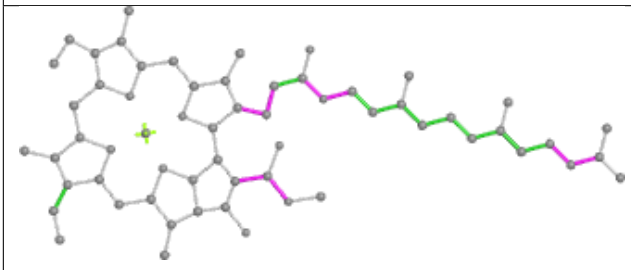
Ligand CLA bA 814



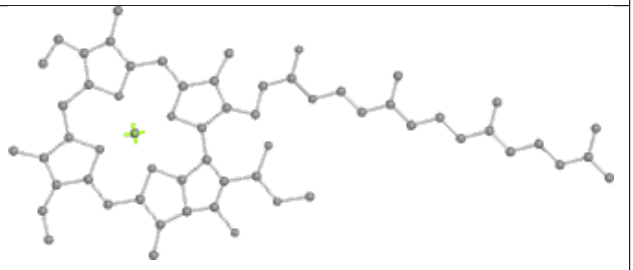
Bond lengths



Bond angles

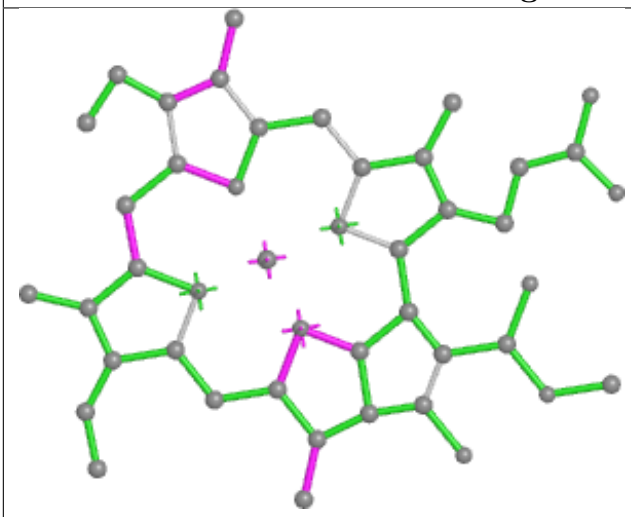


Torsions

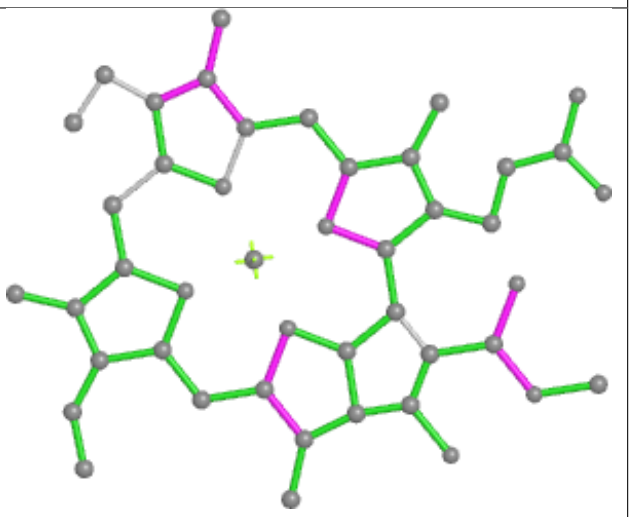


Rings

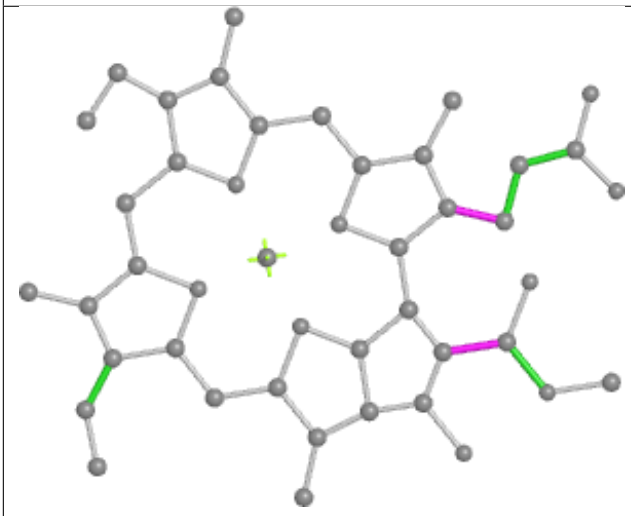
Ligand CLA c4 413



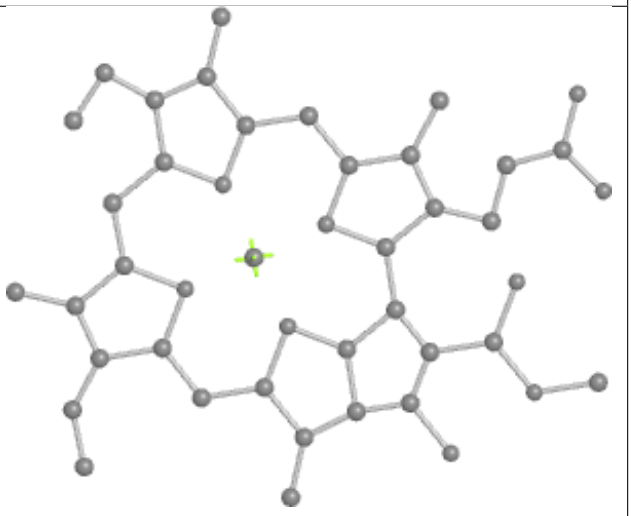
Bond lengths



Bond angles

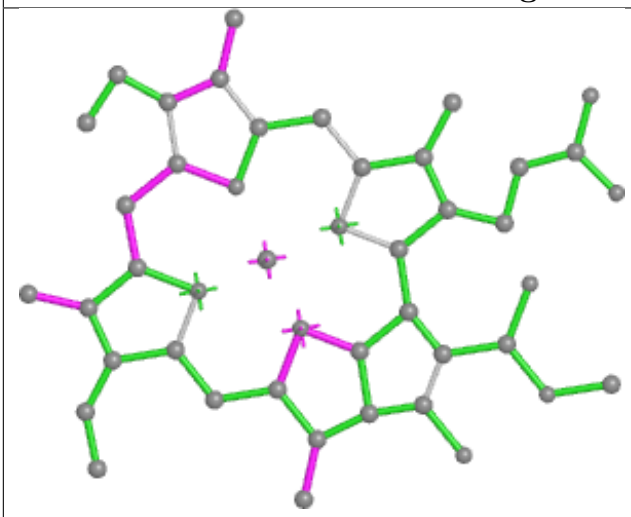


Torsions

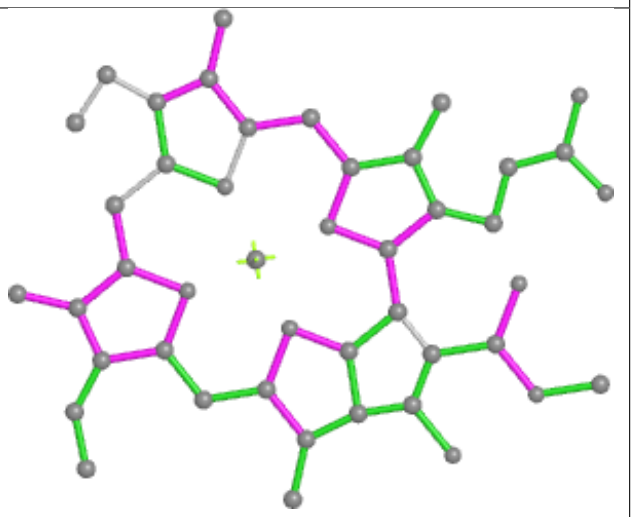


Rings

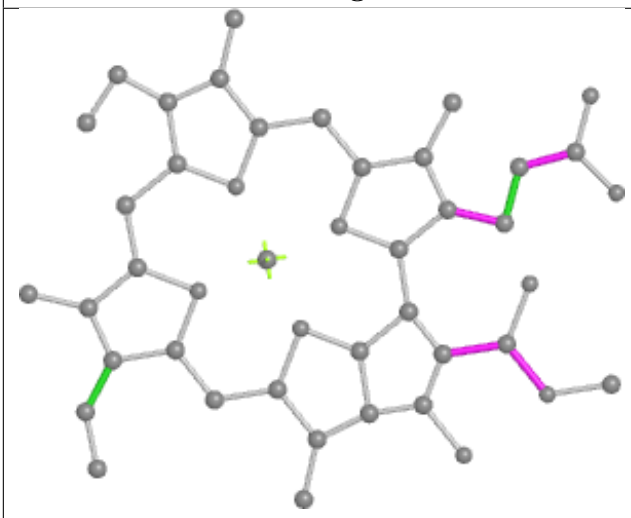
Ligand CLA a4 412



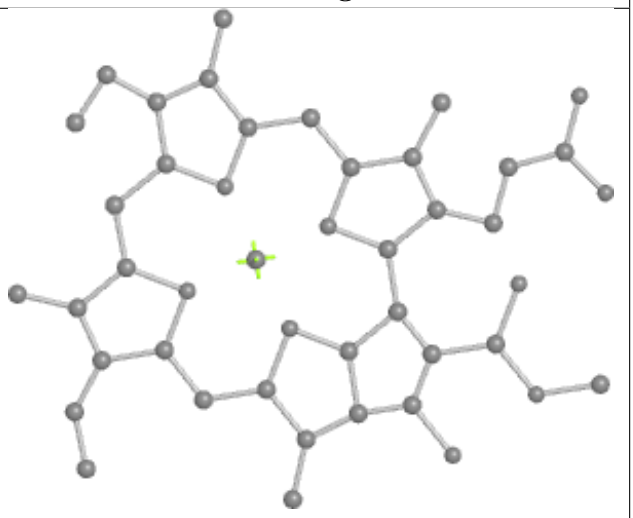
Bond lengths



Bond angles

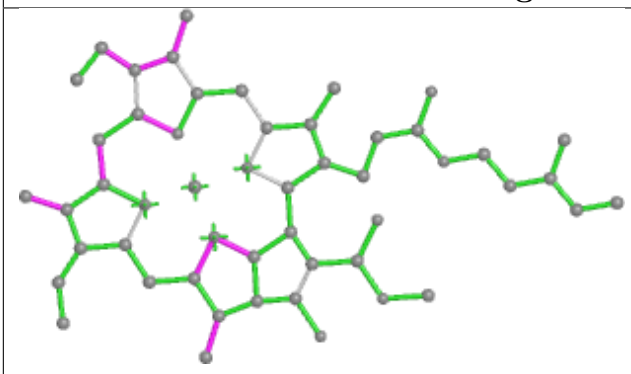


Torsions

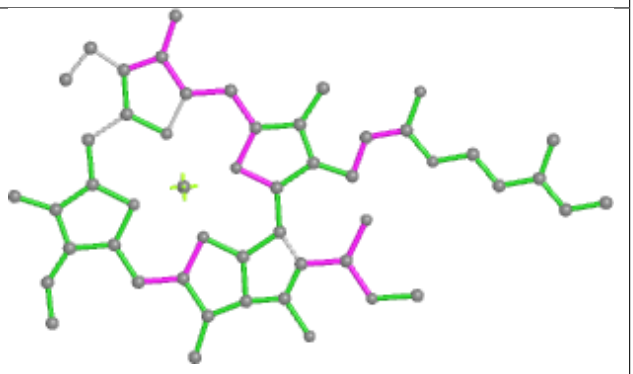


Rings

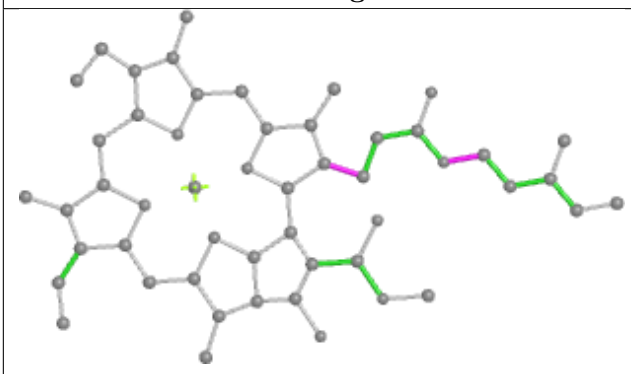
Ligand CLA cA 808



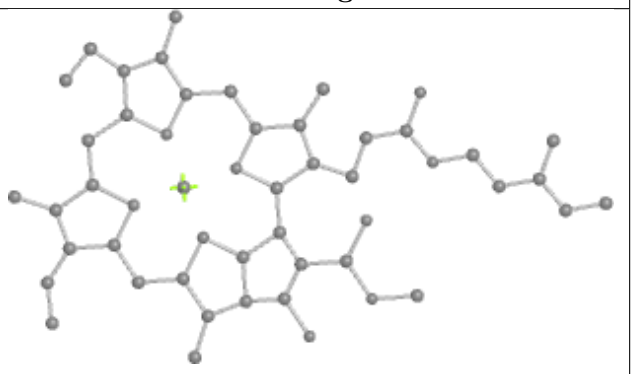
Bond lengths



Bond angles

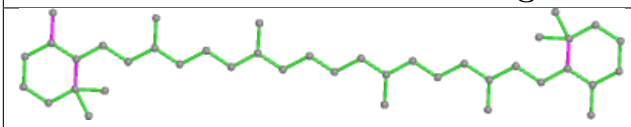


Torsions

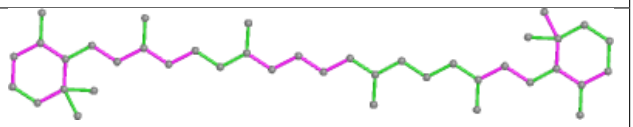


Rings

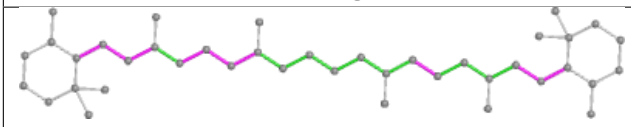
Ligand BCR a4 401



Bond lengths



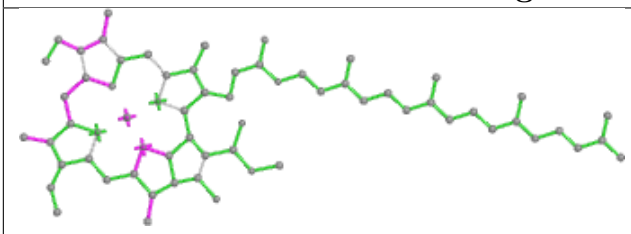
Bond angles



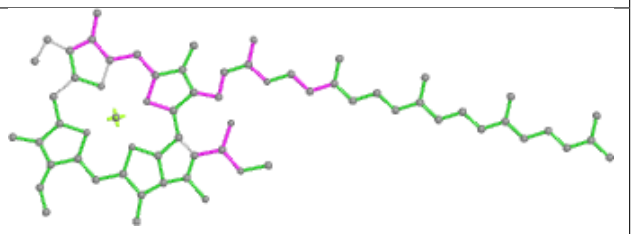
Torsions

Rings

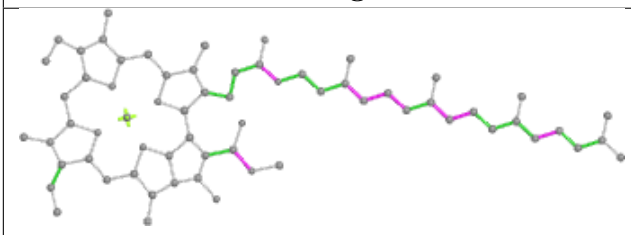
Ligand CLA aB 809



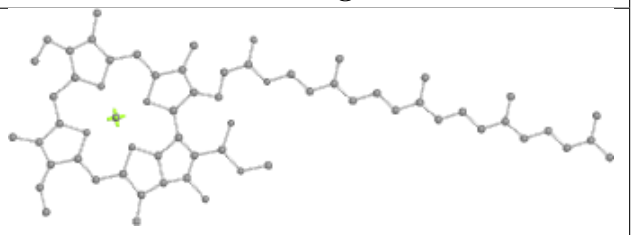
Bond lengths



Bond angles

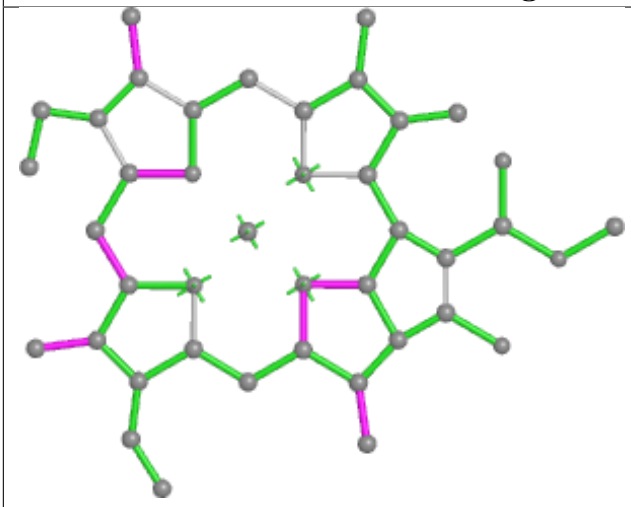


Torsions

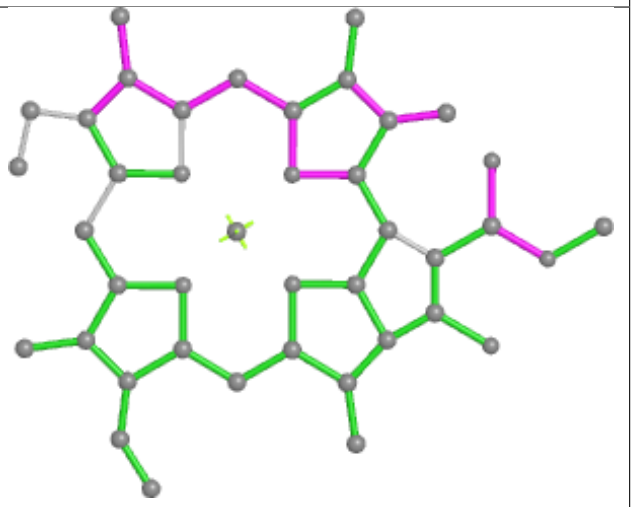


Rings

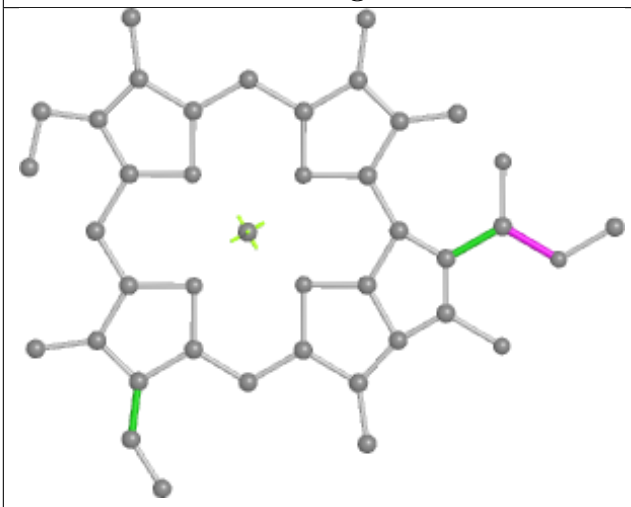
Ligand CLA c1 414



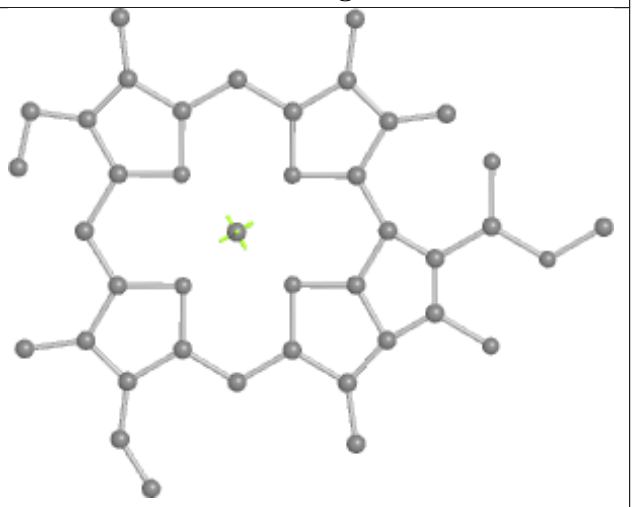
Bond lengths



Bond angles

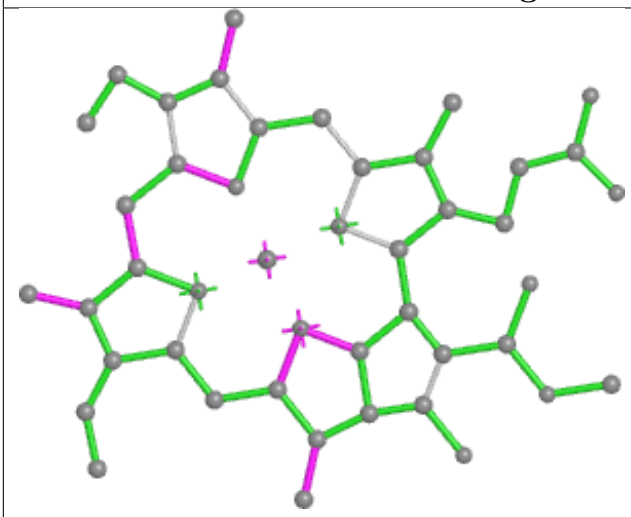


Torsions

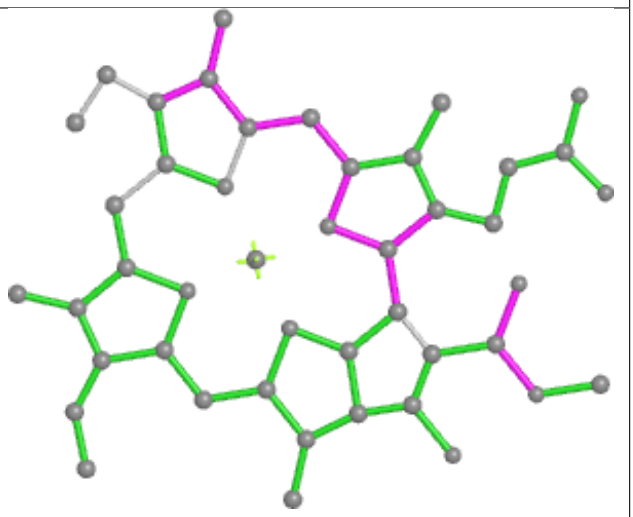


Rings

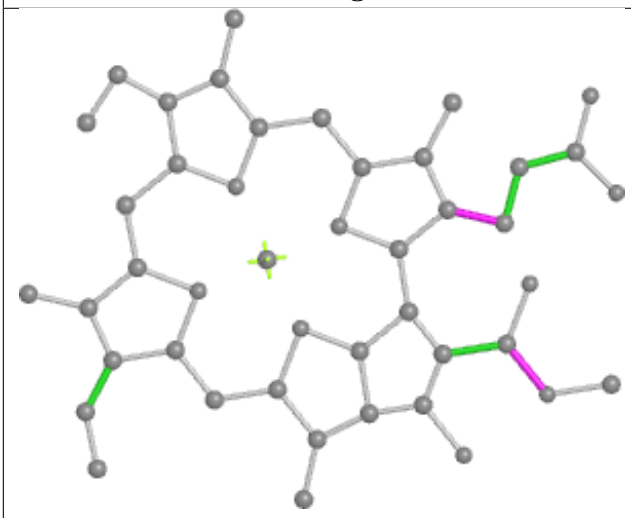
Ligand CLA a1 410



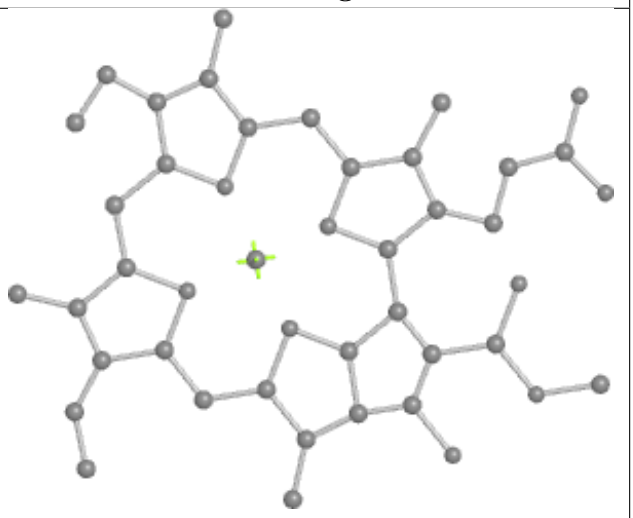
Bond lengths



Bond angles

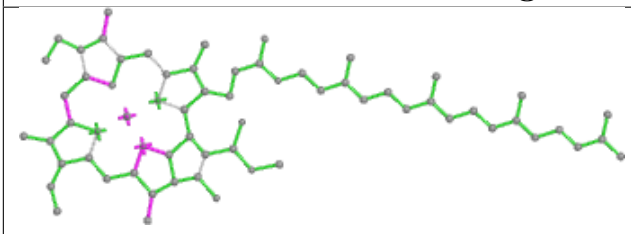


Torsions

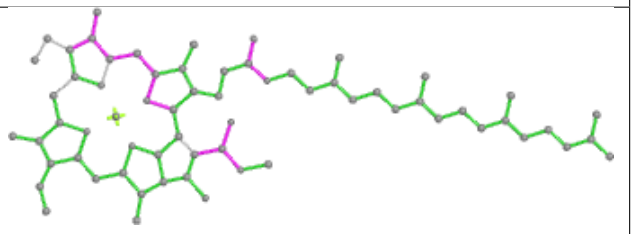


Rings

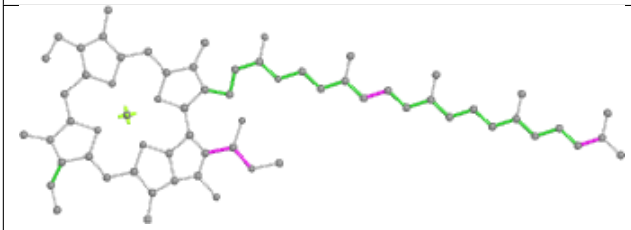
Ligand CLA b6 410



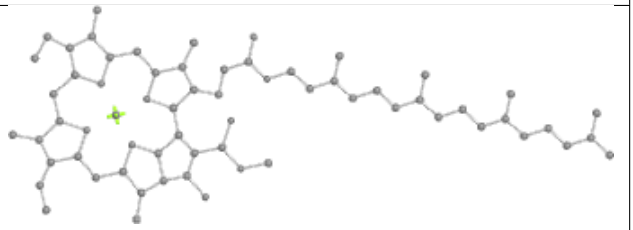
Bond lengths



Bond angles

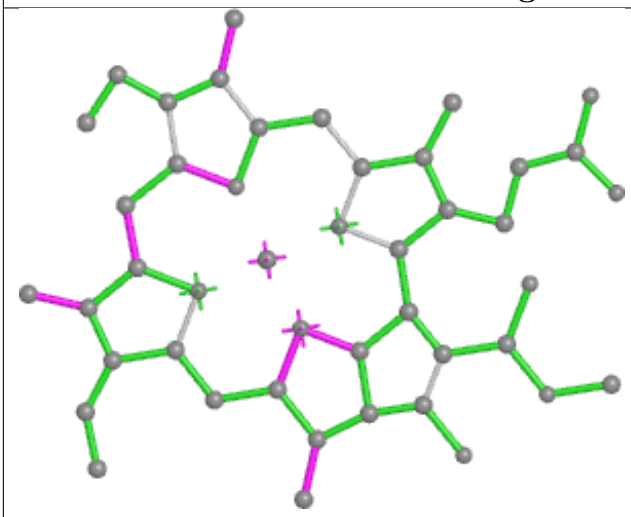


Torsions

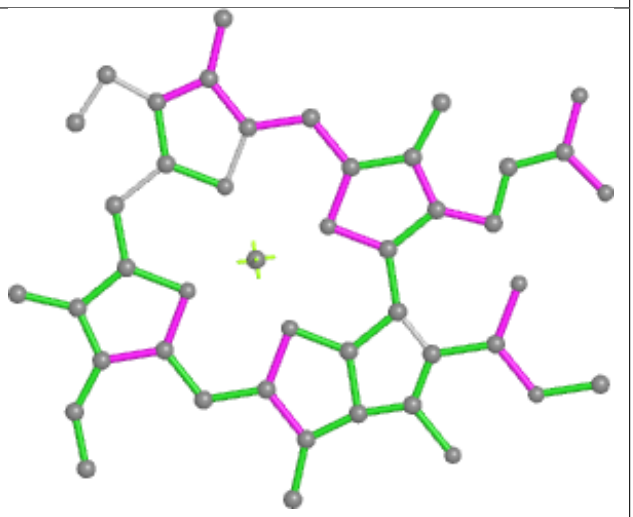


Rings

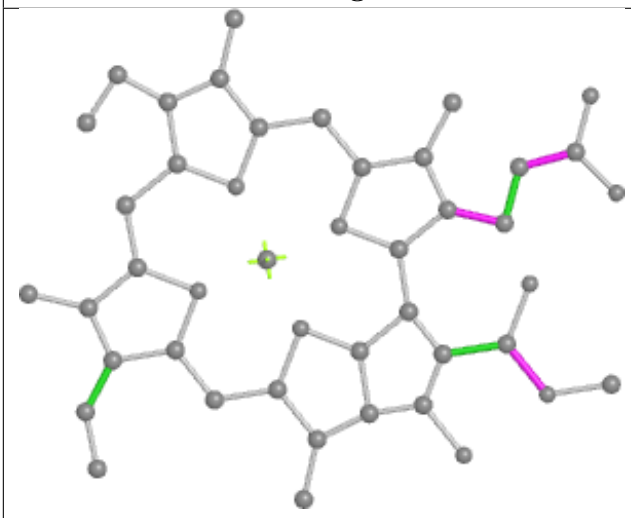
Ligand CLA b3 408



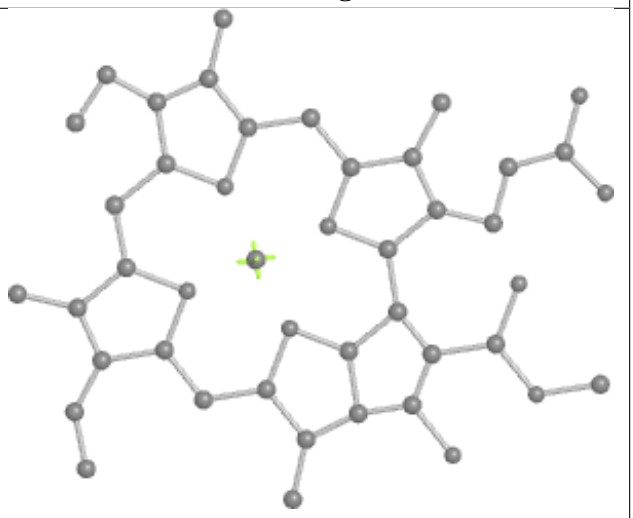
Bond lengths



Bond angles

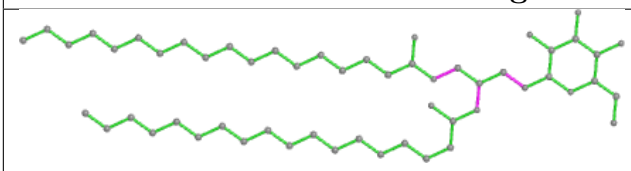


Torsions

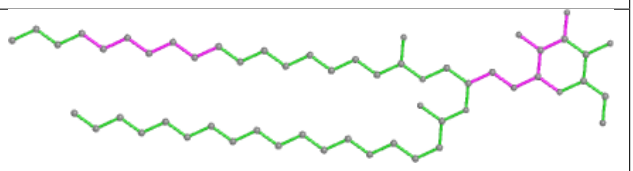


Rings

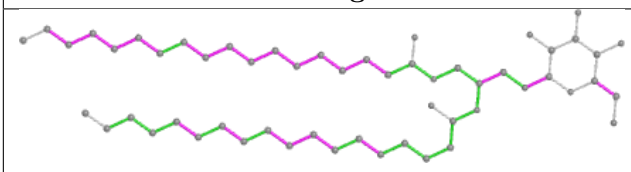
Ligand LMG bB 851



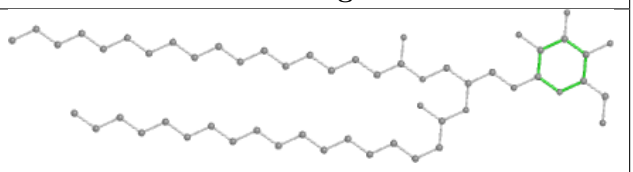
Bond lengths



Bond angles

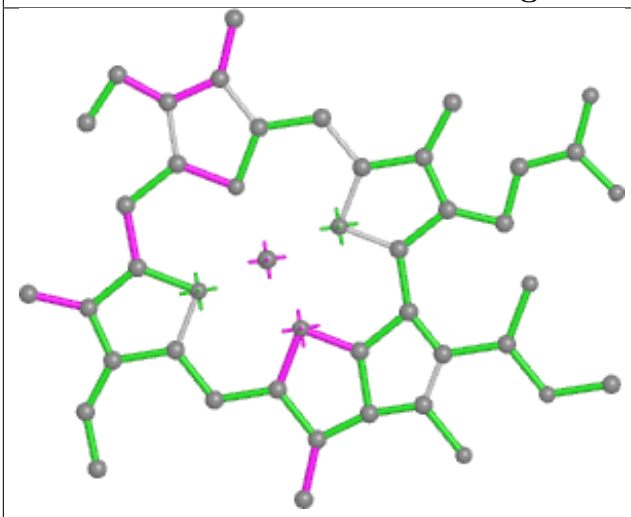


Torsions

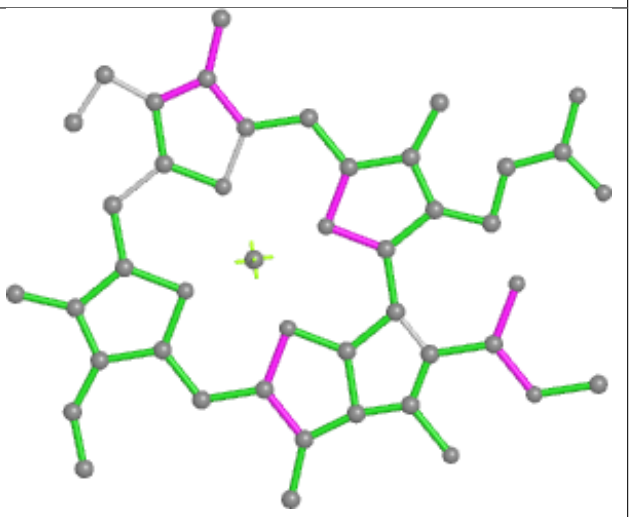


Rings

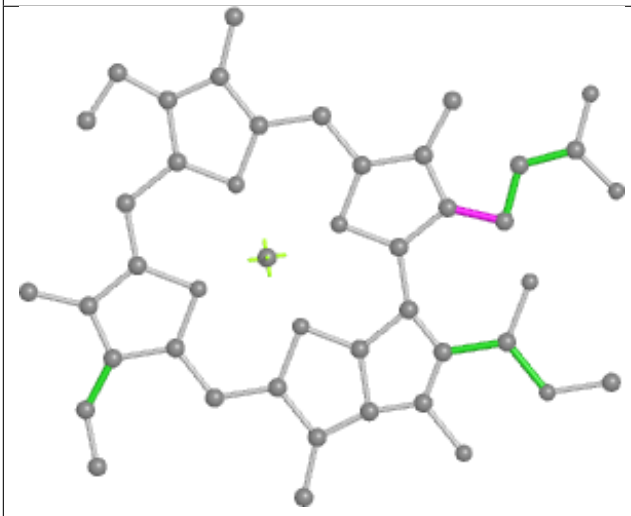
Ligand CLA c5 413



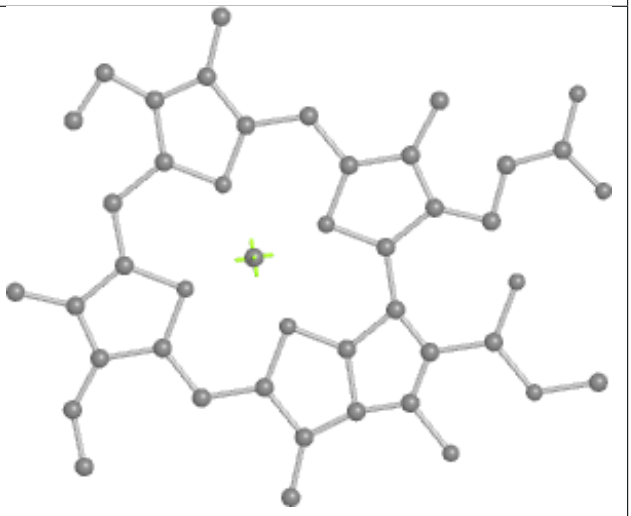
Bond lengths



Bond angles

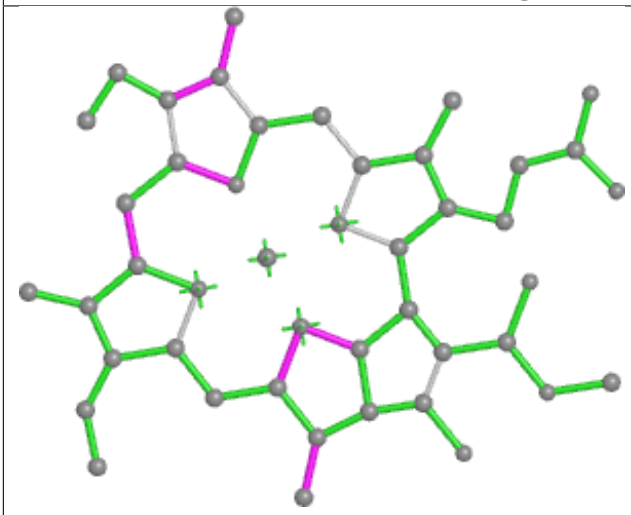


Torsions

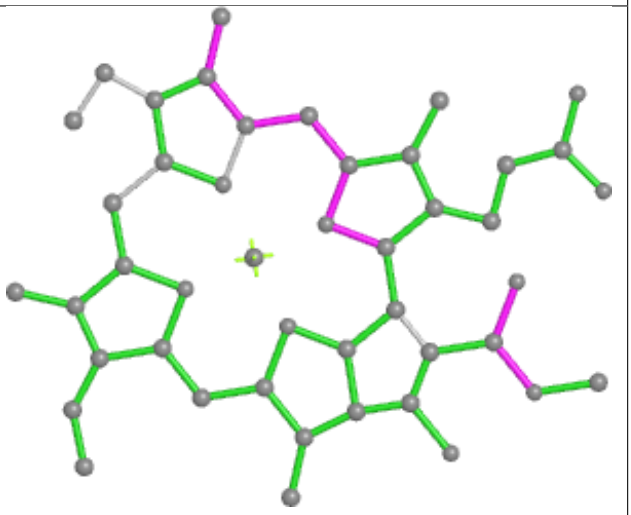


Rings

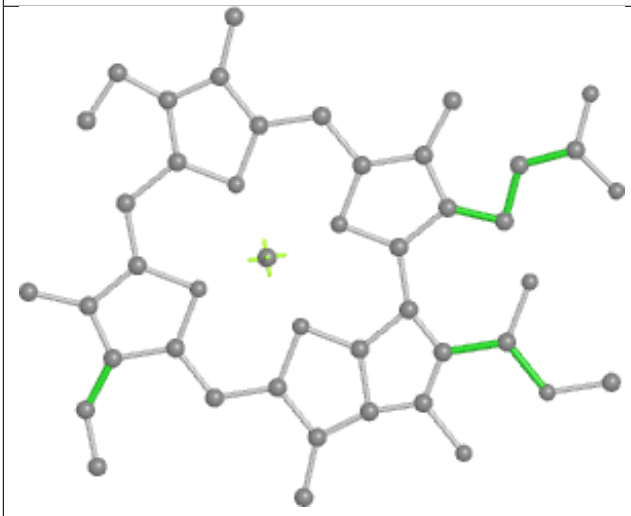
Ligand CLA aB 842



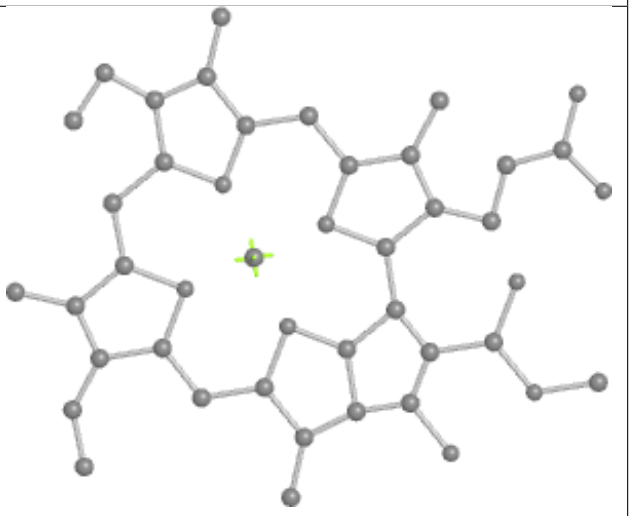
Bond lengths



Bond angles

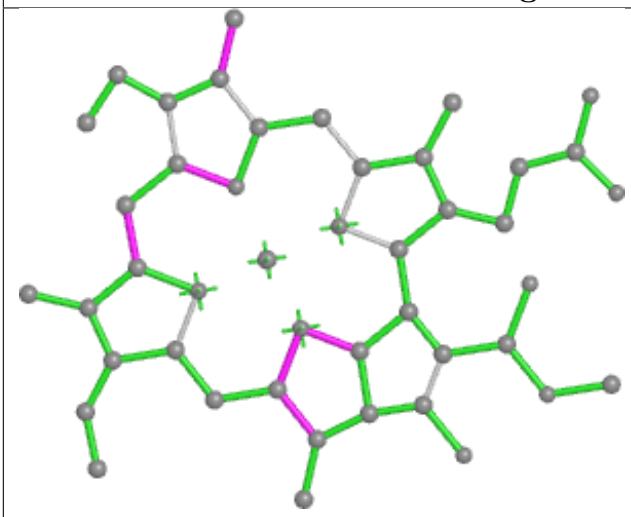


Torsions

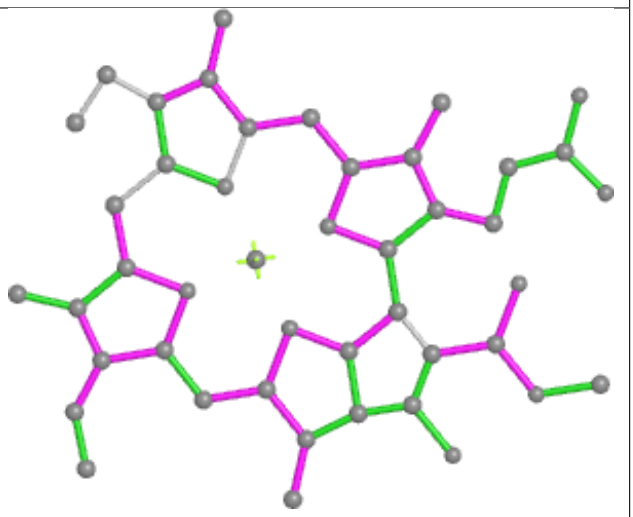


Rings

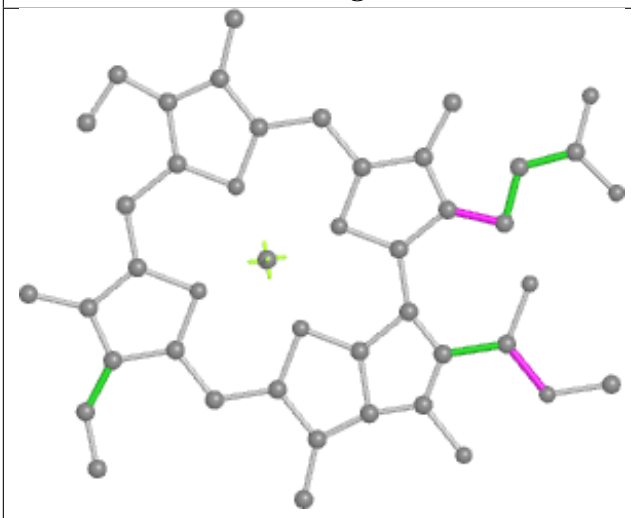
Ligand CLA a6 406



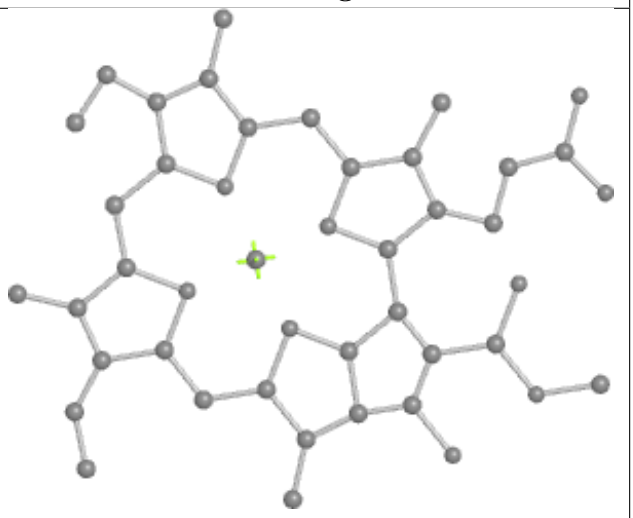
Bond lengths



Bond angles

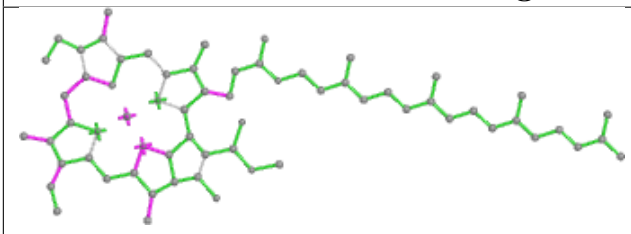


Torsions

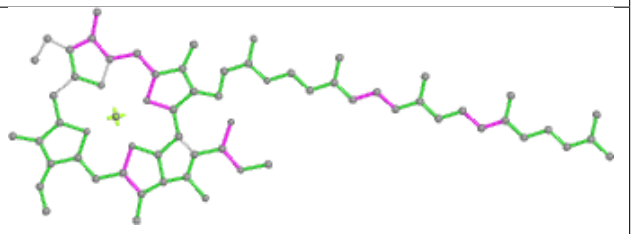


Rings

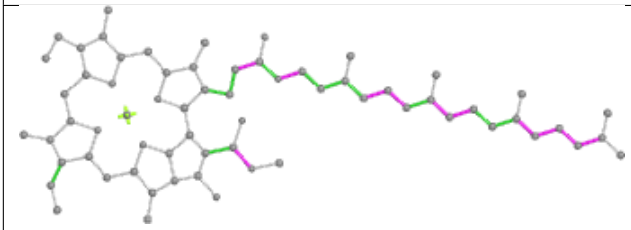
Ligand CLA aB 807



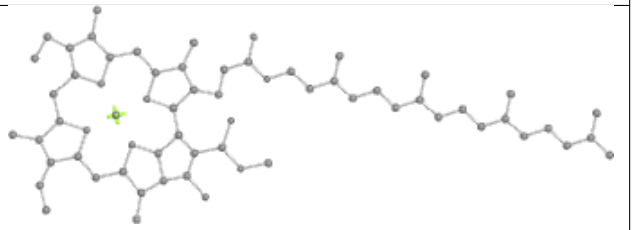
Bond lengths



Bond angles

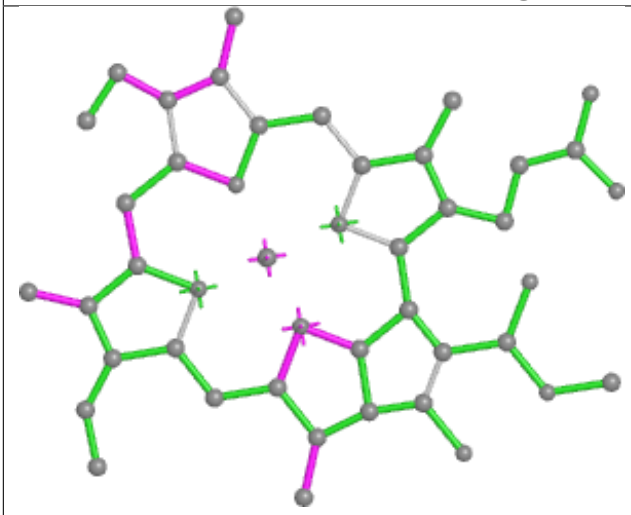


Torsions

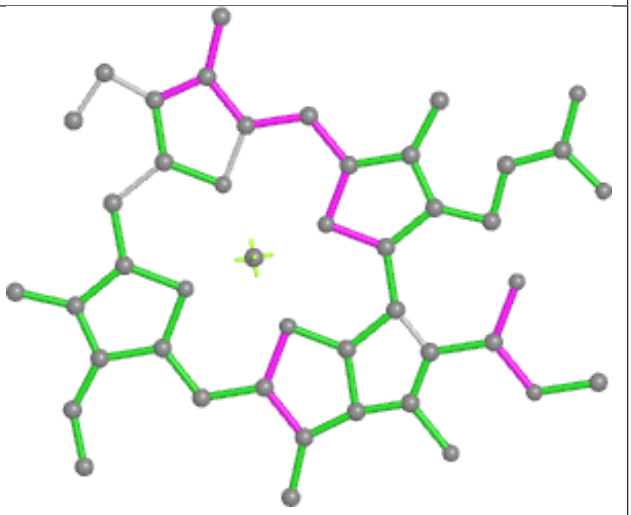


Rings

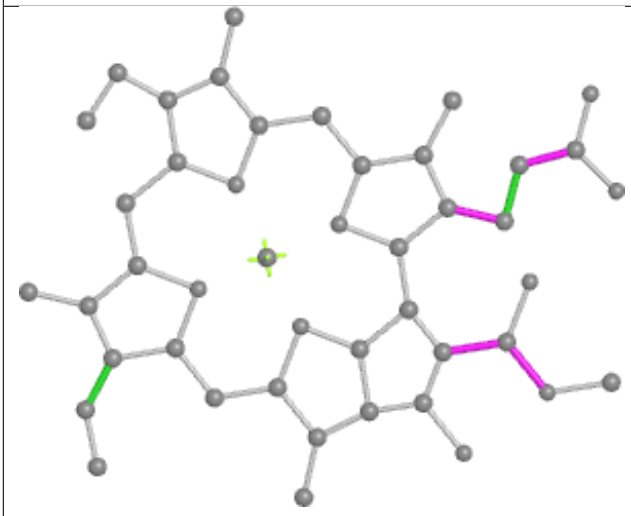
Ligand CLA aA 811



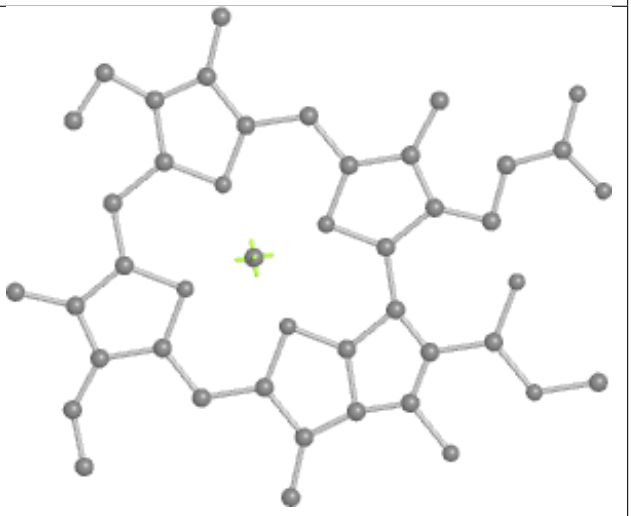
Bond lengths



Bond angles

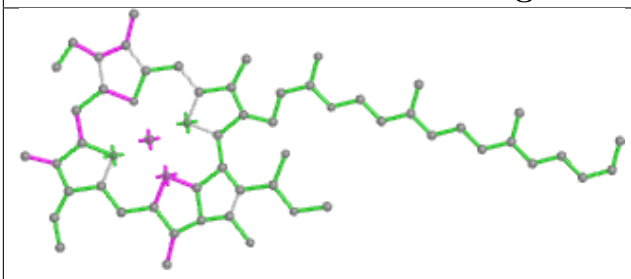


Torsions

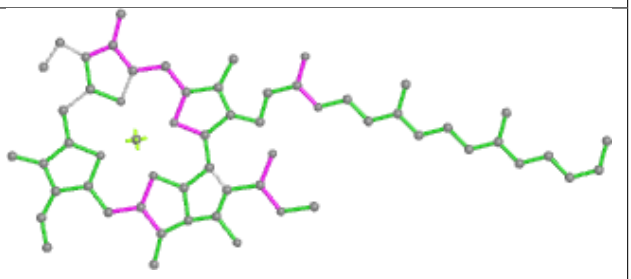


Rings

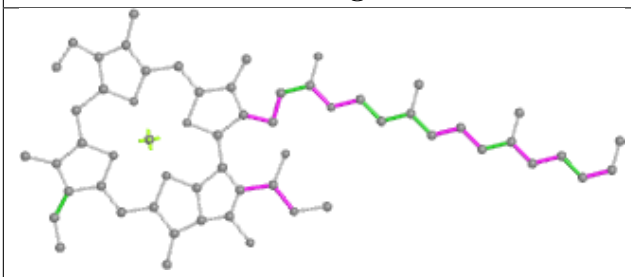
Ligand CLA cA 825



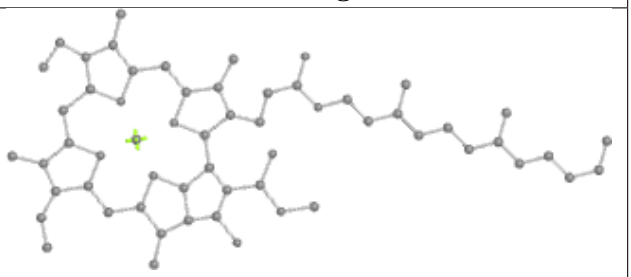
Bond lengths



Bond angles

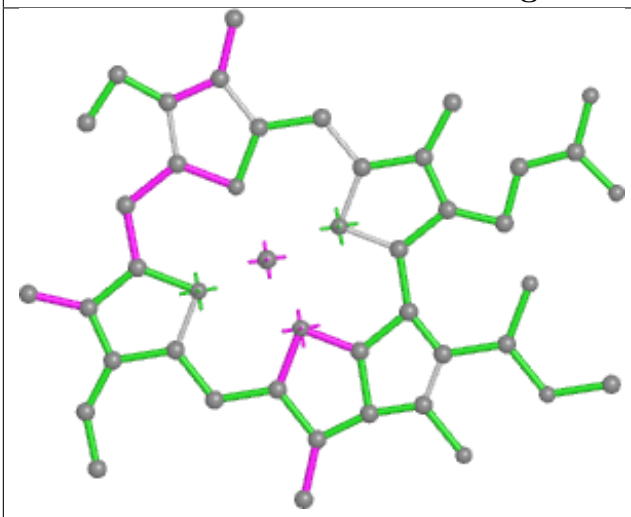


Torsions

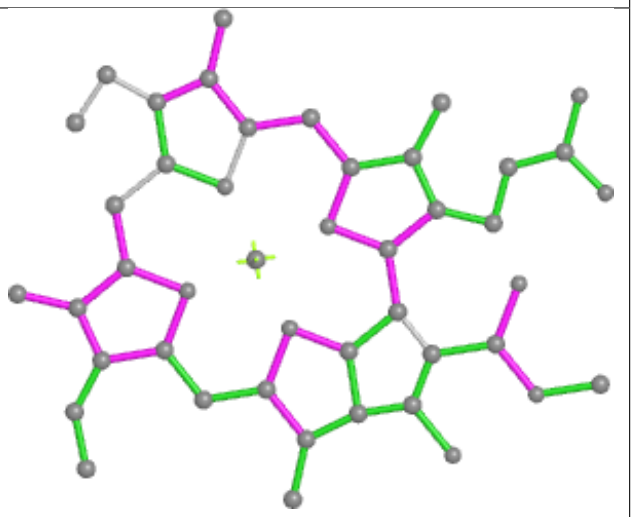


Rings

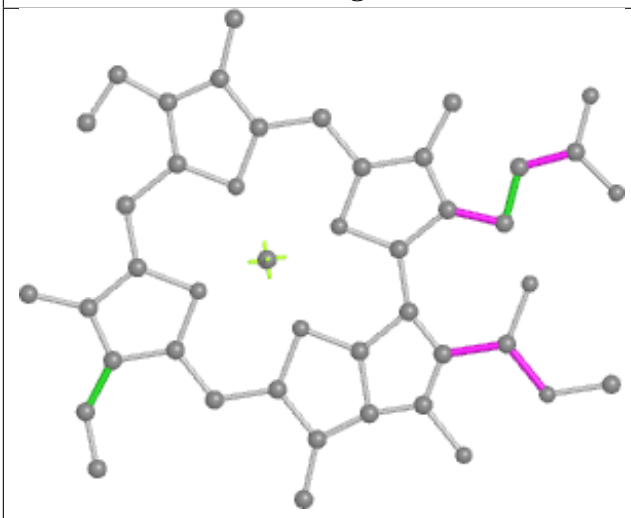
Ligand CLA c1 412



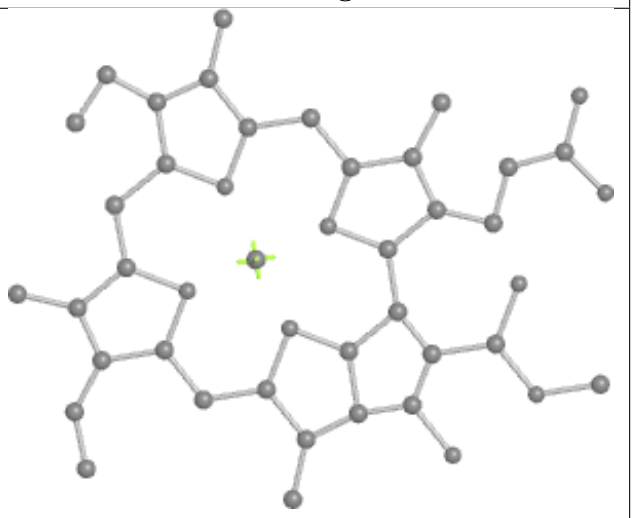
Bond lengths



Bond angles

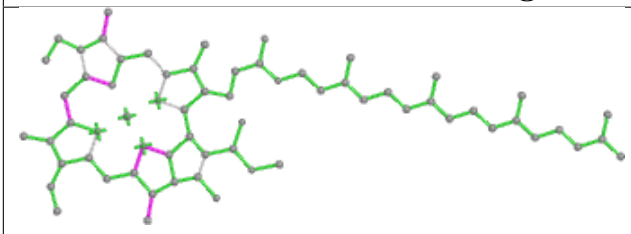


Torsions

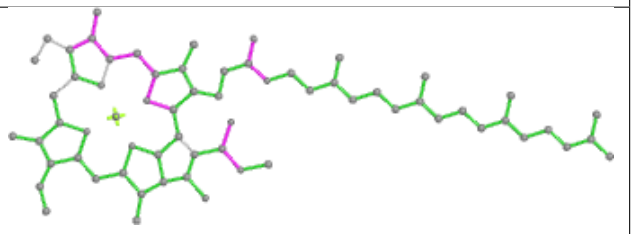


Rings

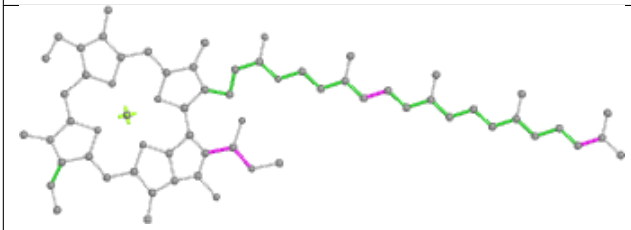
Ligand CLA b1 409



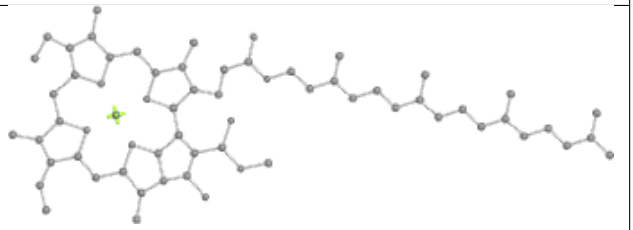
Bond lengths



Bond angles

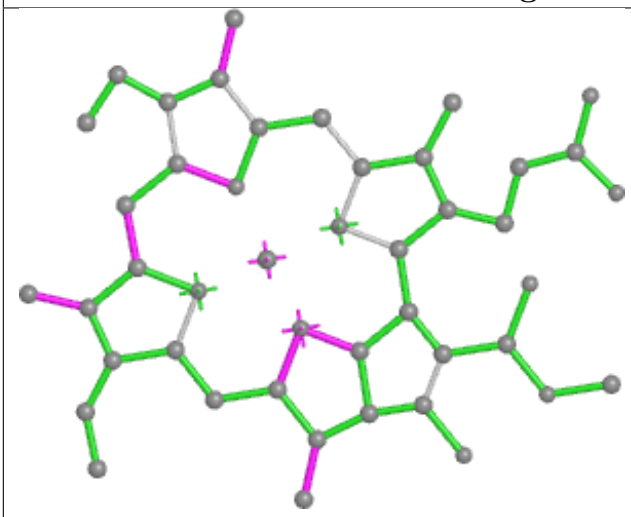


Torsions

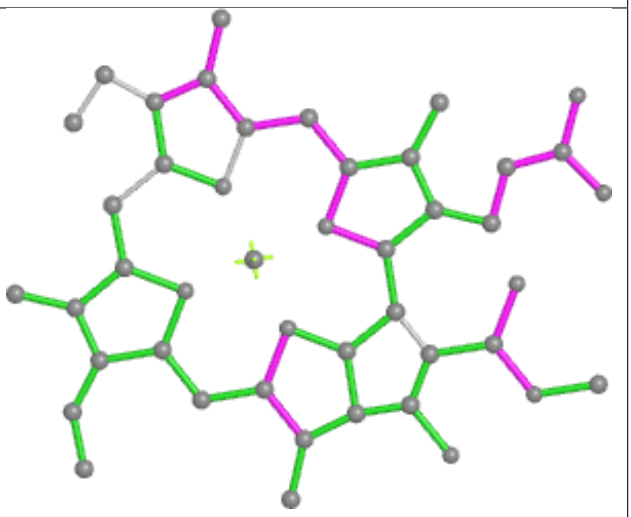


Rings

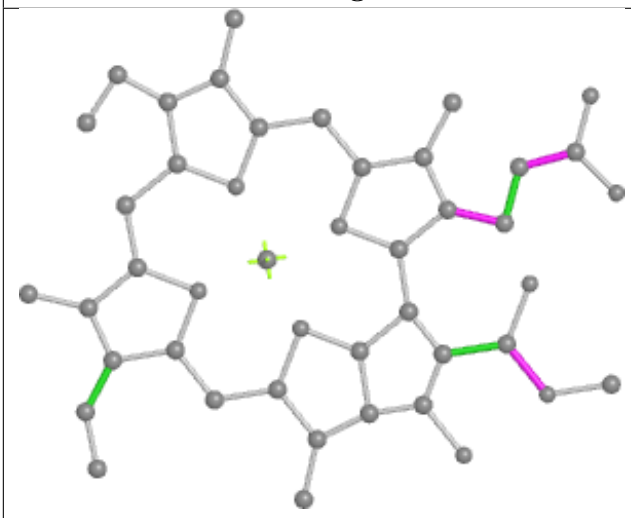
Ligand CLA a5 408



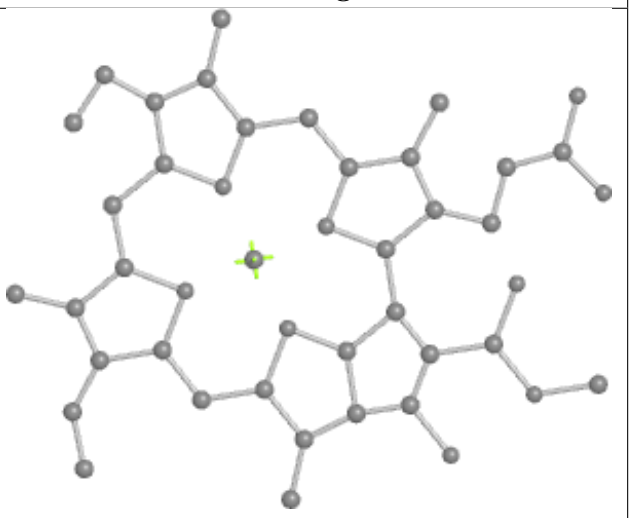
Bond lengths



Bond angles

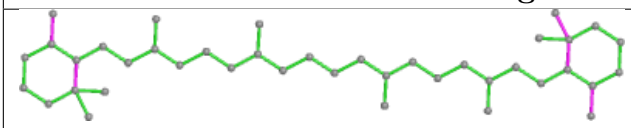


Torsions

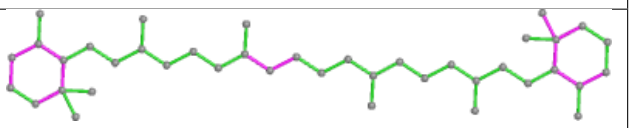


Rings

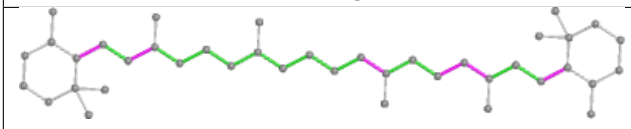
Ligand BCR a1 417



Bond lengths



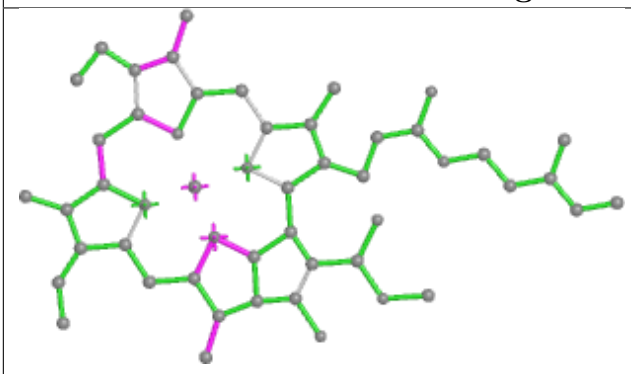
Bond angles



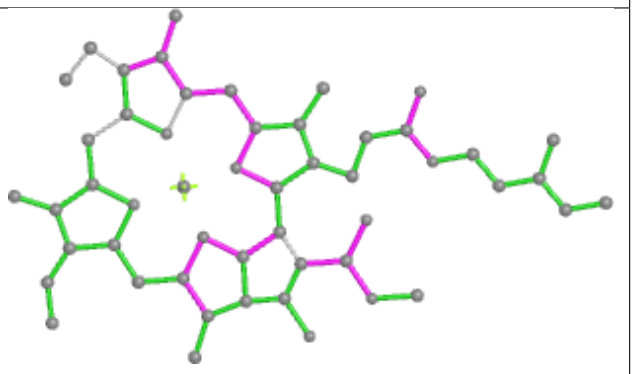
Torsions

Rings

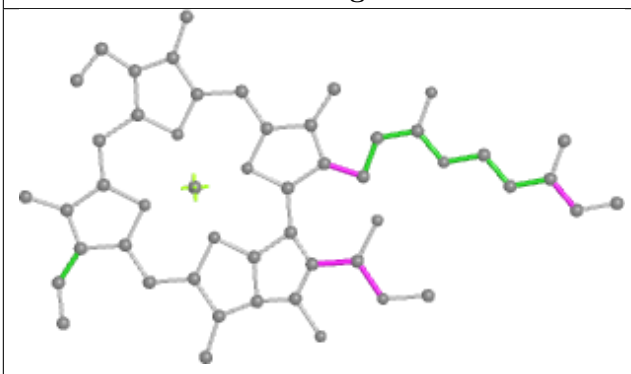
Ligand CLA aA 842



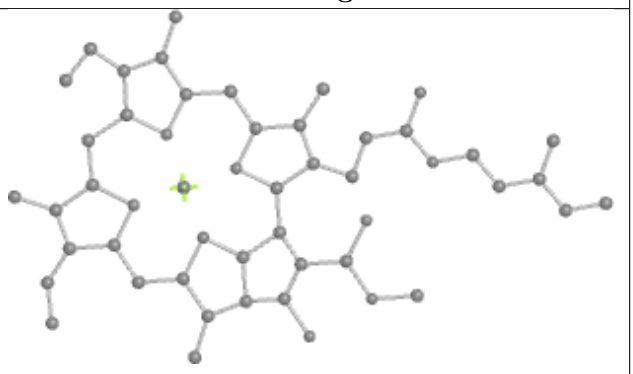
Bond lengths



Bond angles

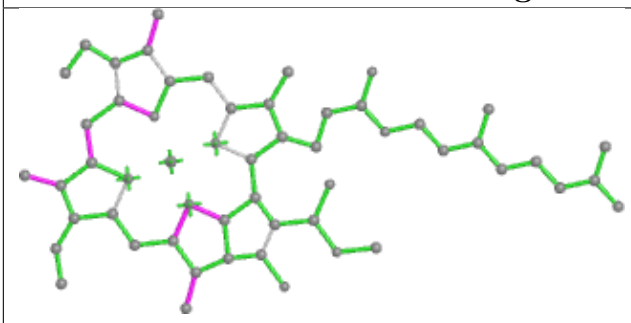


Torsions

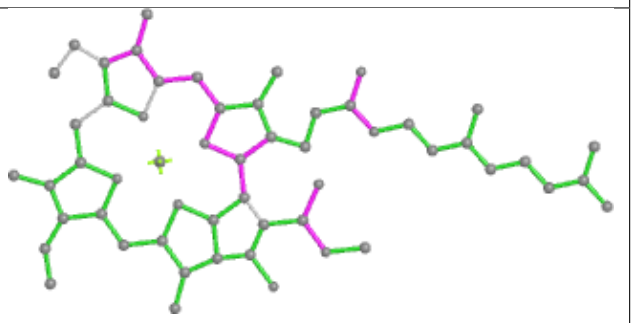


Rings

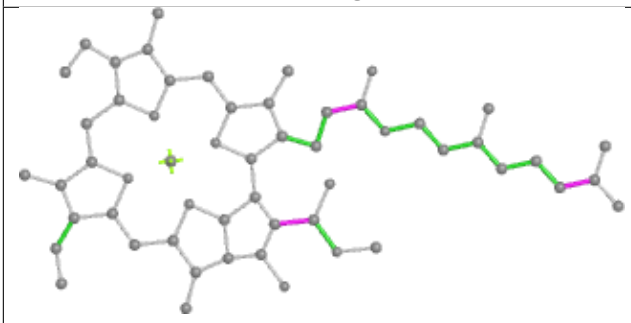
Ligand CLA bB 823



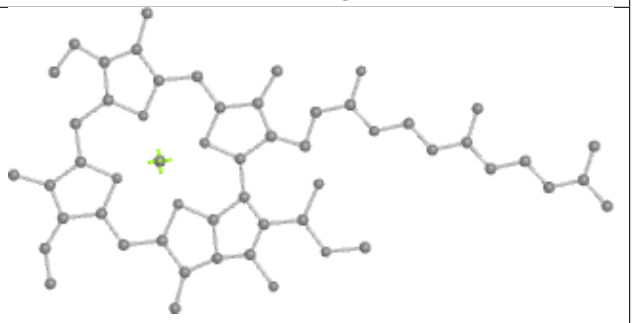
Bond lengths



Bond angles

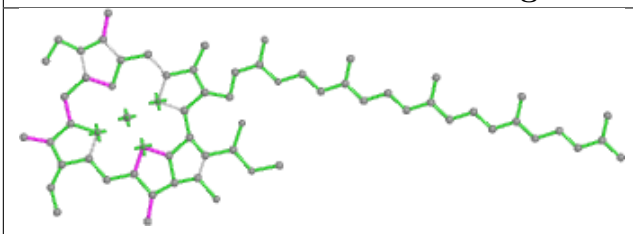


Torsions

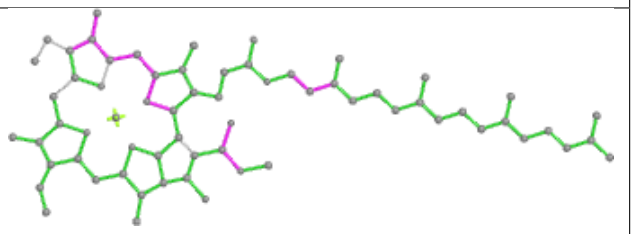


Rings

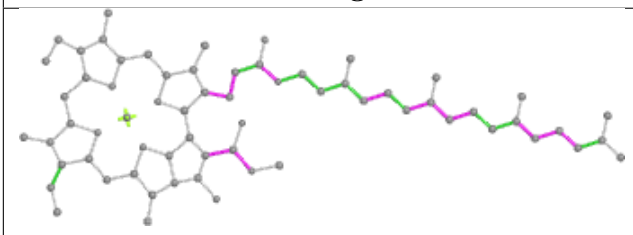
Ligand CLA c1 402



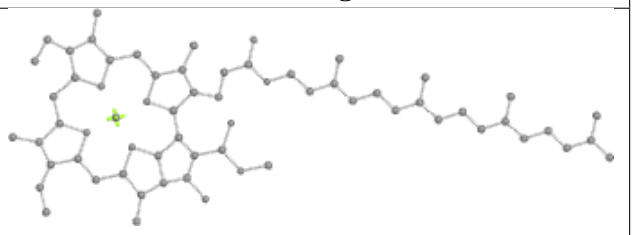
Bond lengths



Bond angles

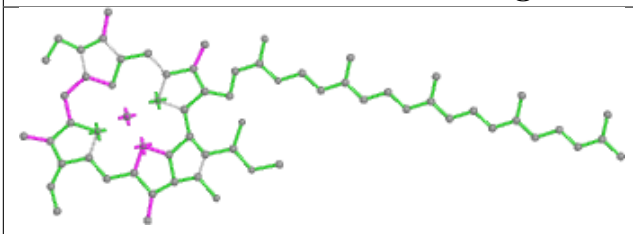


Torsions

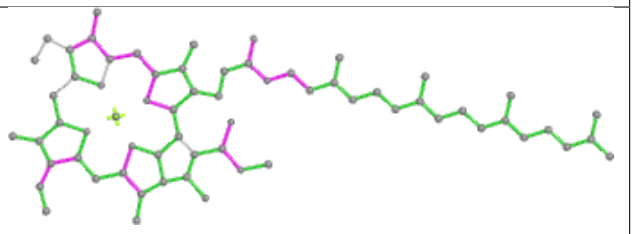


Rings

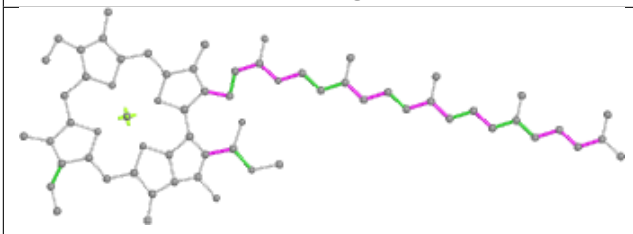
Ligand CLA bB 806



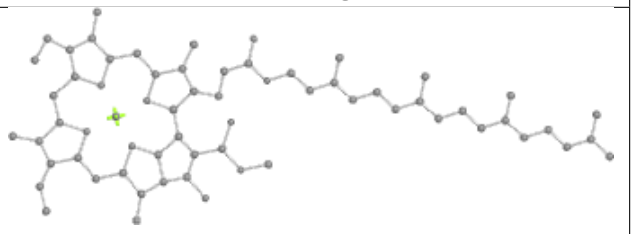
Bond lengths



Bond angles

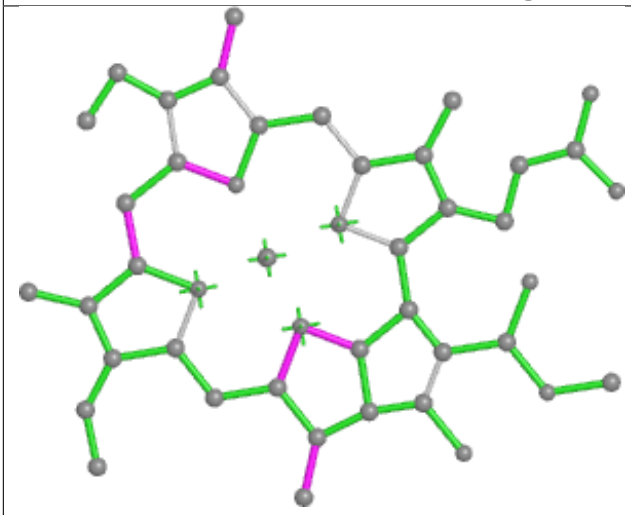


Torsions

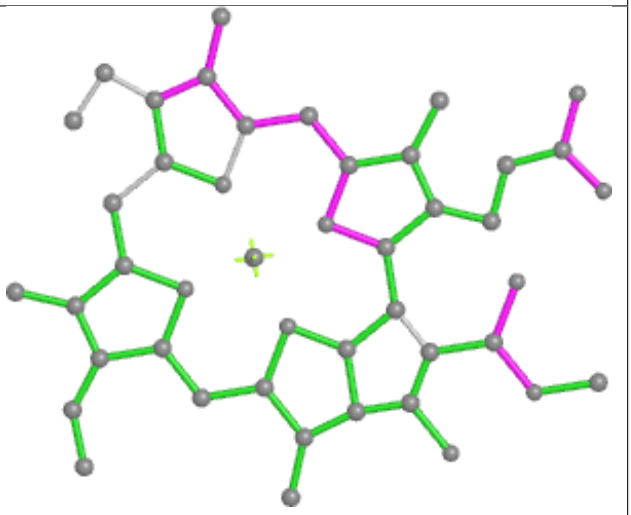


Rings

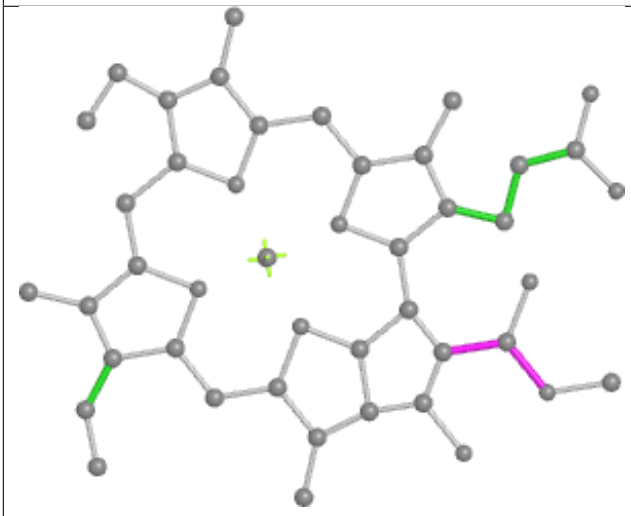
Ligand CLA a2 407



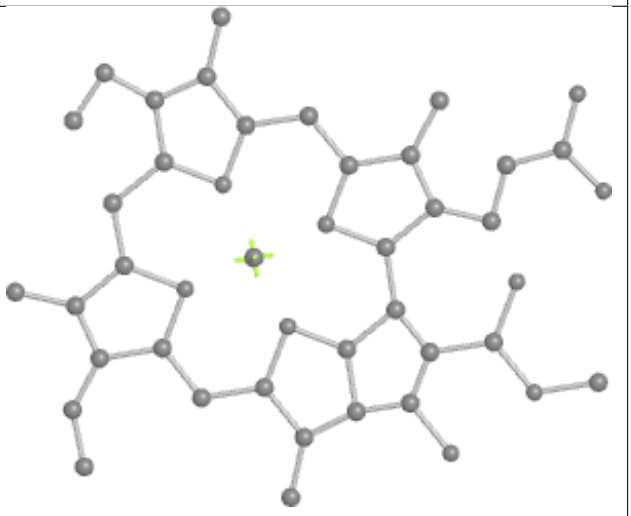
Bond lengths



Bond angles

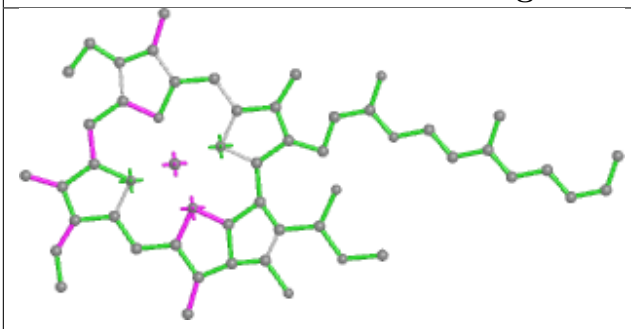


Torsions

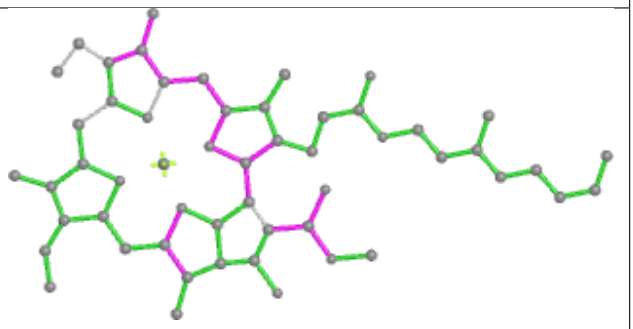


Rings

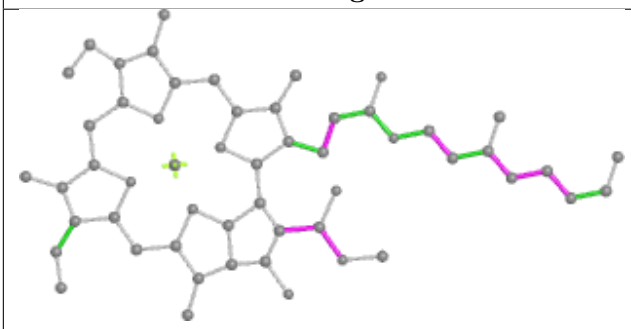
Ligand CLA cB 825



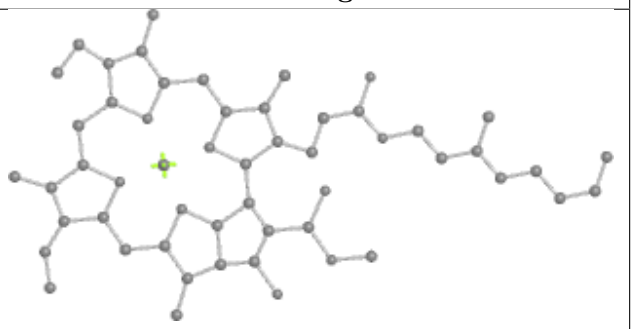
Bond lengths



Bond angles

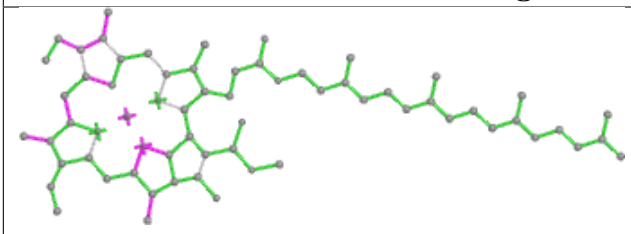


Torsions

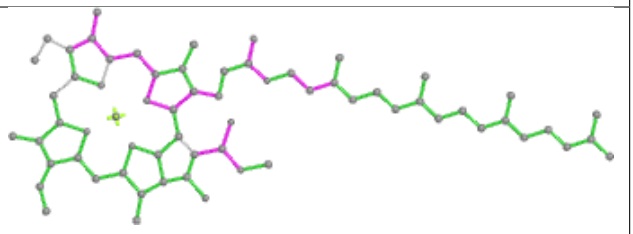


Rings

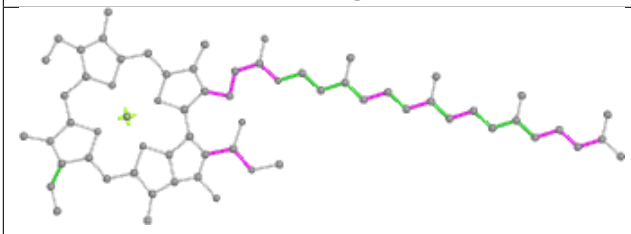
Ligand CLA aA 809



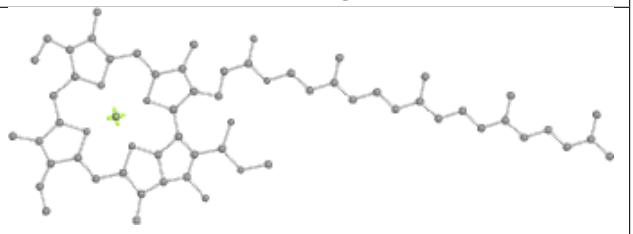
Bond lengths



Bond angles

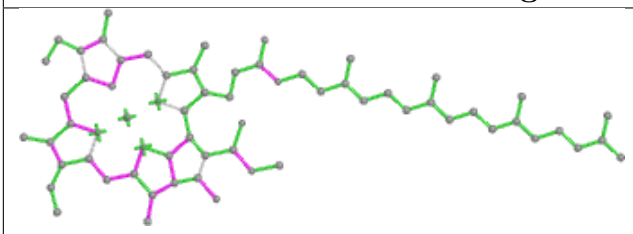


Torsions

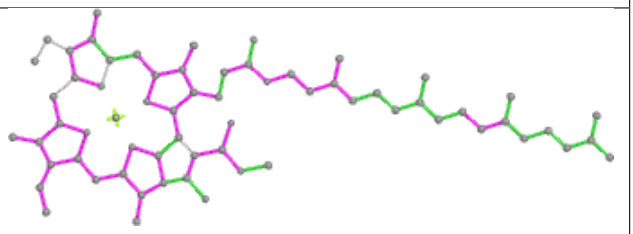


Rings

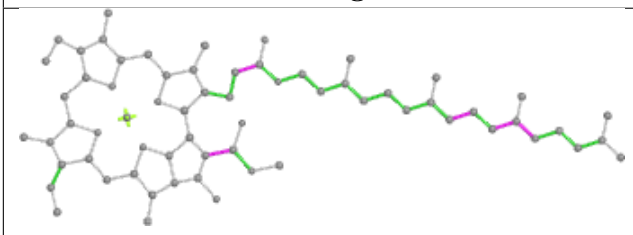
Ligand CL0 cA 801



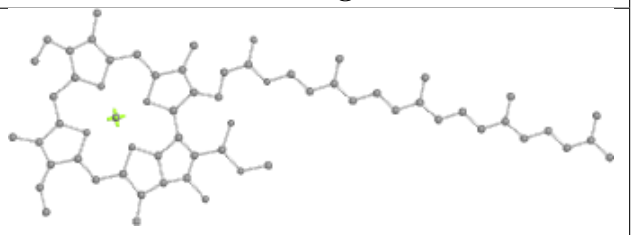
Bond lengths



Bond angles

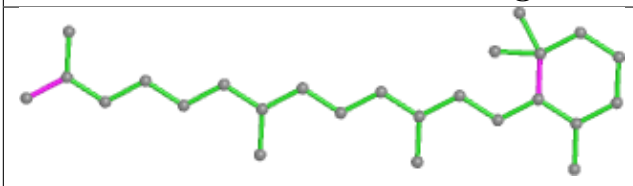


Torsions

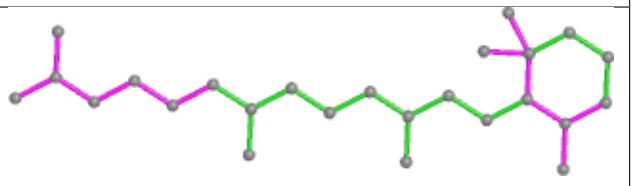


Rings

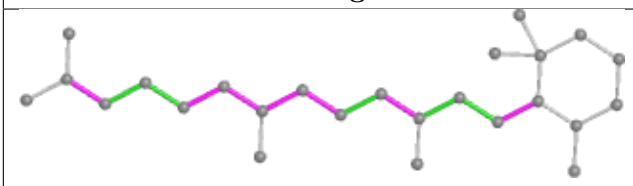
Ligand BCR aB 847



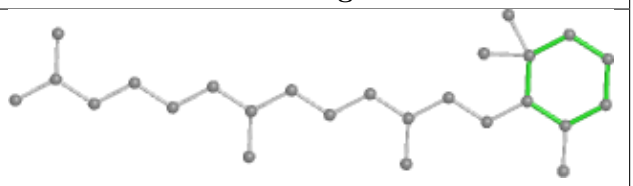
Bond lengths



Bond angles

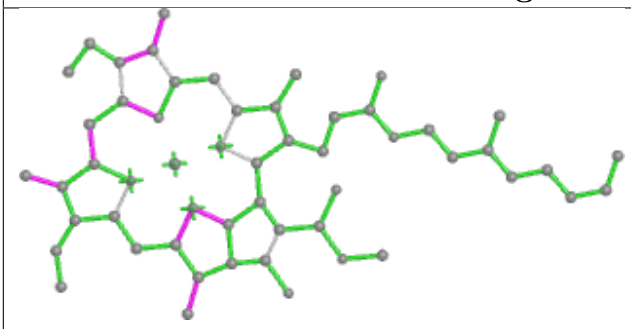


Torsions

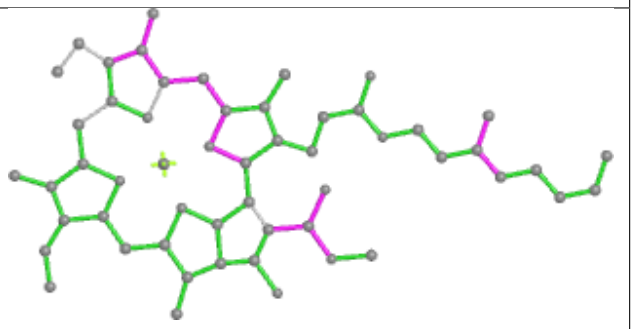


Rings

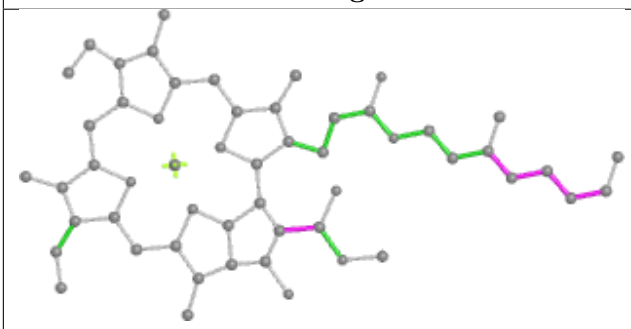
Ligand CLA cA 818



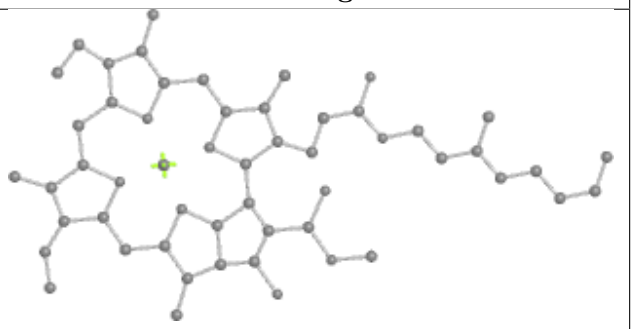
Bond lengths



Bond angles

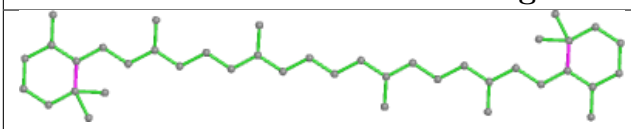


Torsions

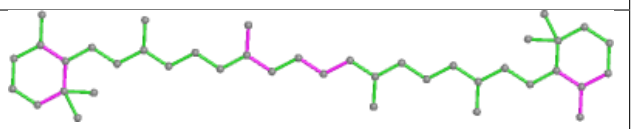


Rings

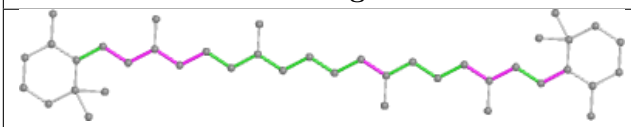
Ligand BCR bI 101



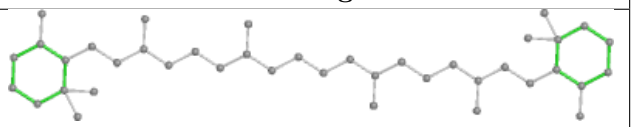
Bond lengths



Bond angles

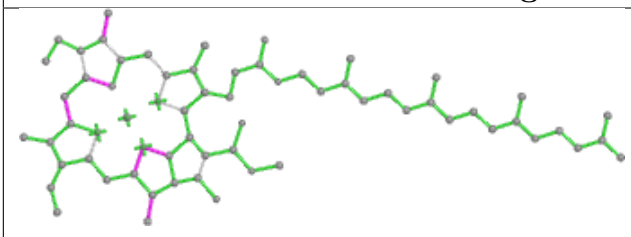


Torsions

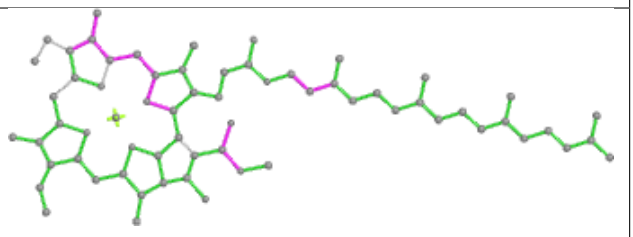


Rings

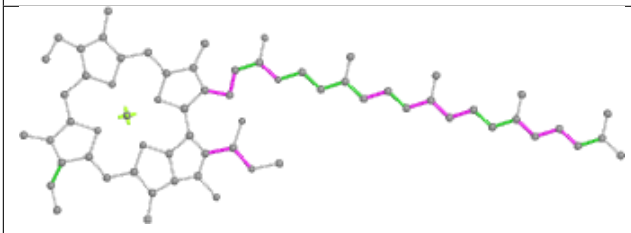
Ligand CLA c6 403



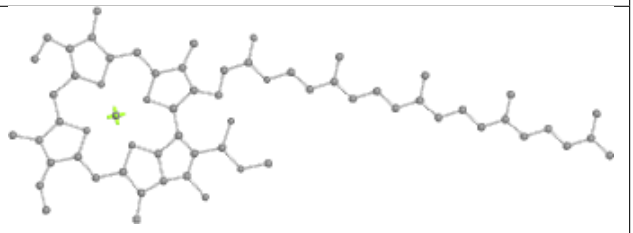
Bond lengths



Bond angles

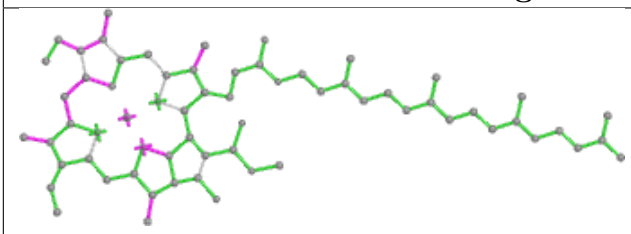


Torsions

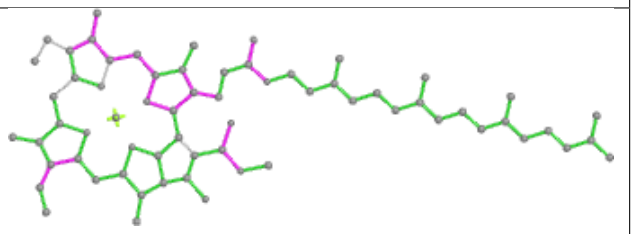


Rings

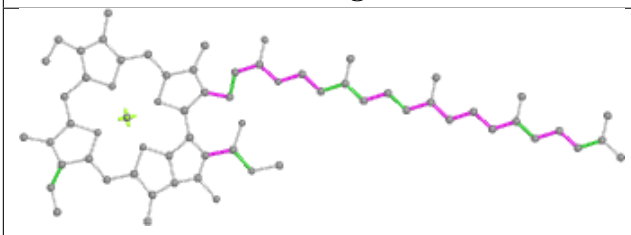
Ligand CLA aA 806



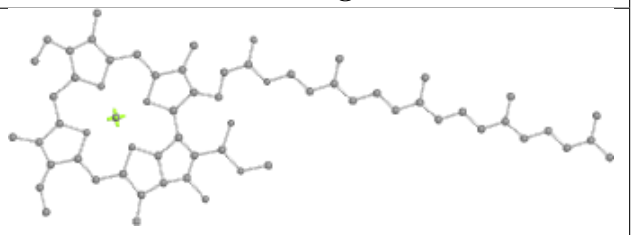
Bond lengths



Bond angles

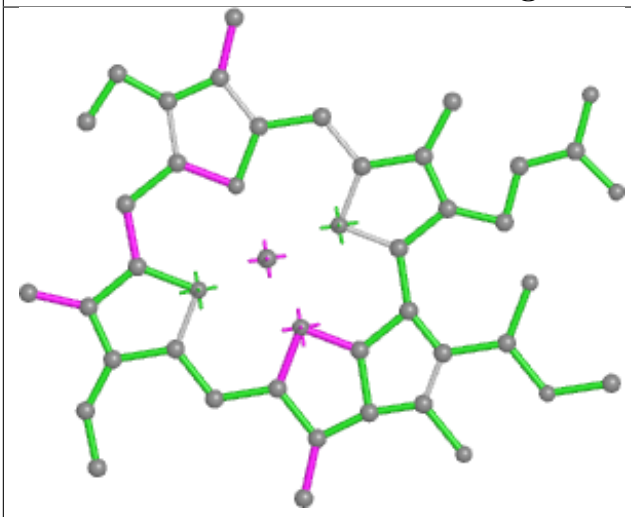


Torsions

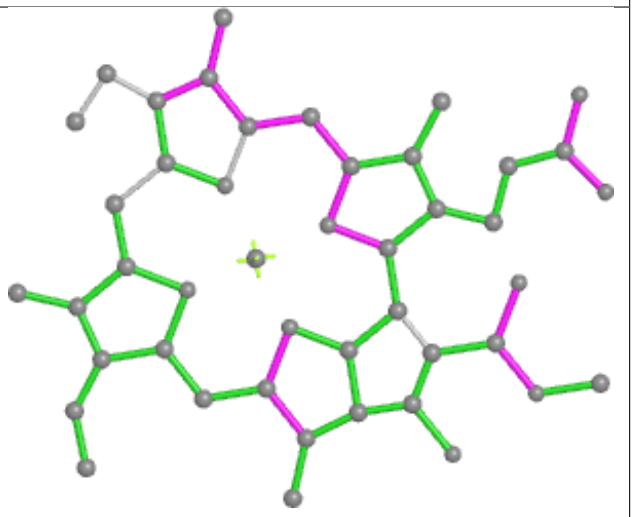


Rings

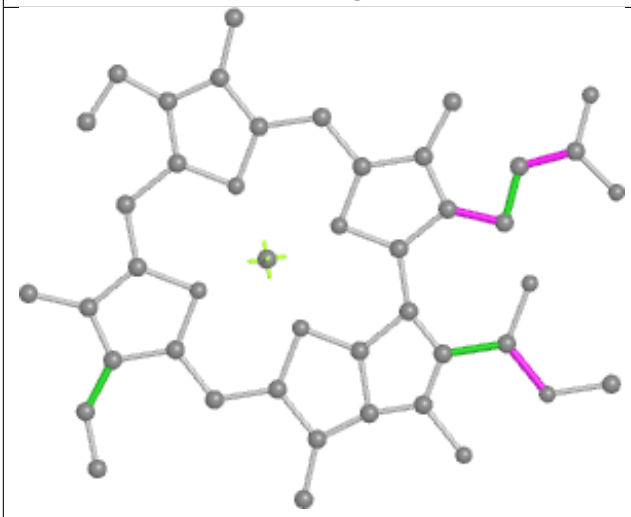
Ligand CLA a4 408



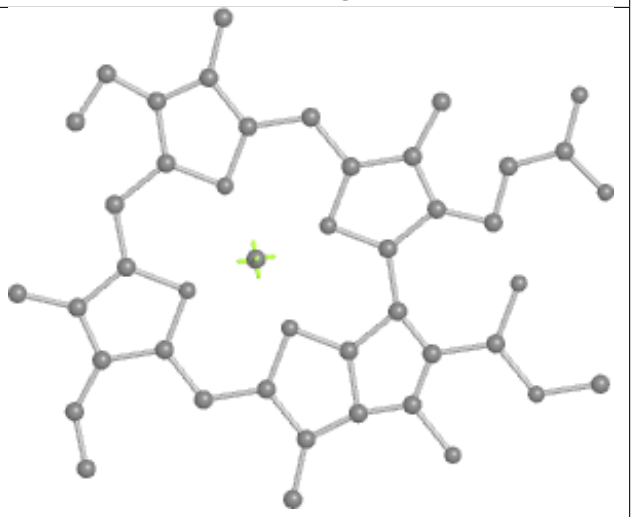
Bond lengths



Bond angles

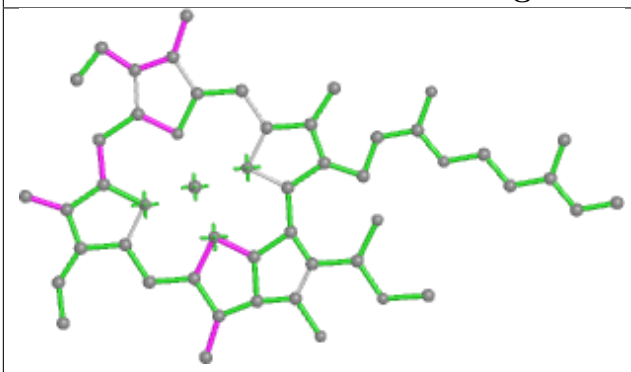


Torsions

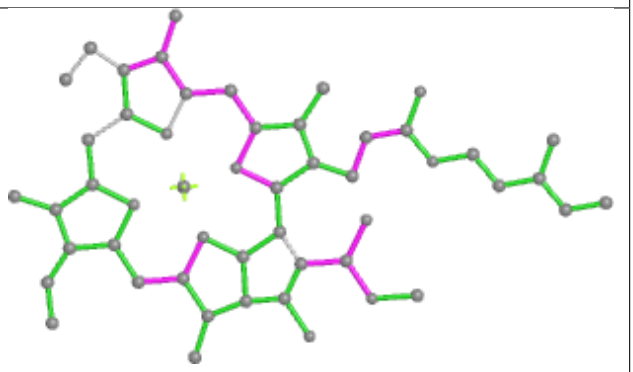


Rings

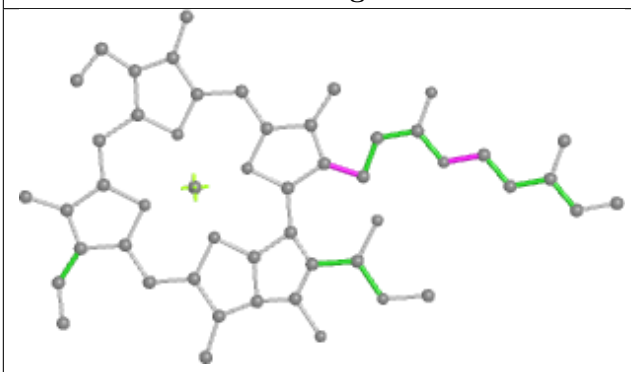
Ligand CLA bA 808



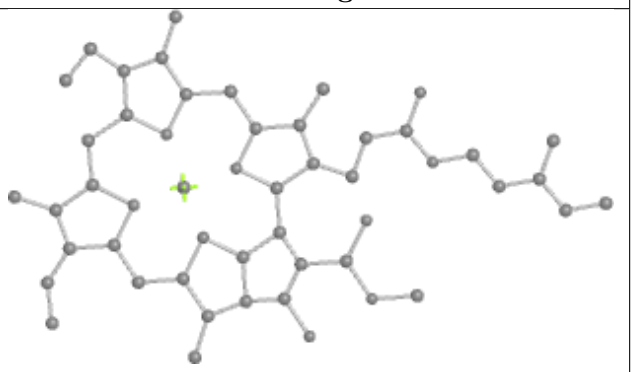
Bond lengths



Bond angles

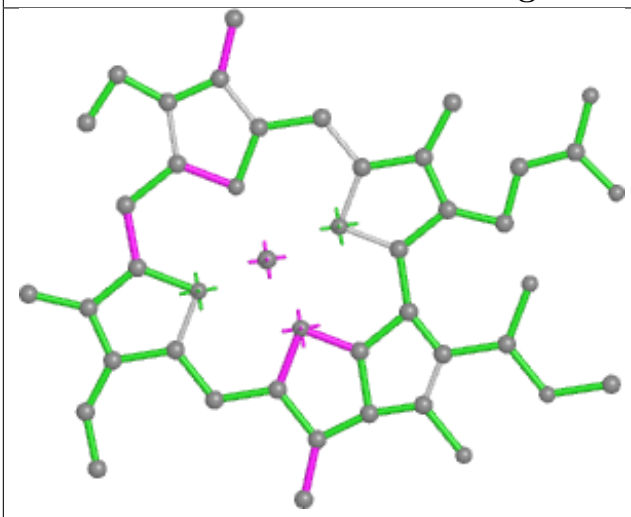


Torsions

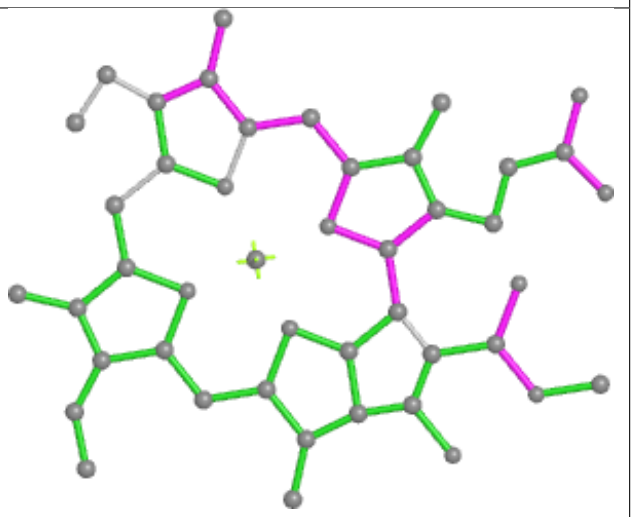


Rings

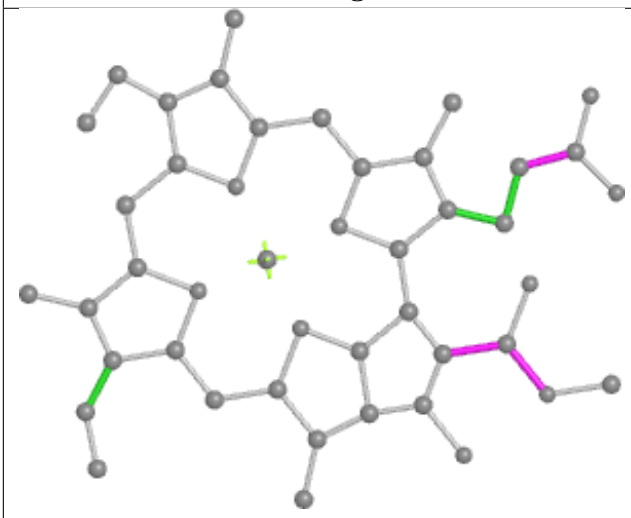
Ligand CLA b6 408



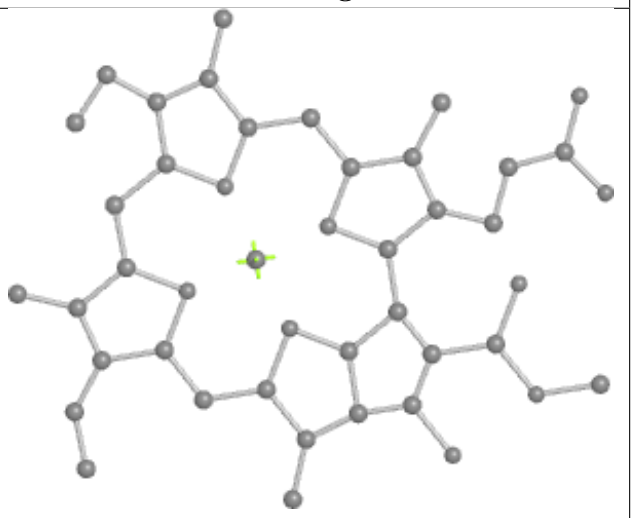
Bond lengths



Bond angles

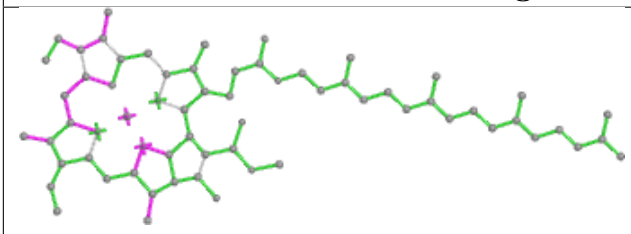


Torsions

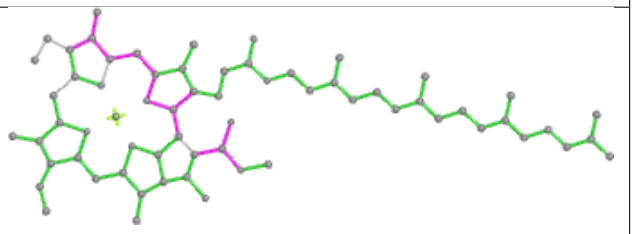


Rings

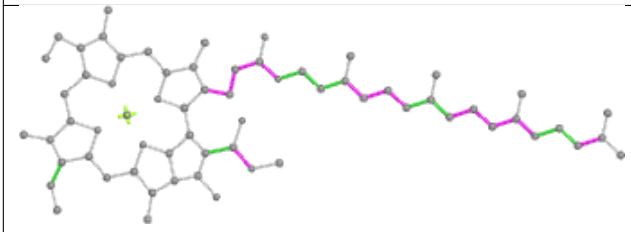
Ligand CLA bB 828



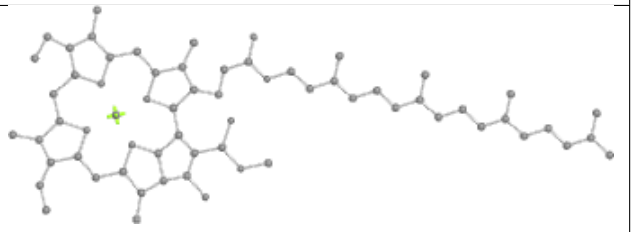
Bond lengths



Bond angles

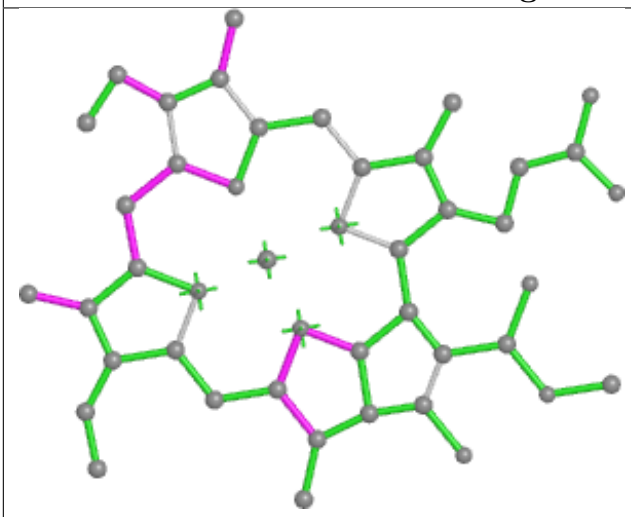


Torsions

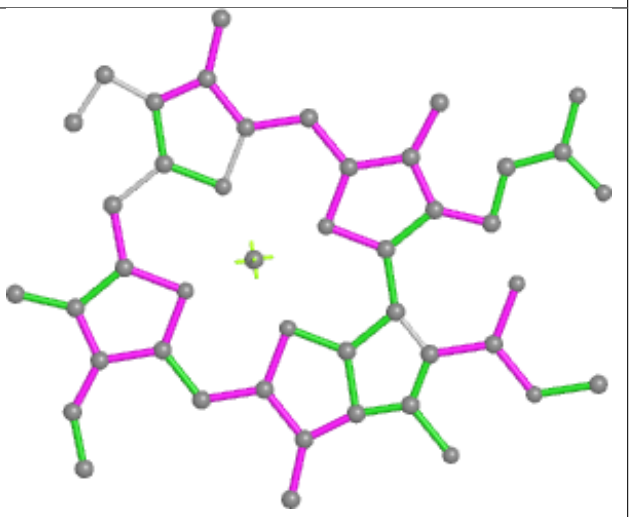


Rings

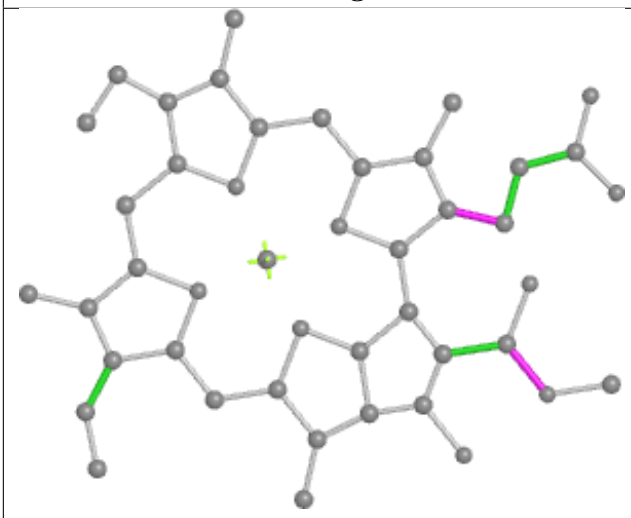
Ligand CLA a1 404



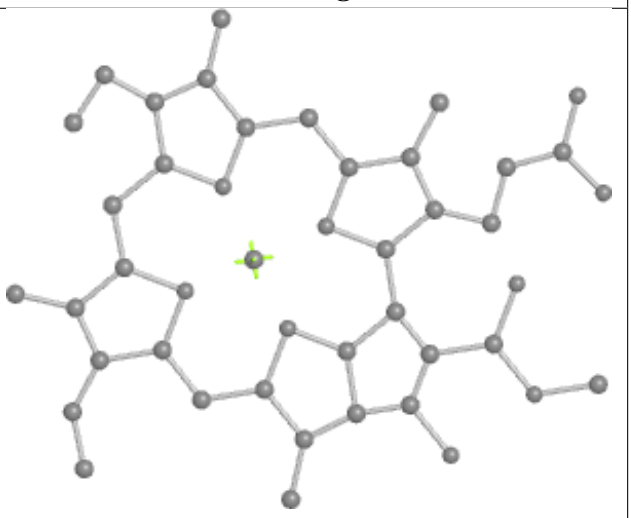
Bond lengths



Bond angles

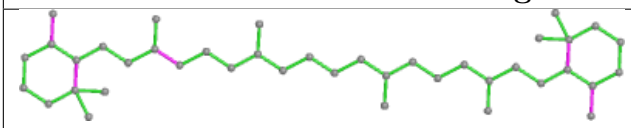


Torsions

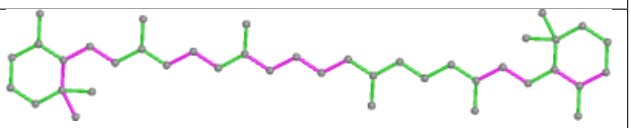


Rings

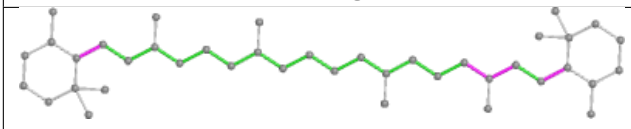
Ligand BCR cA 850



Bond lengths



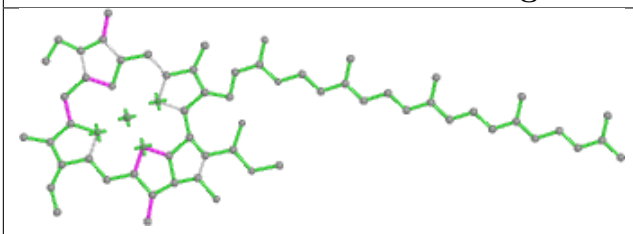
Bond angles



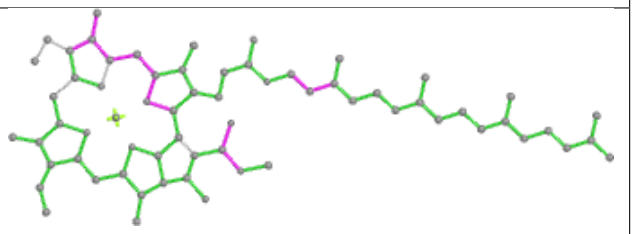
Torsions

Rings

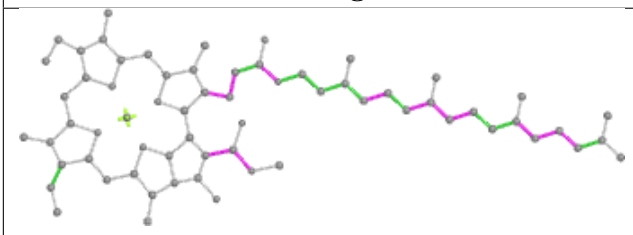
Ligand CLA c2 402



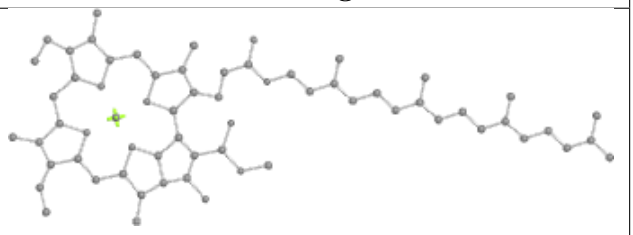
Bond lengths



Bond angles

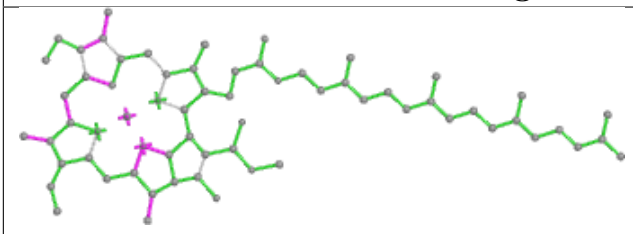


Torsions

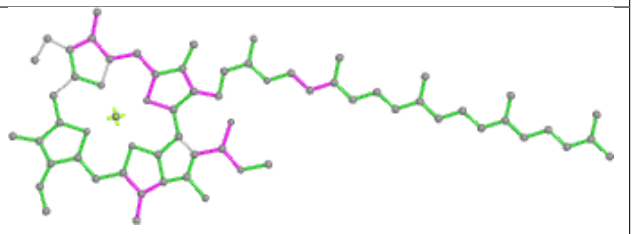


Rings

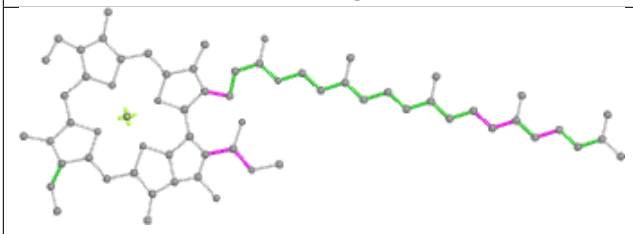
Ligand CLA bA 804



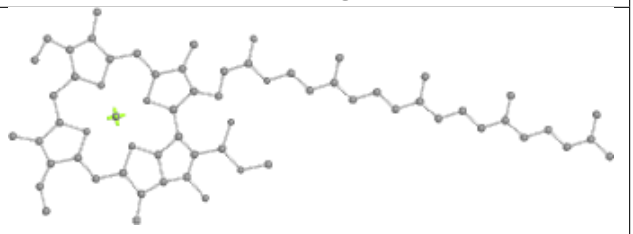
Bond lengths



Bond angles

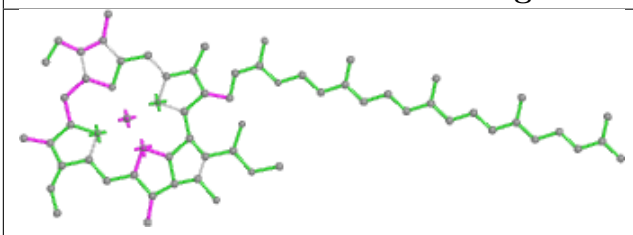


Torsions

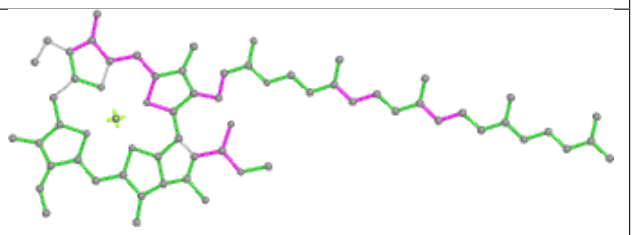


Rings

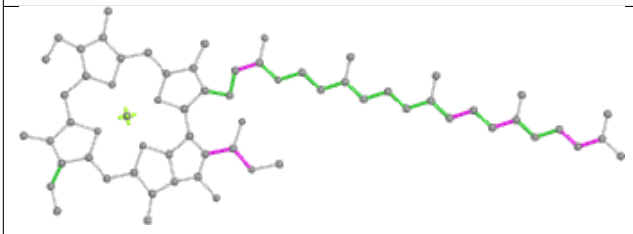
Ligand CLA bB 802



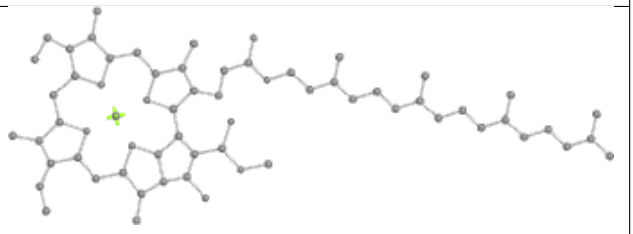
Bond lengths



Bond angles

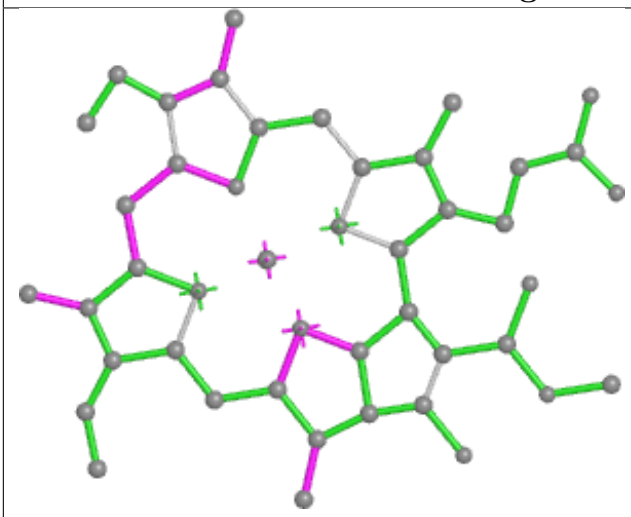


Torsions

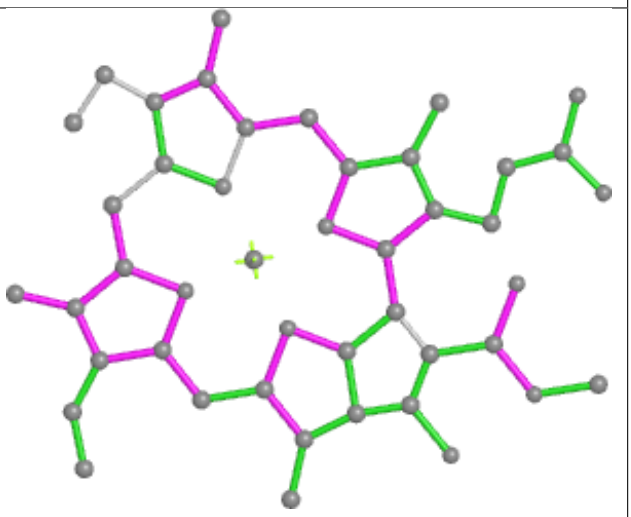


Rings

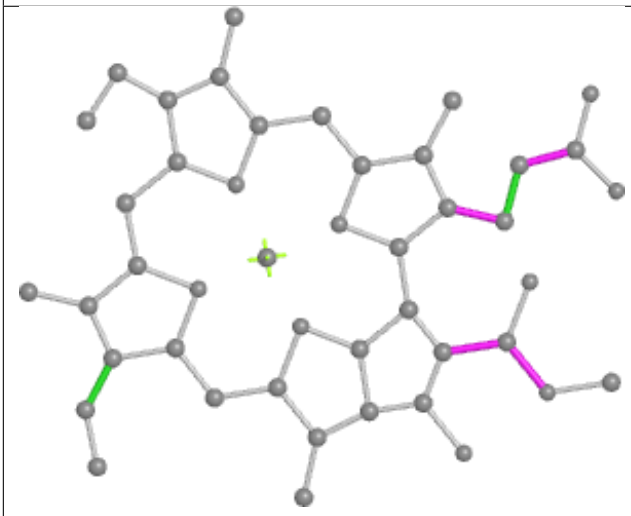
Ligand CLA a2 413



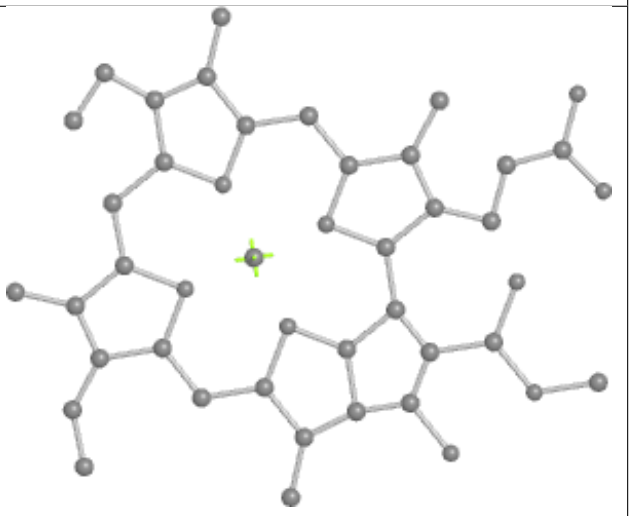
Bond lengths



Bond angles

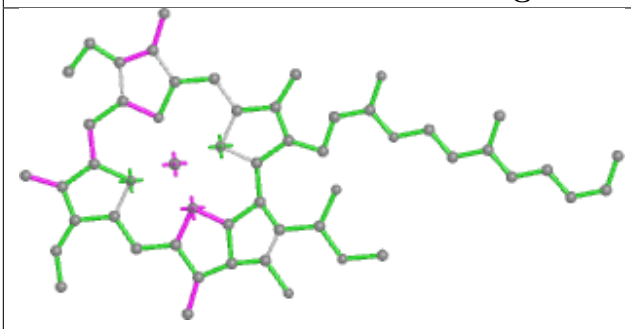


Torsions

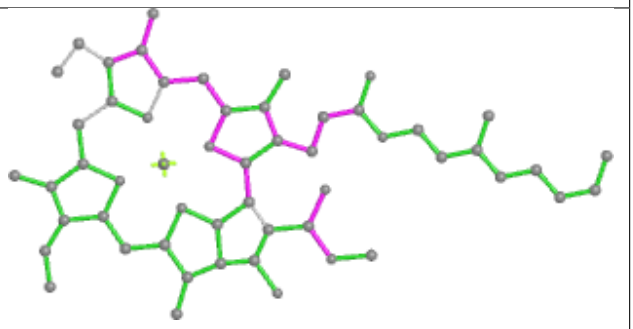


Rings

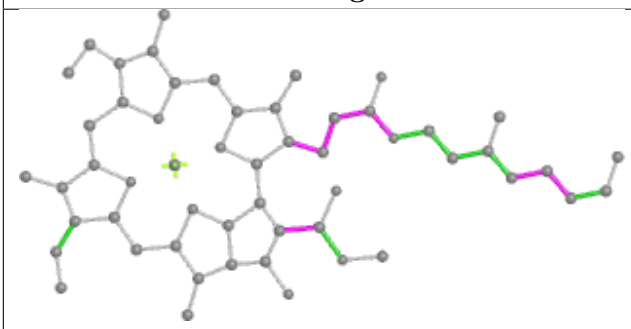
Ligand CLA bA 813



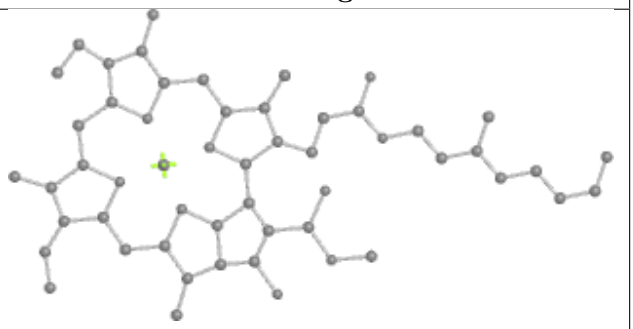
Bond lengths



Bond angles

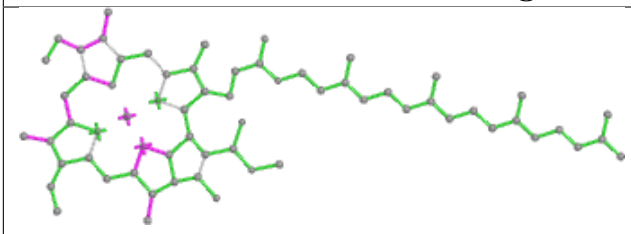


Torsions

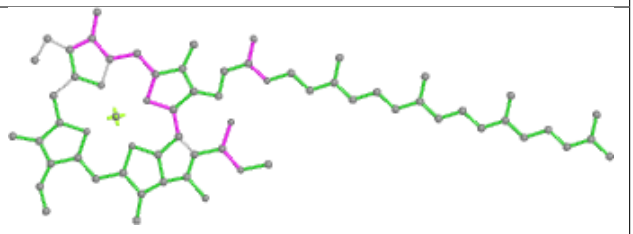


Rings

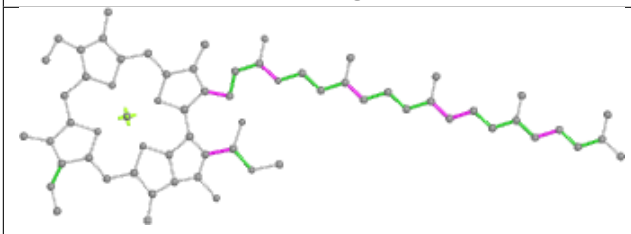
Ligand CLA aL 201



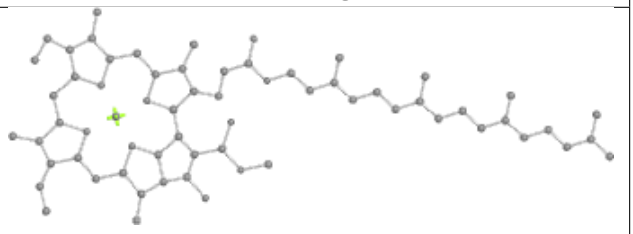
Bond lengths



Bond angles

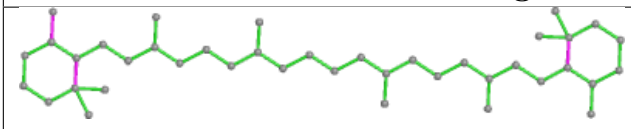


Torsions

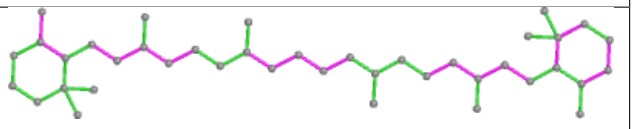


Rings

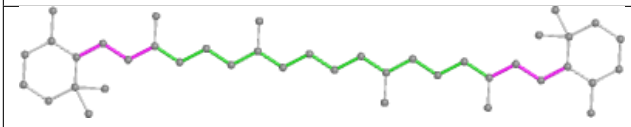
Ligand BCR cK 101



Bond lengths



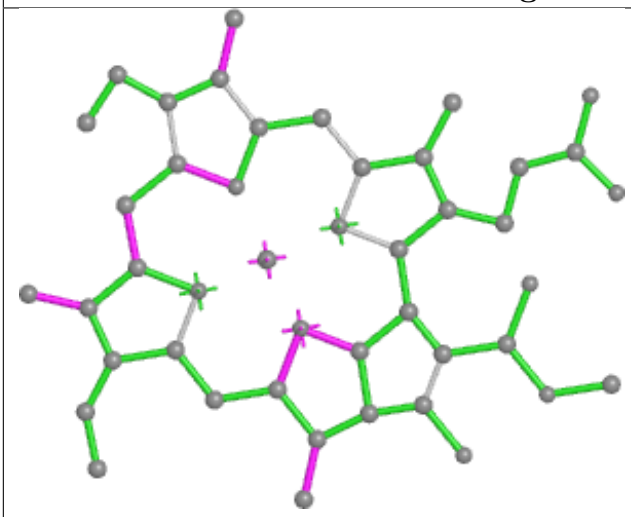
Bond angles



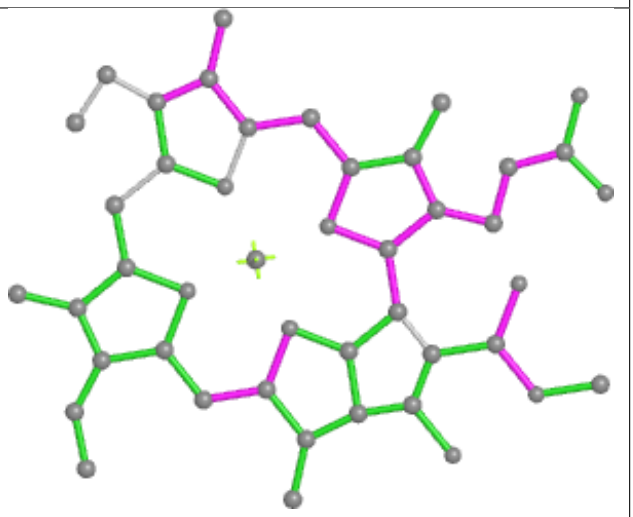
Torsions

Rings

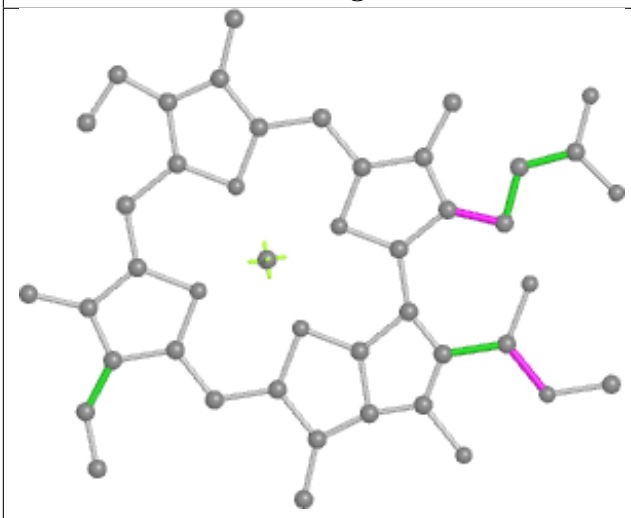
Ligand CLA a6 412



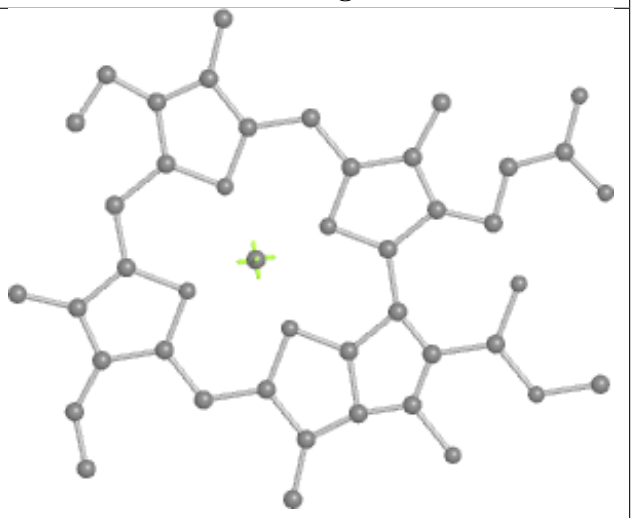
Bond lengths



Bond angles

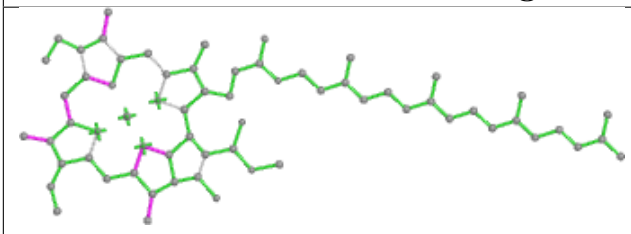


Torsions

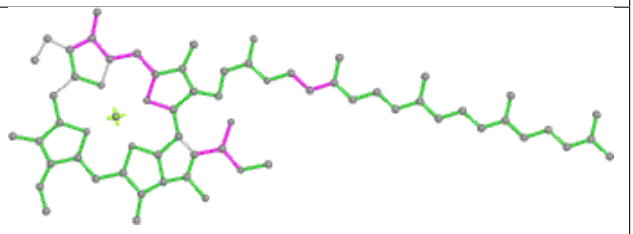


Rings

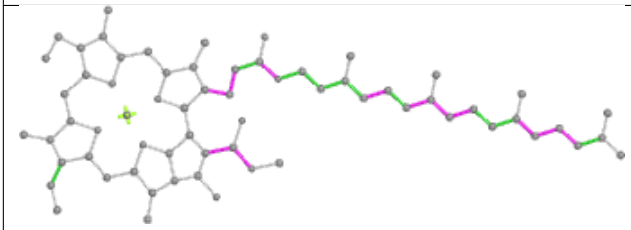
Ligand CLA b4 402



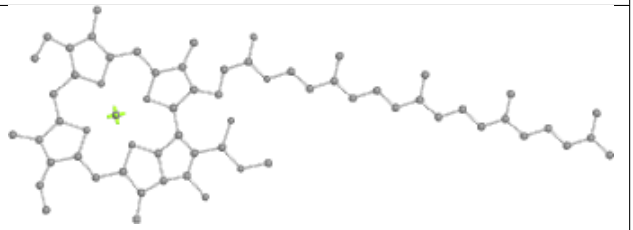
Bond lengths



Bond angles

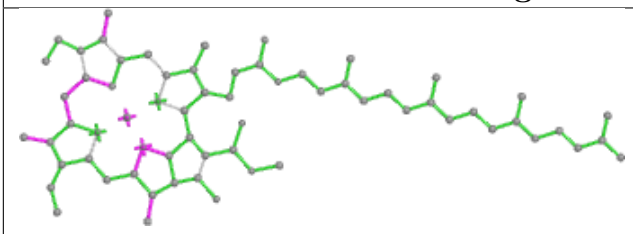


Torsions

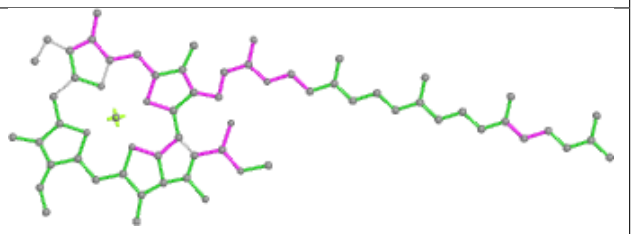


Rings

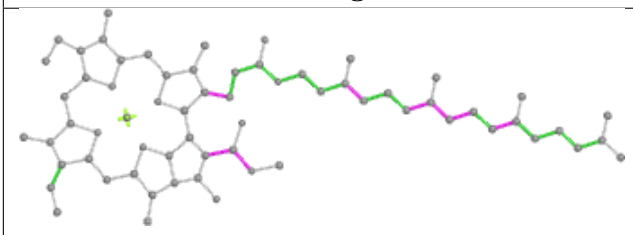
Ligand CLA bB 827



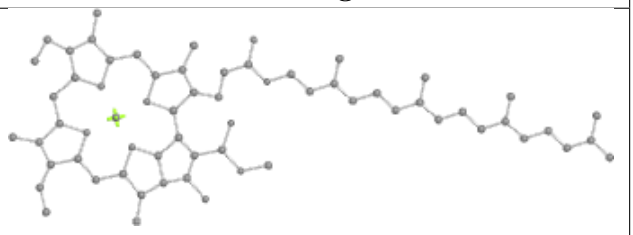
Bond lengths



Bond angles

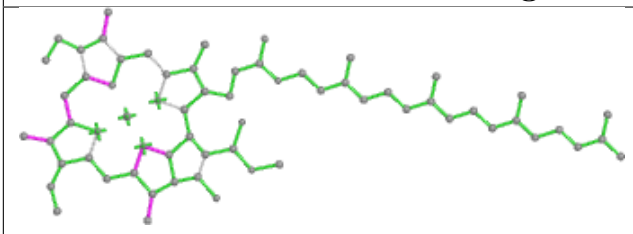


Torsions

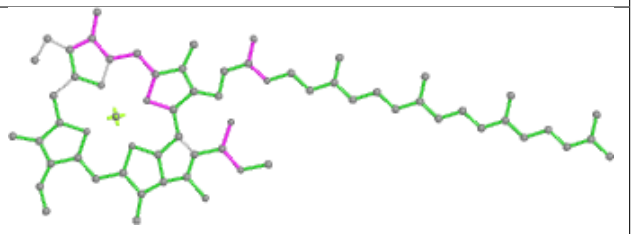


Rings

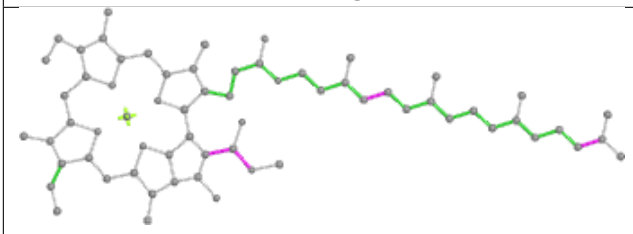
Ligand CLA c5 409



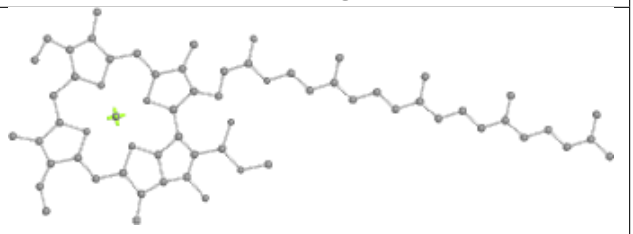
Bond lengths



Bond angles

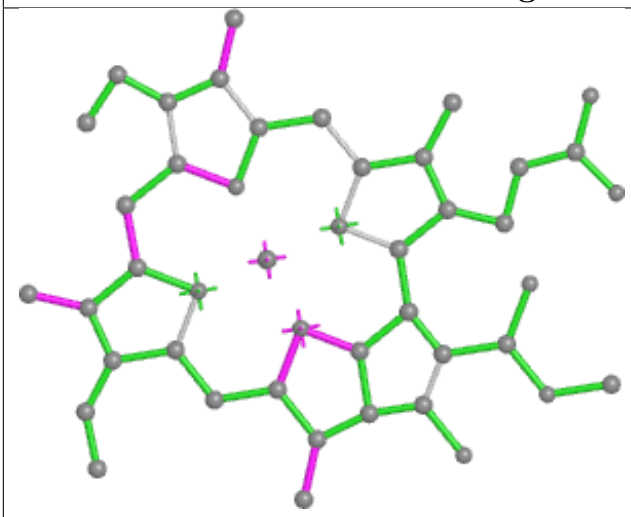


Torsions

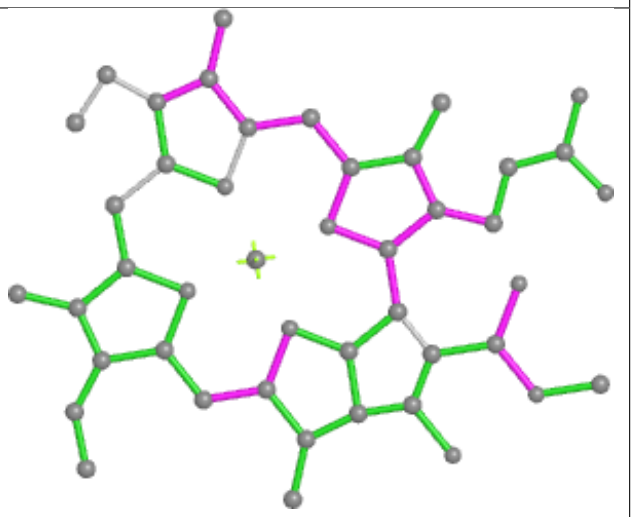


Rings

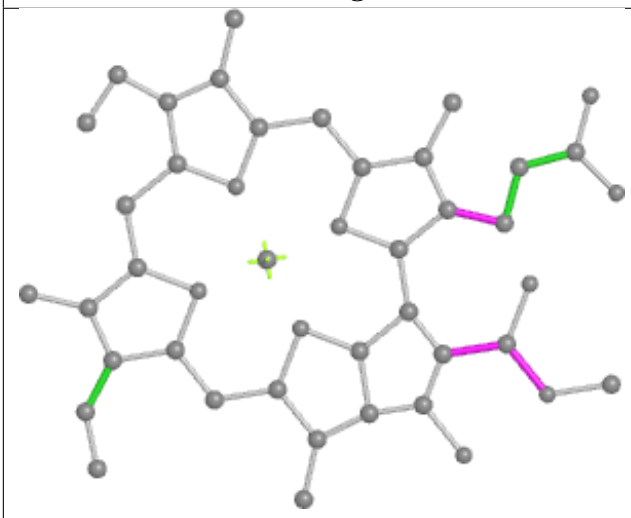
Ligand CLA b3 411



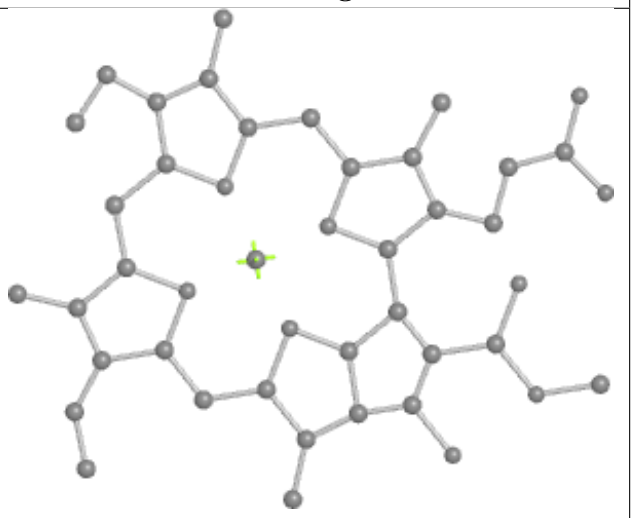
Bond lengths



Bond angles

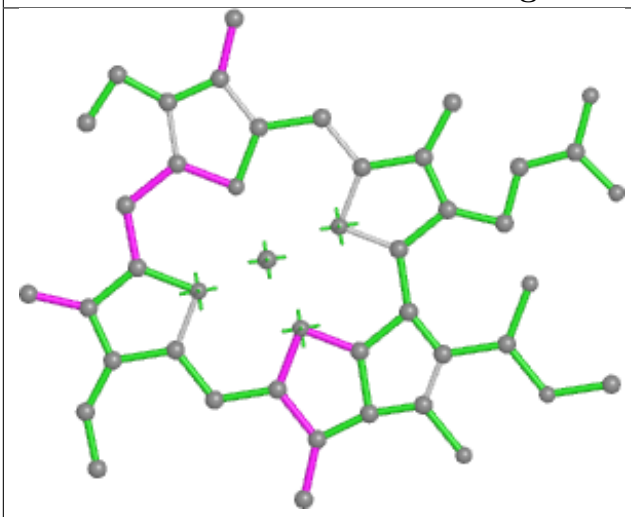


Torsions

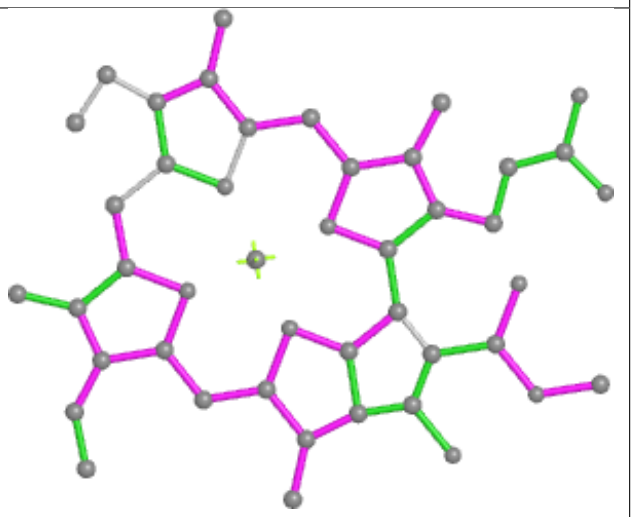


Rings

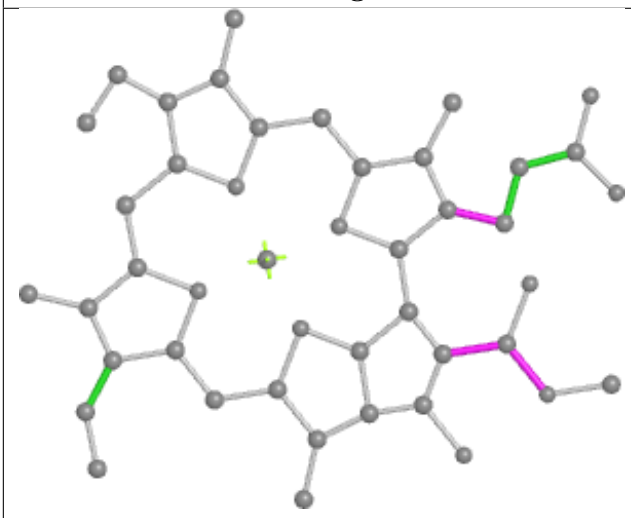
Ligand CLA a4 405



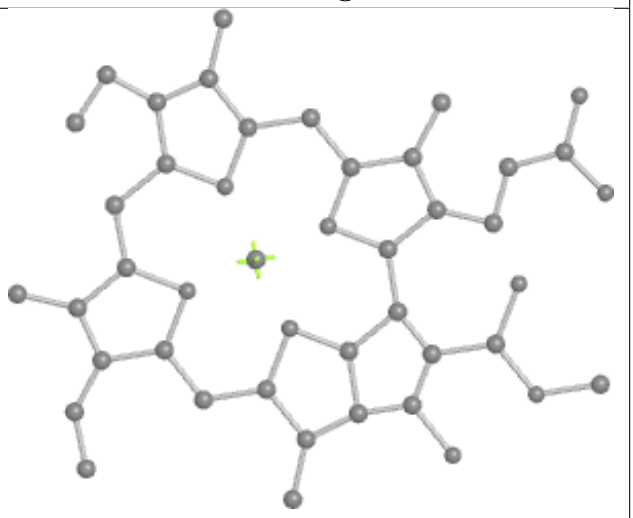
Bond lengths



Bond angles

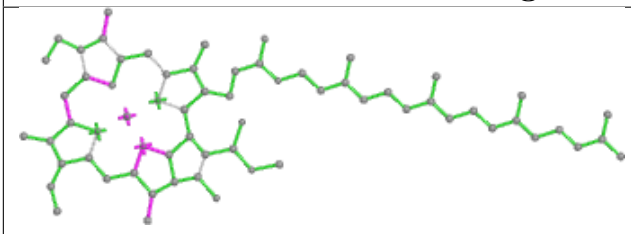


Torsions

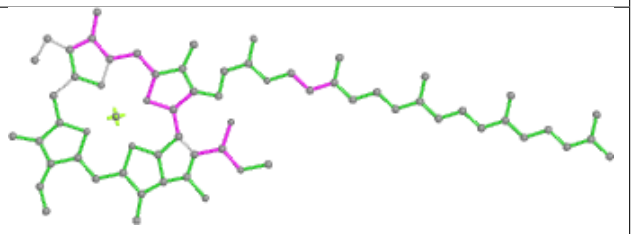


Rings

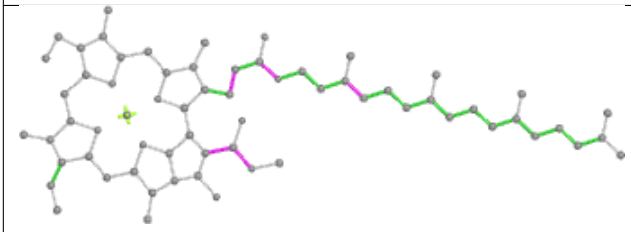
Ligand CLA a5 404



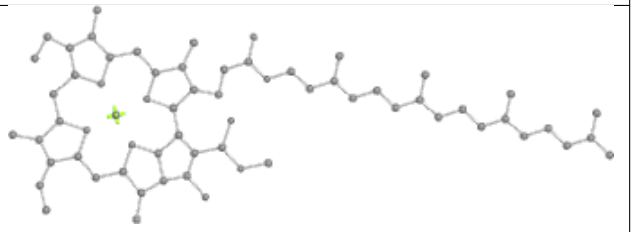
Bond lengths



Bond angles

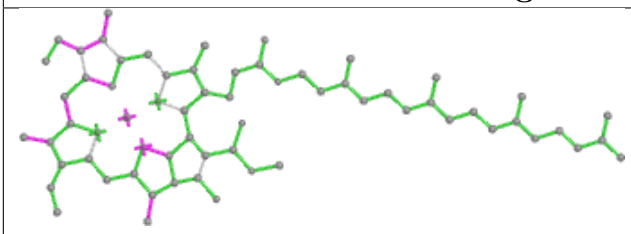


Torsions

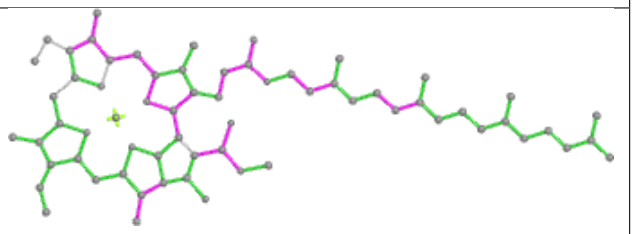


Rings

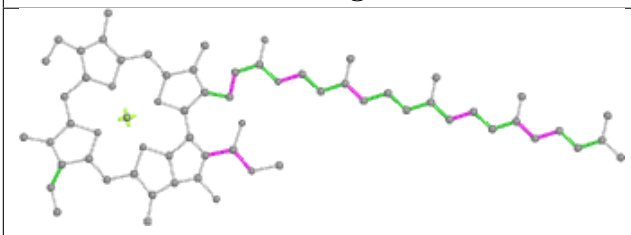
Ligand CLA aB 803



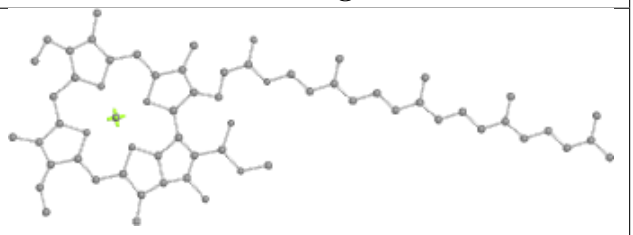
Bond lengths



Bond angles

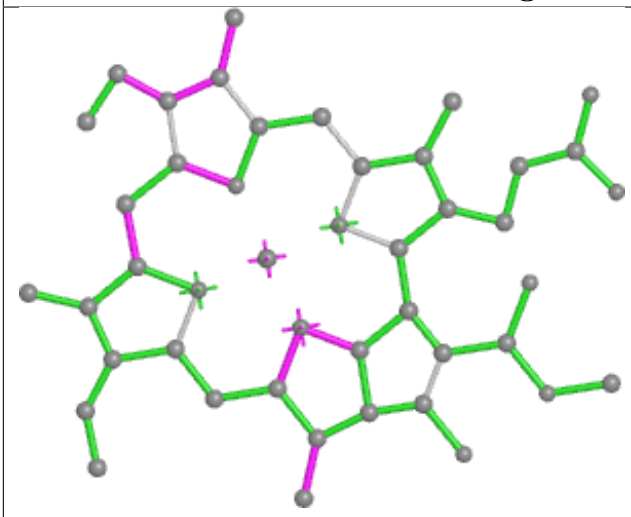


Torsions

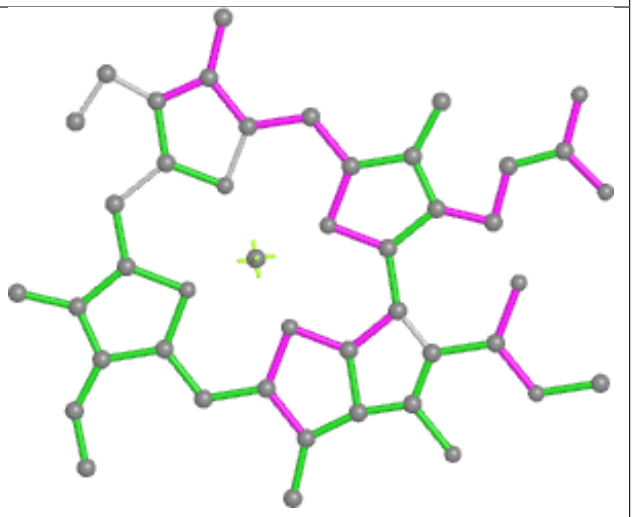


Rings

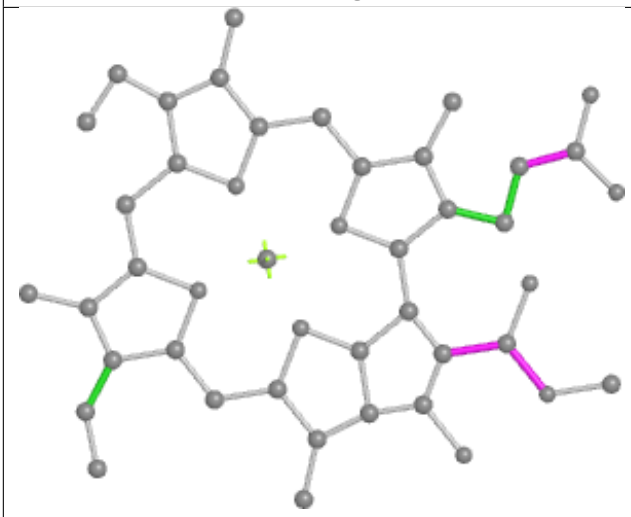
Ligand CLA b6 416



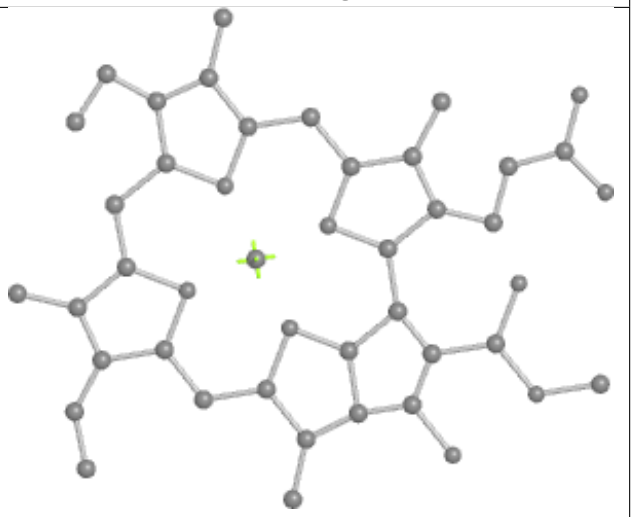
Bond lengths



Bond angles

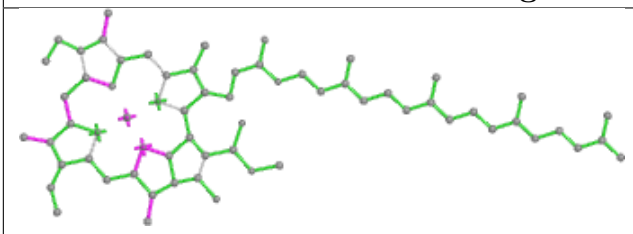


Torsions

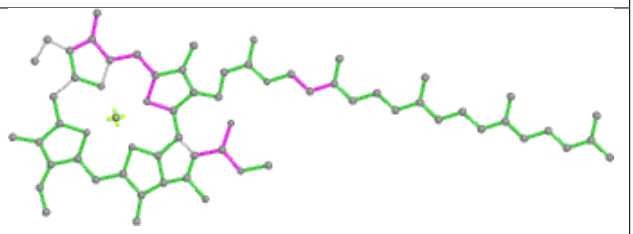


Rings

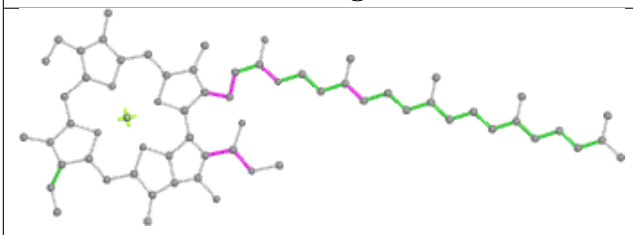
Ligand CLA a4 404



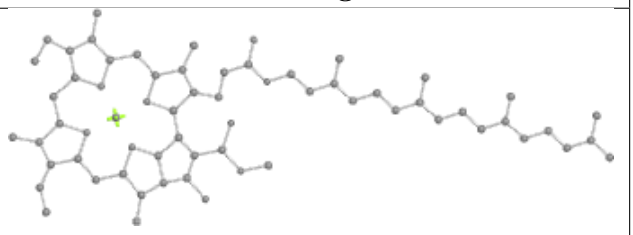
Bond lengths



Bond angles

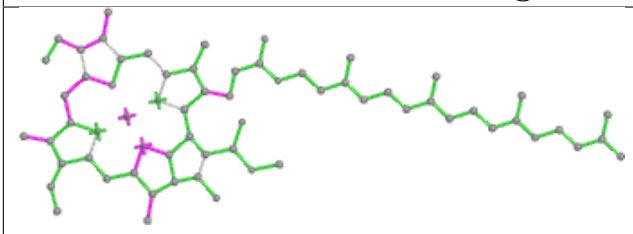


Torsions

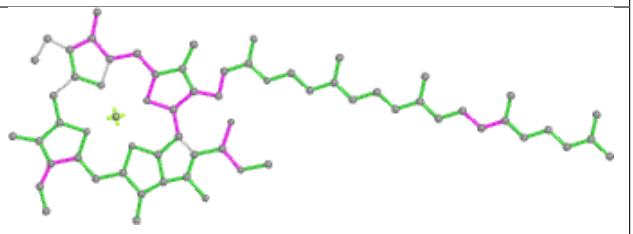


Rings

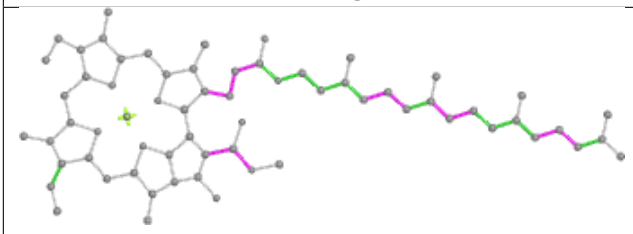
Ligand CLA bB 810



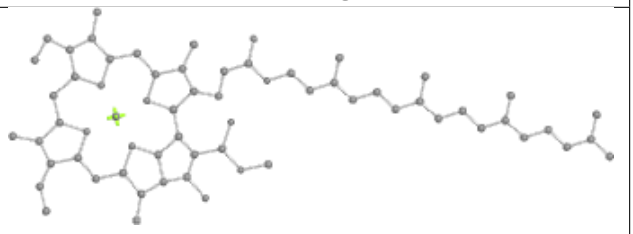
Bond lengths



Bond angles

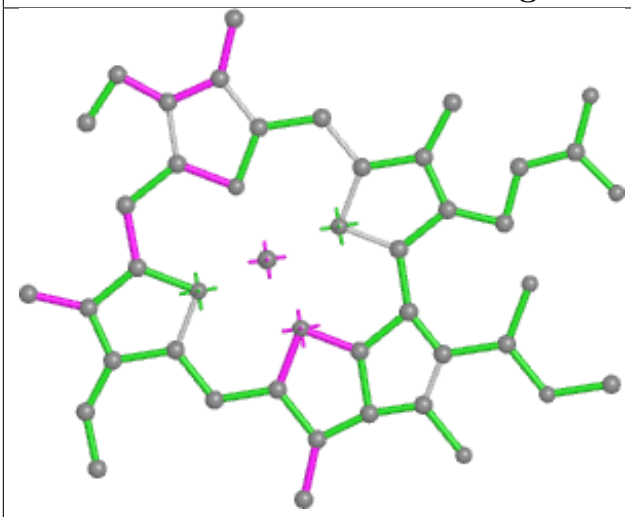


Torsions

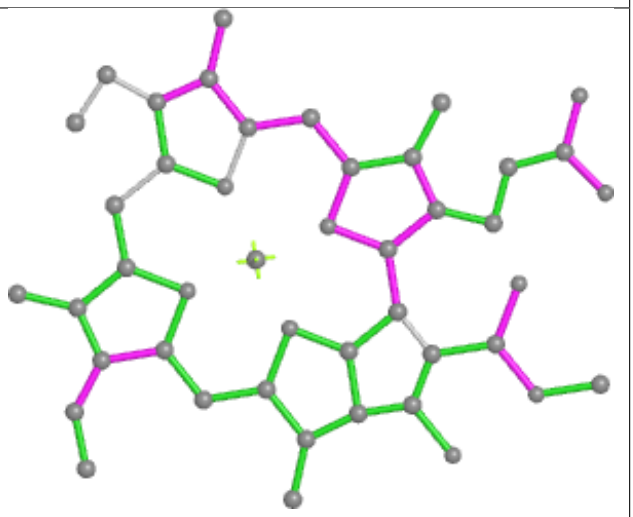


Rings

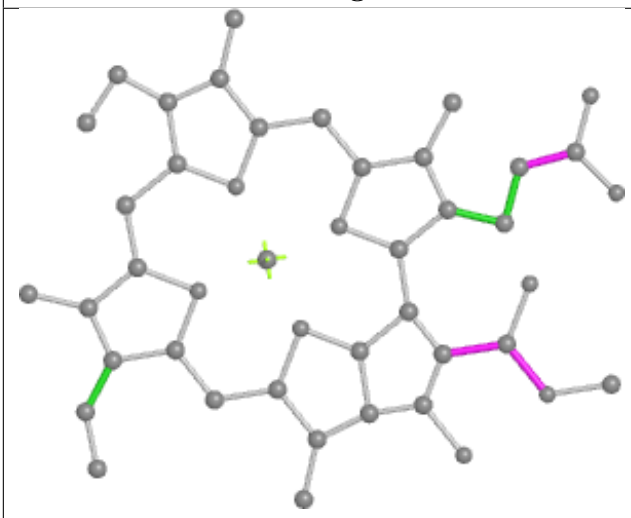
Ligand CLA aJ 201



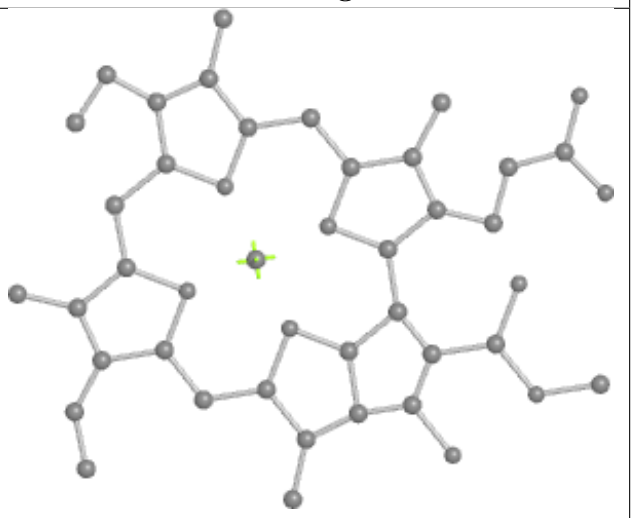
Bond lengths



Bond angles

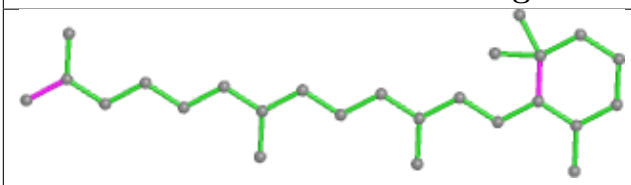


Torsions

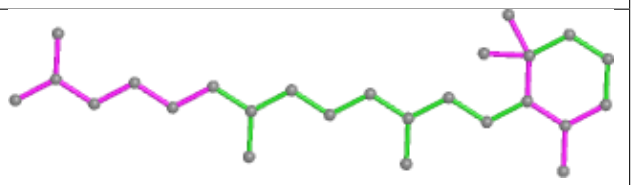


Rings

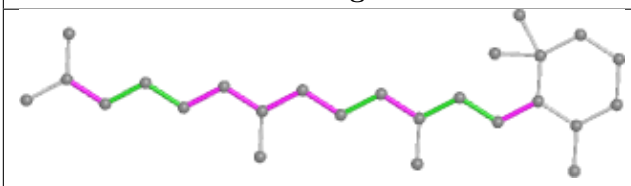
Ligand BCR bB 847



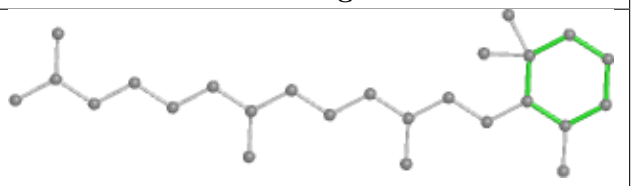
Bond lengths



Bond angles

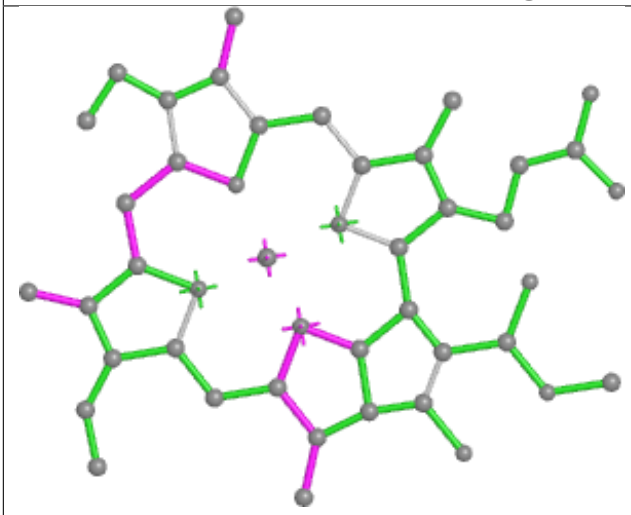


Torsions

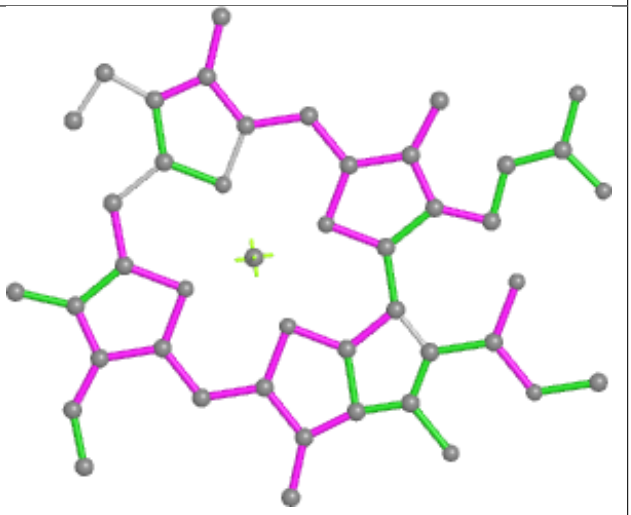


Rings

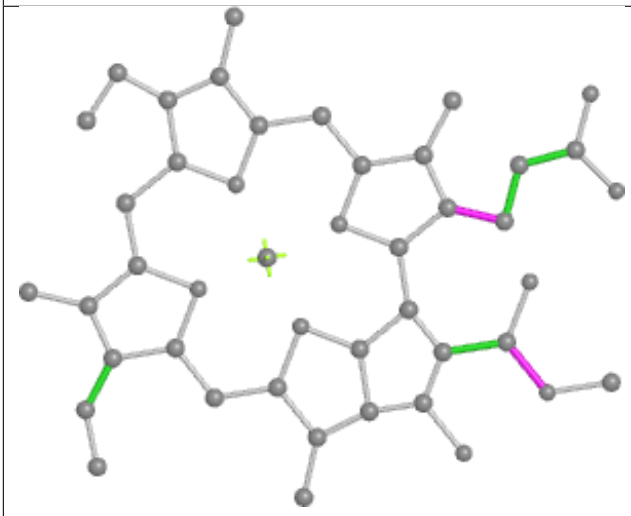
Ligand CLA c3 405



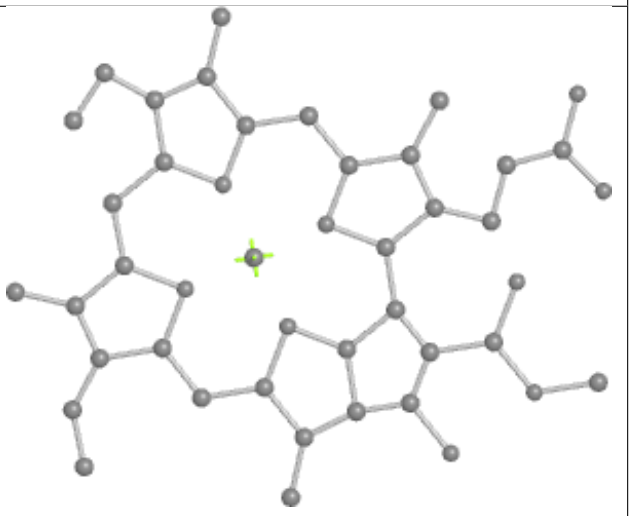
Bond lengths



Bond angles

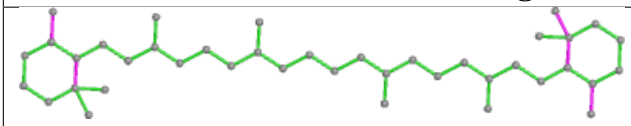


Torsions

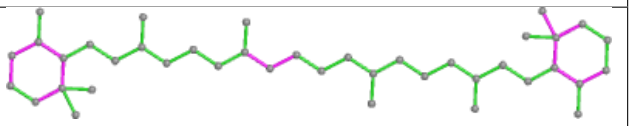


Rings

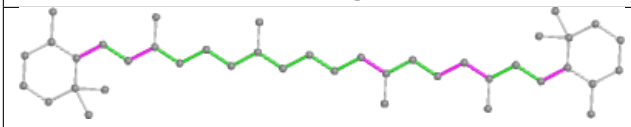
Ligand BCR b1 418



Bond lengths



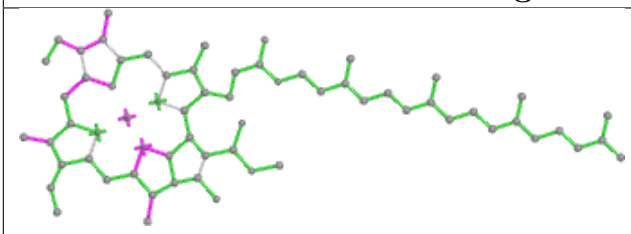
Bond angles



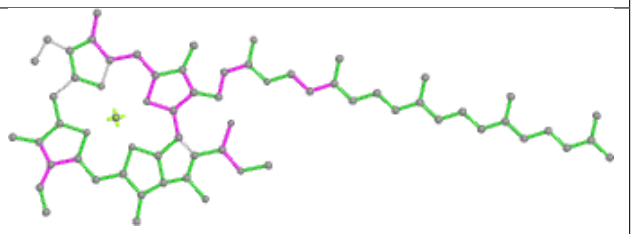
Torsions

Rings

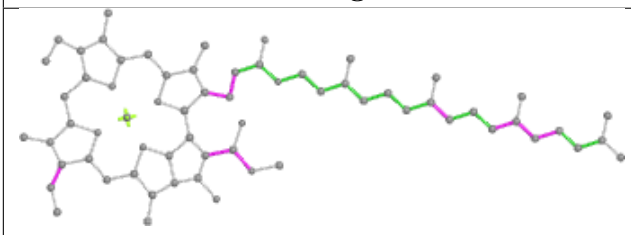
Ligand CLA bB 840



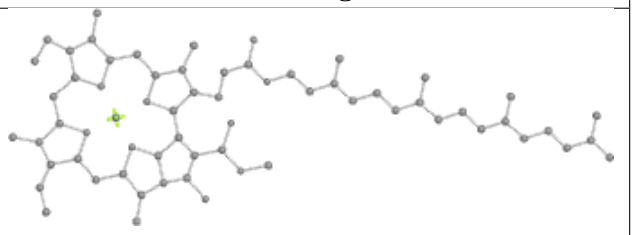
Bond lengths



Bond angles

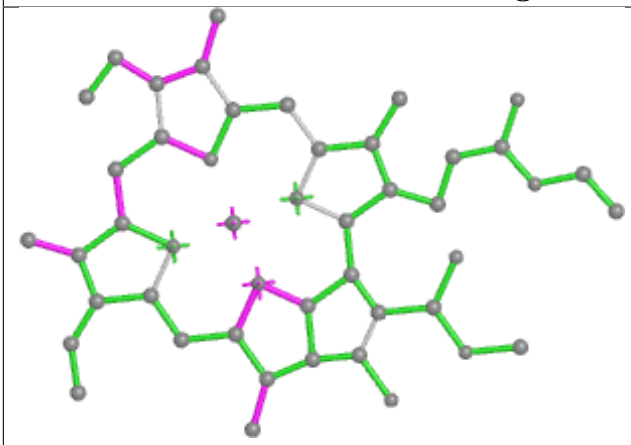


Torsions

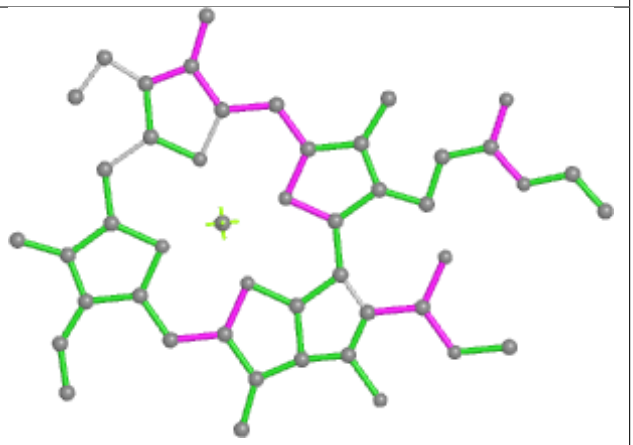


Rings

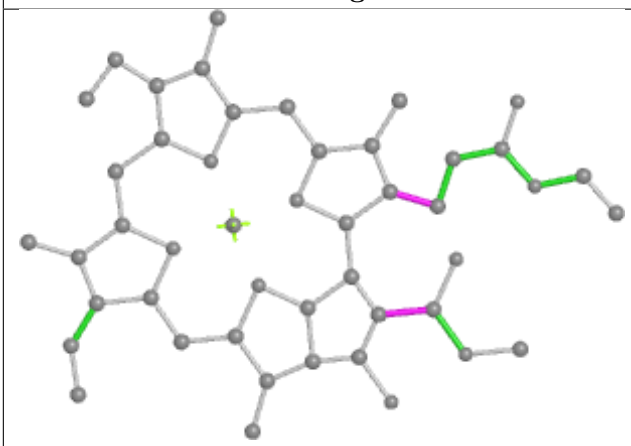
Ligand CLA bB 838



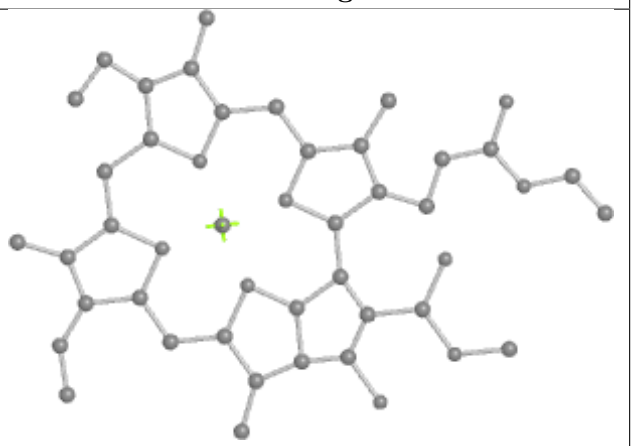
Bond lengths



Bond angles

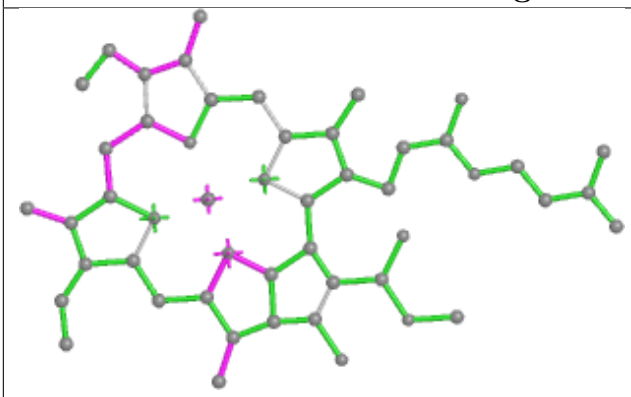


Torsions

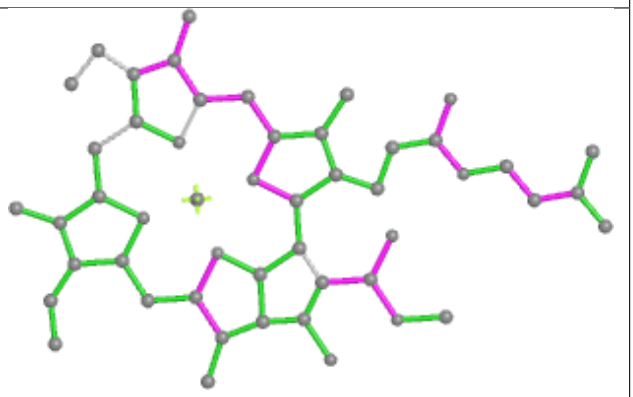


Rings

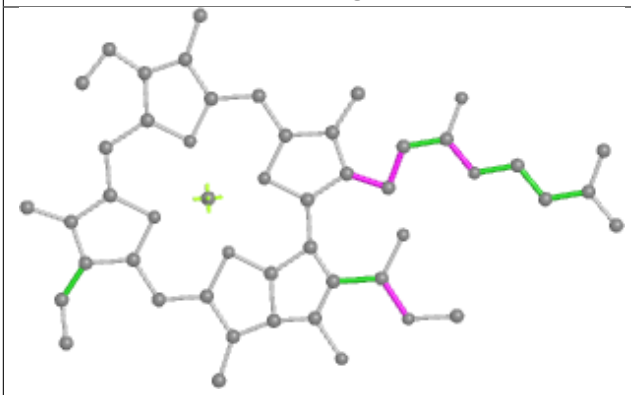
Ligand CLA bA 832



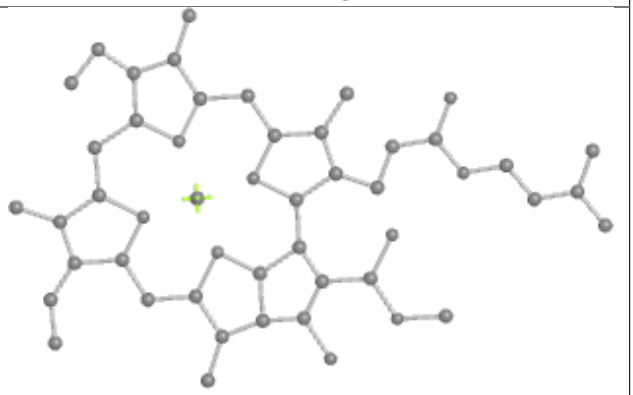
Bond lengths



Bond angles

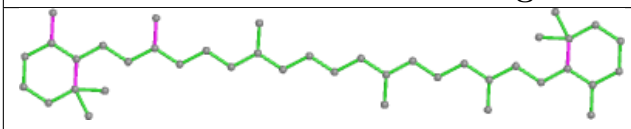


Torsions

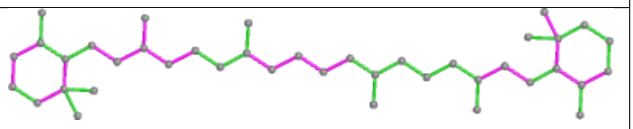


Rings

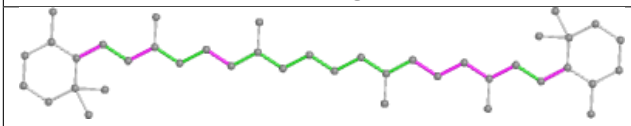
Ligand BCR b1 419



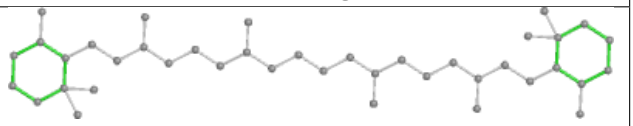
Bond lengths



Bond angles

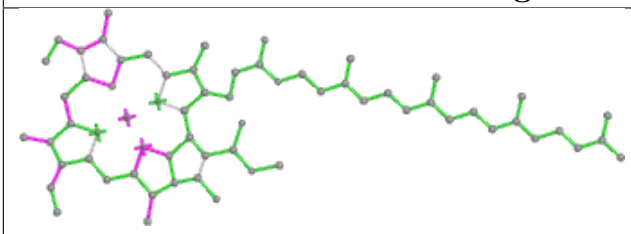


Torsions

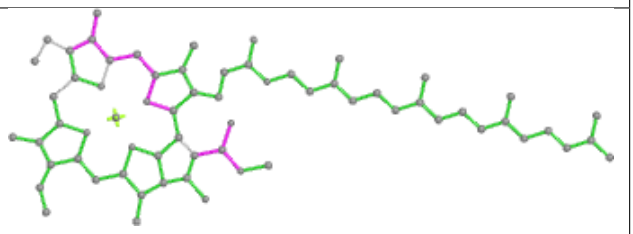


Rings

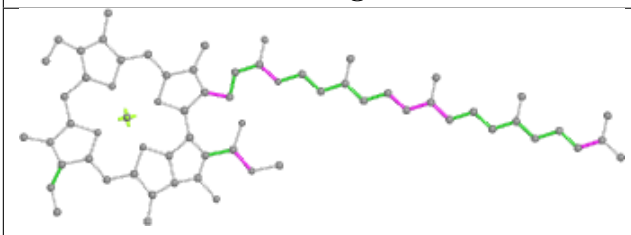
Ligand CLA bA 833



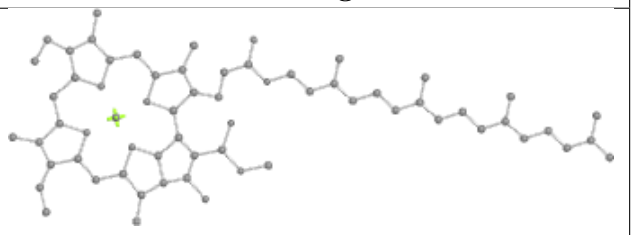
Bond lengths



Bond angles

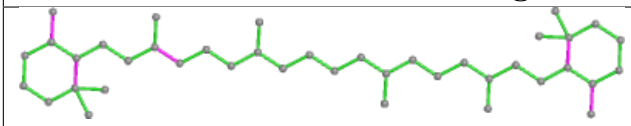


Torsions

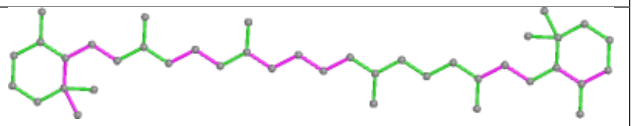


Rings

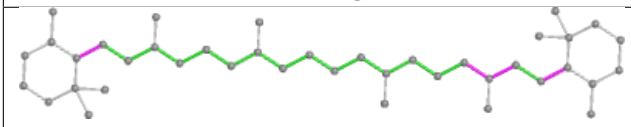
Ligand BCR bA 852



Bond lengths



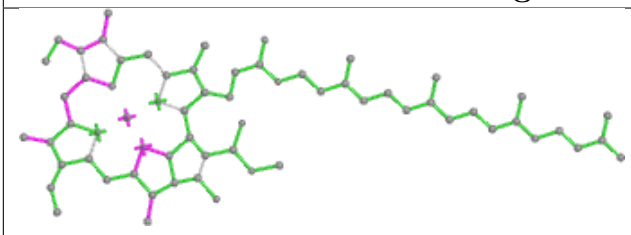
Bond angles



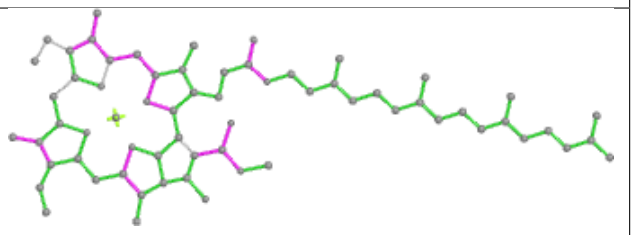
Torsions

Rings

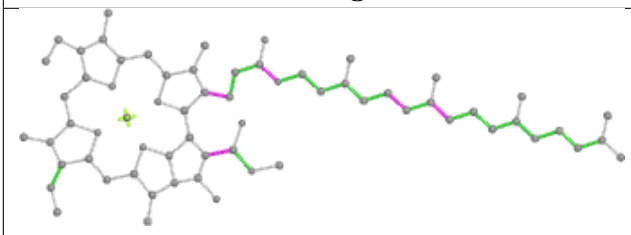
Ligand CLA bA 831



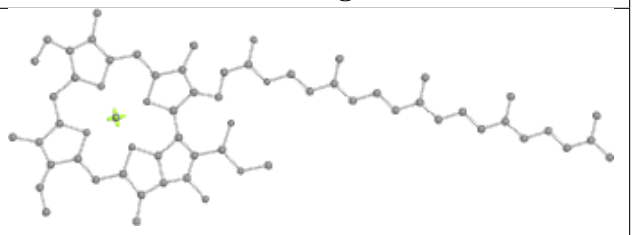
Bond lengths



Bond angles

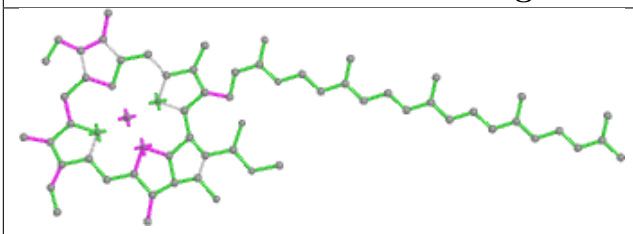


Torsions

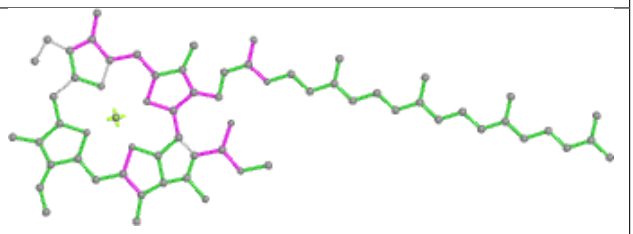


Rings

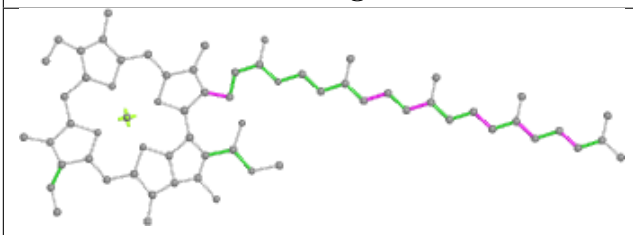
Ligand CLA aA 807



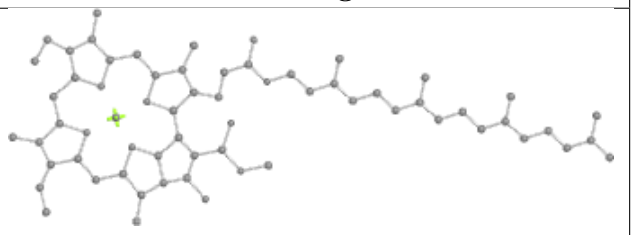
Bond lengths



Bond angles

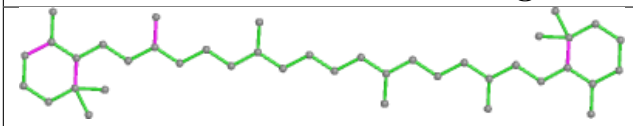


Torsions

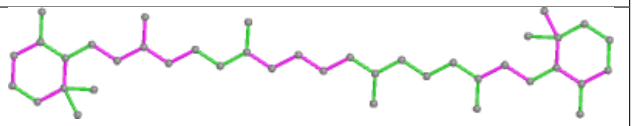


Rings

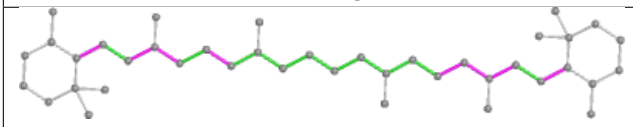
Ligand BCR b6 401



Bond lengths



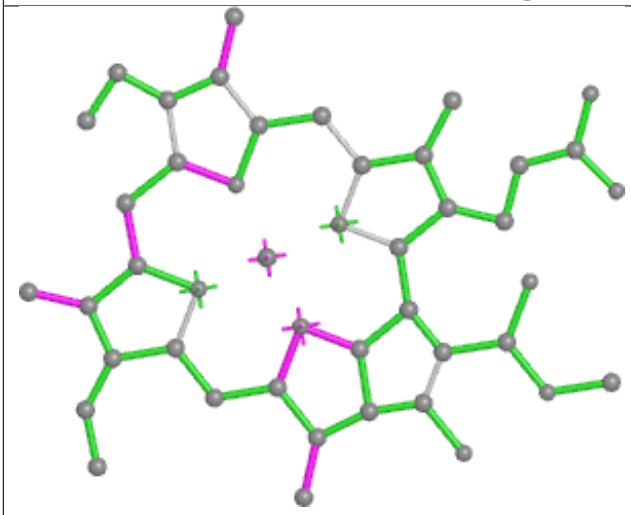
Bond angles



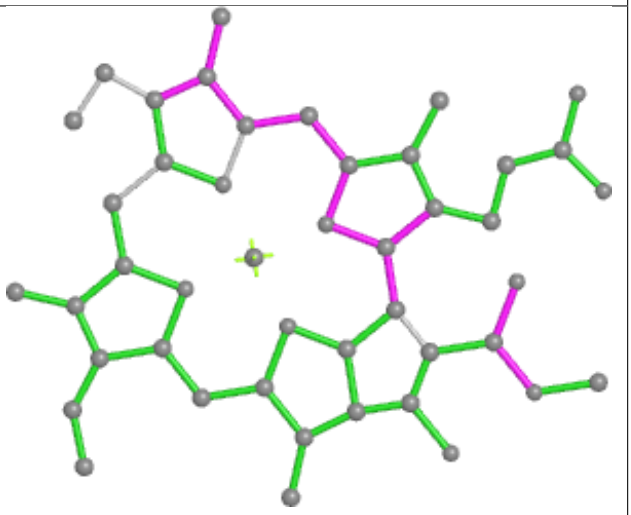
Torsions

Rings

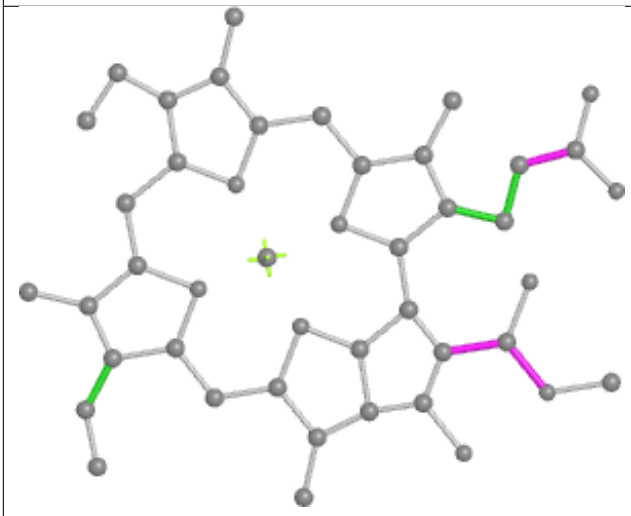
Ligand CLA b3 407



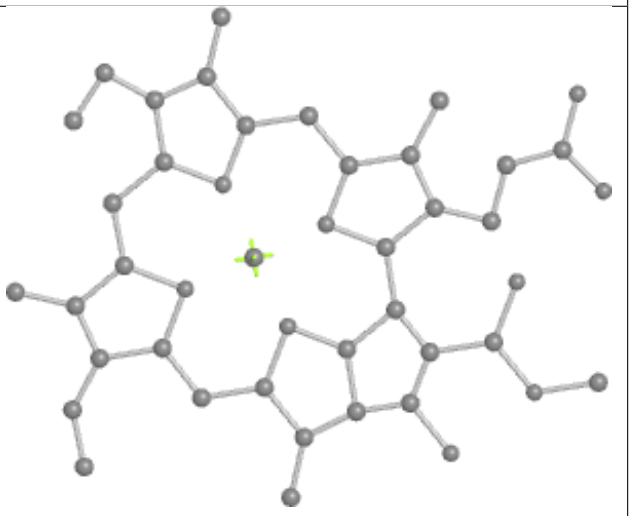
Bond lengths



Bond angles

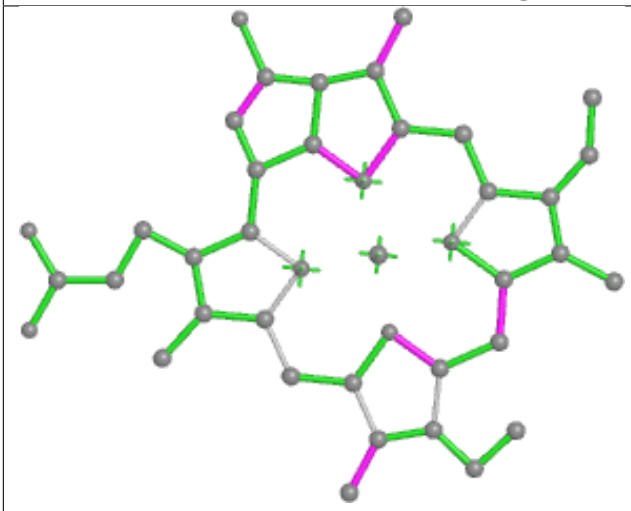


Torsions

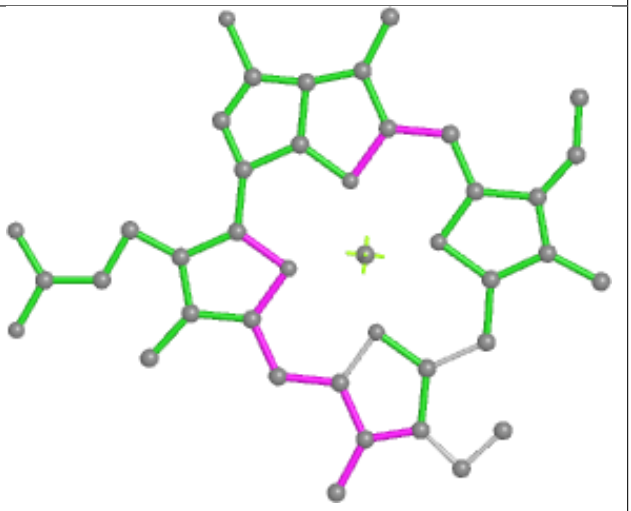


Rings

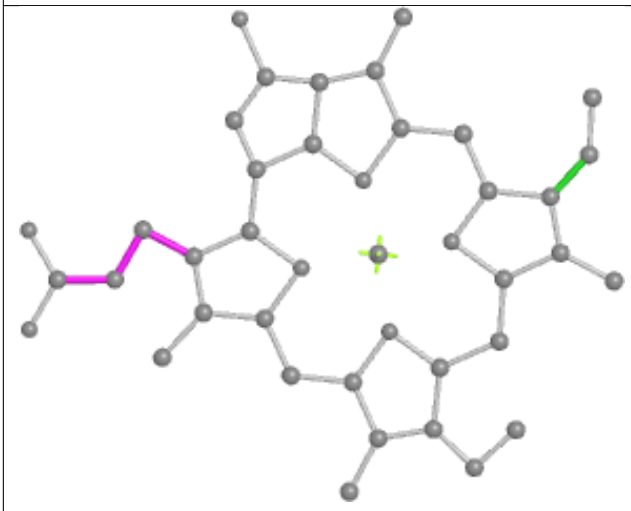
Ligand CLA aA 844



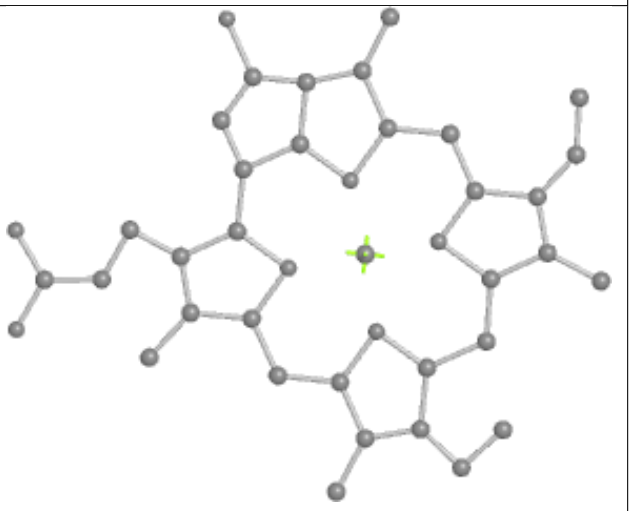
Bond lengths



Bond angles

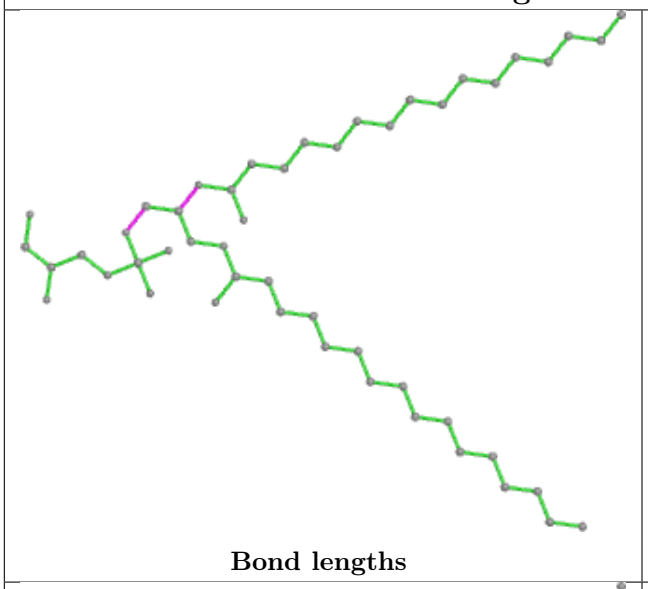


Torsions

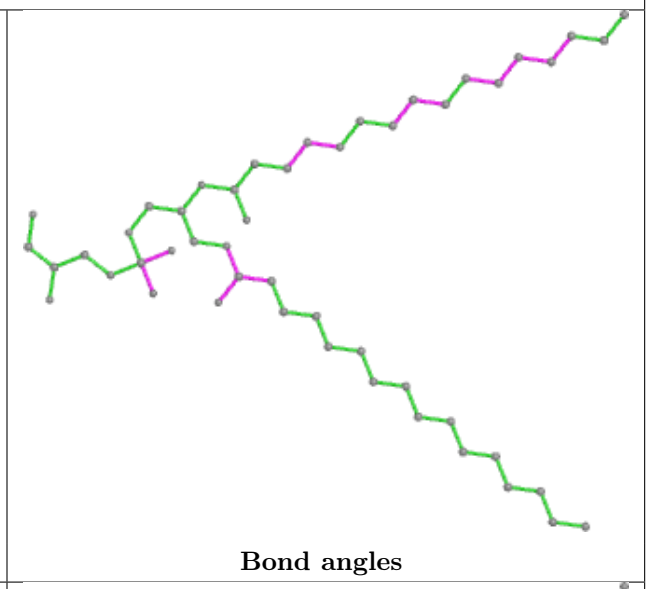


Rings

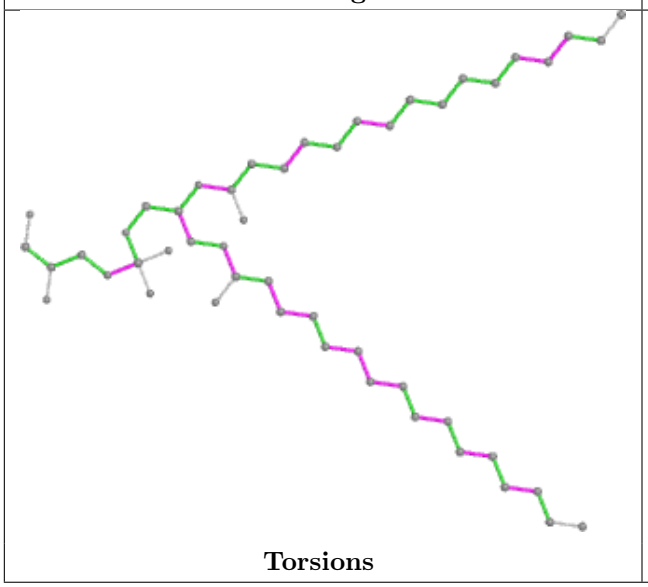
Ligand LHG bA 854



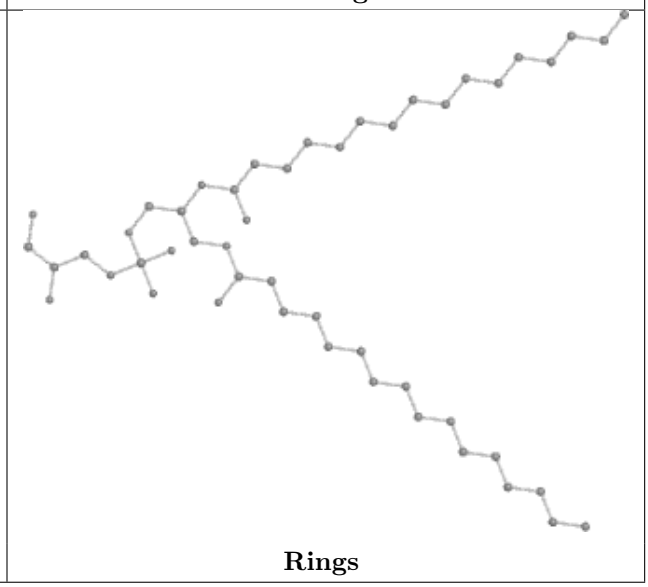
Bond lengths



Bond angles

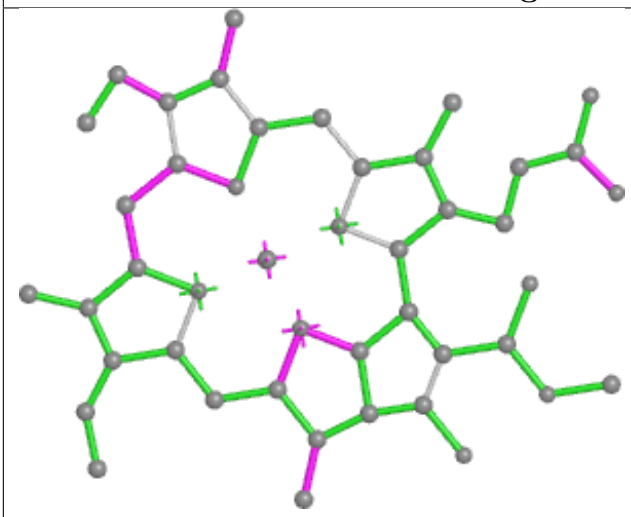


Torsions

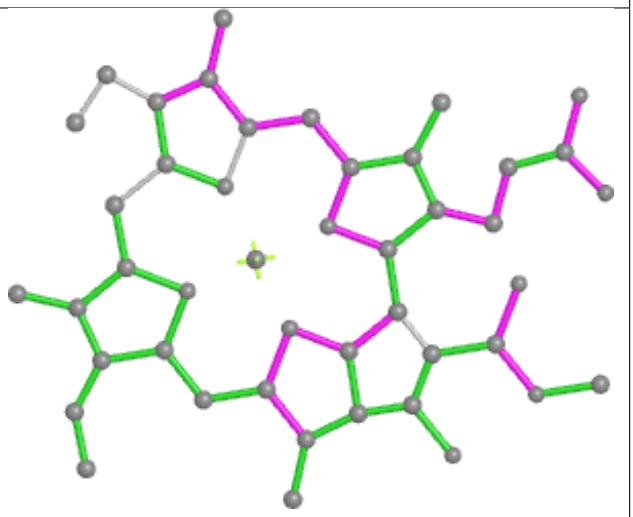


Rings

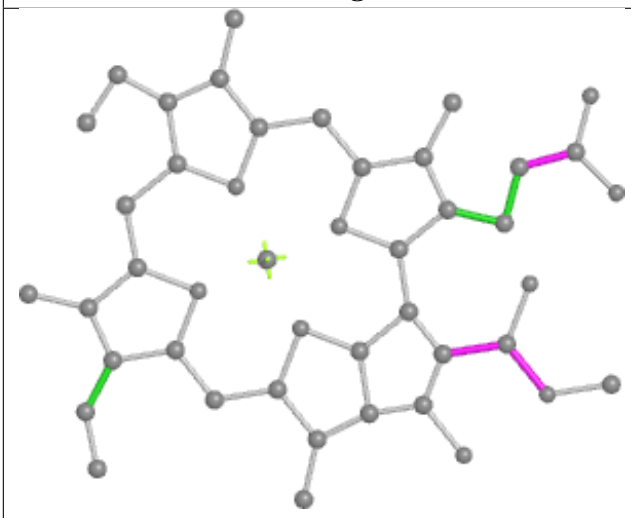
Ligand CLA c3 415



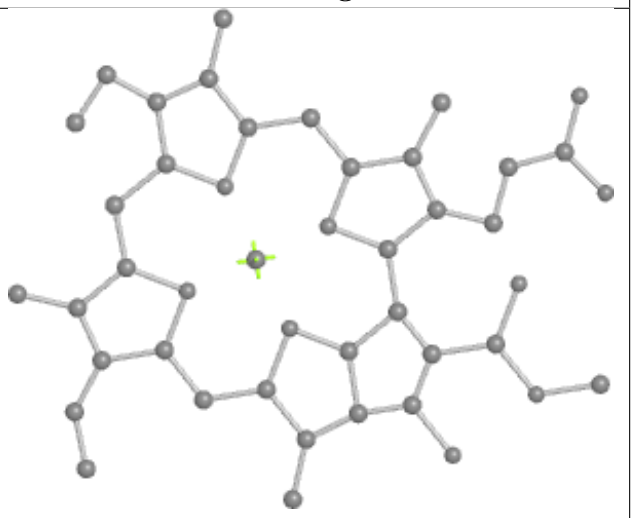
Bond lengths



Bond angles

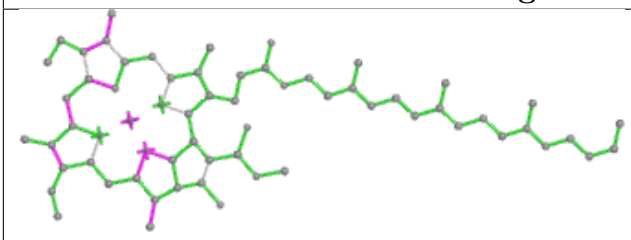


Torsions

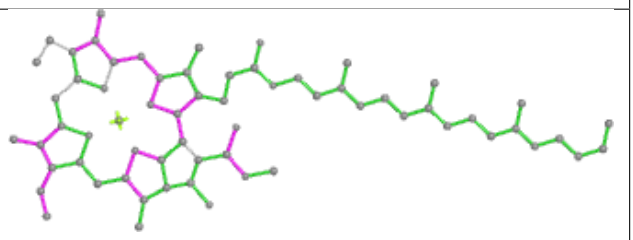


Rings

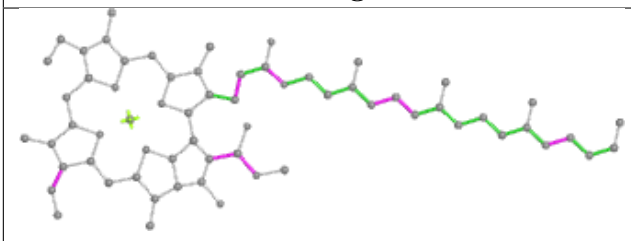
Ligand CLA b2 411



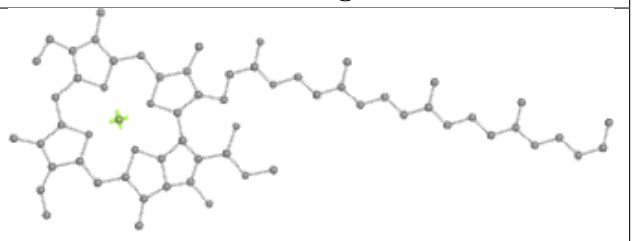
Bond lengths



Bond angles

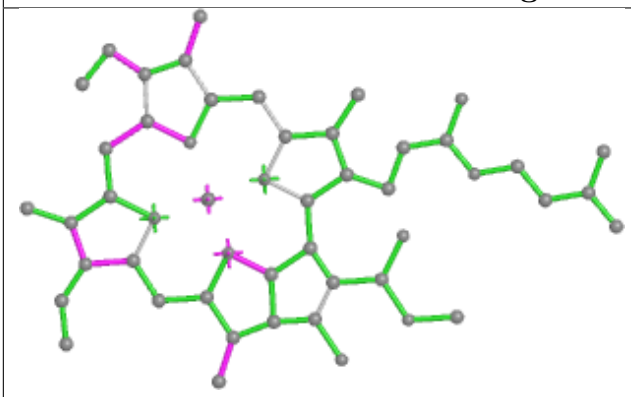


Torsions

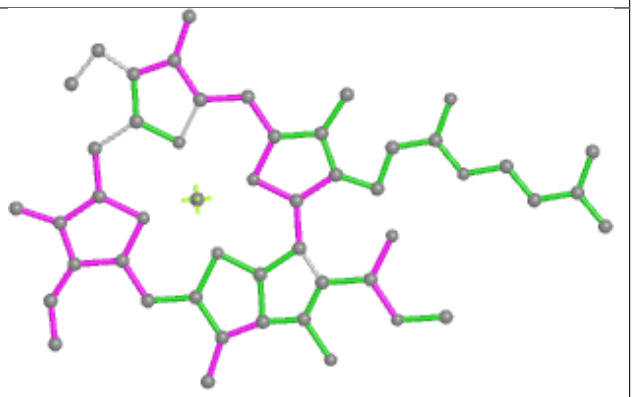


Rings

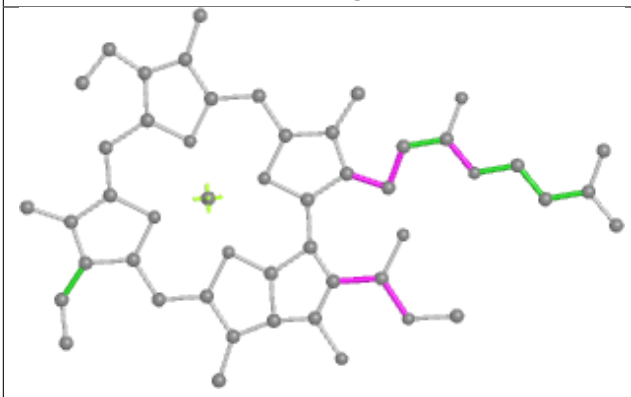
Ligand CLA c5 416



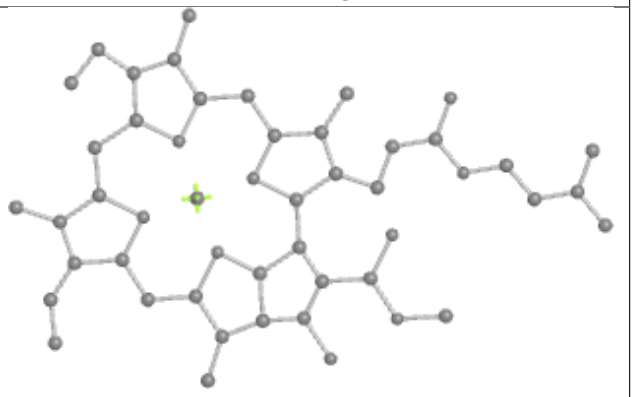
Bond lengths



Bond angles

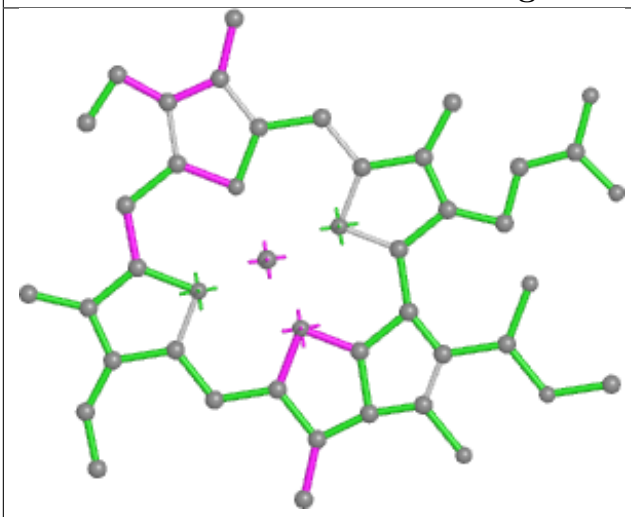


Torsions

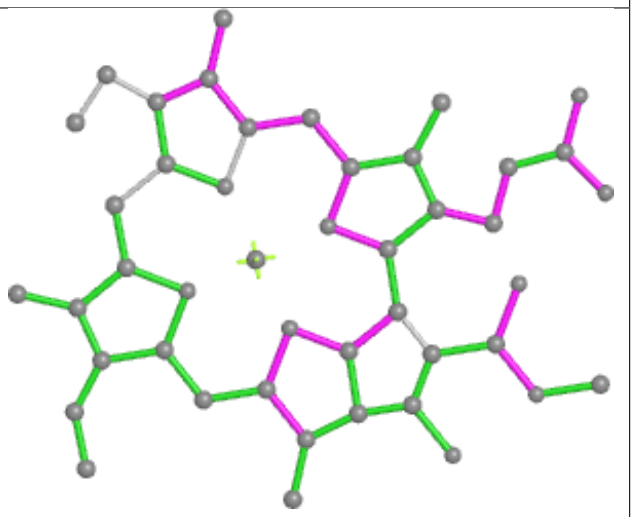


Rings

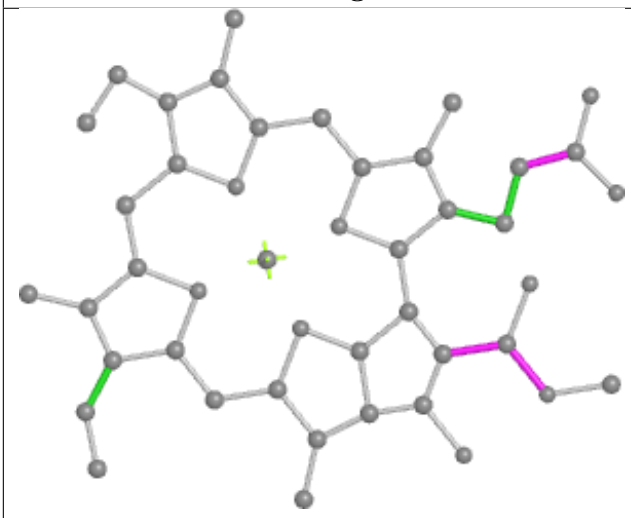
Ligand CLA b1 415



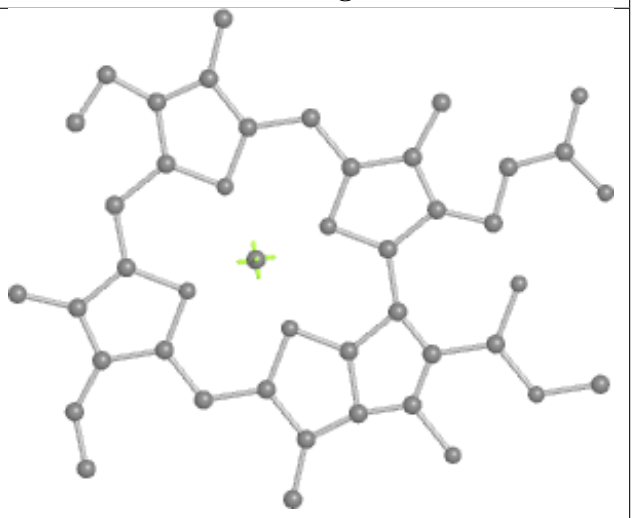
Bond lengths



Bond angles

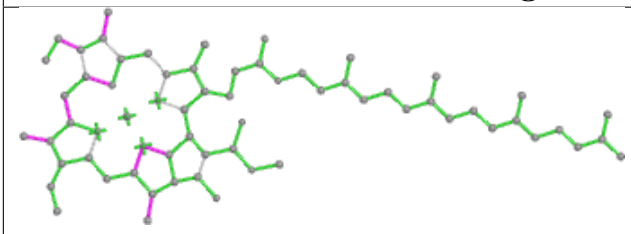


Torsions

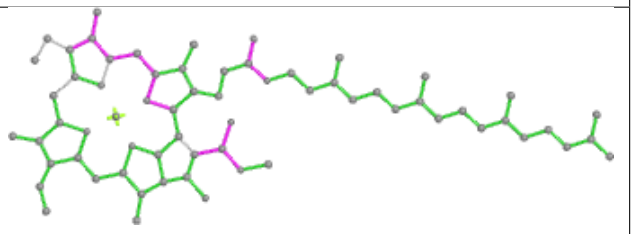


Rings

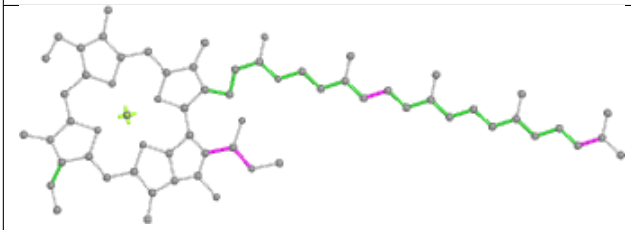
Ligand CLA a3 409



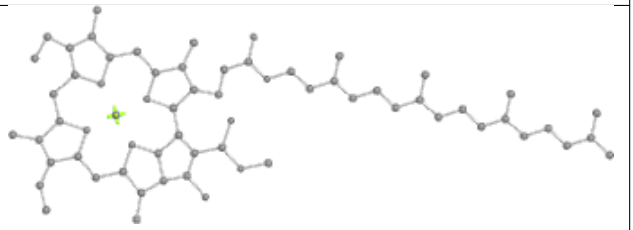
Bond lengths



Bond angles

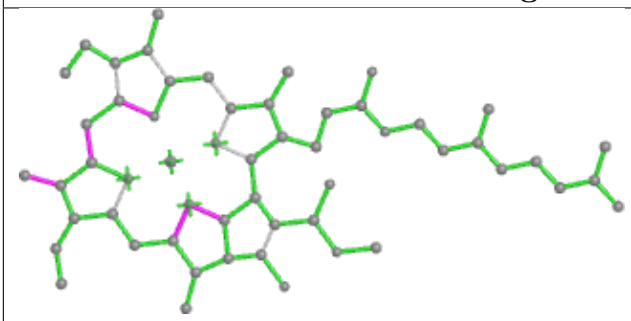


Torsions

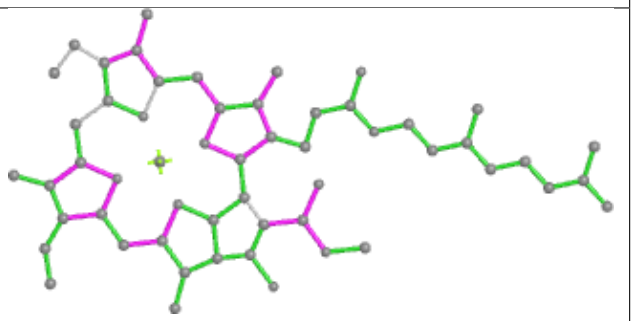


Rings

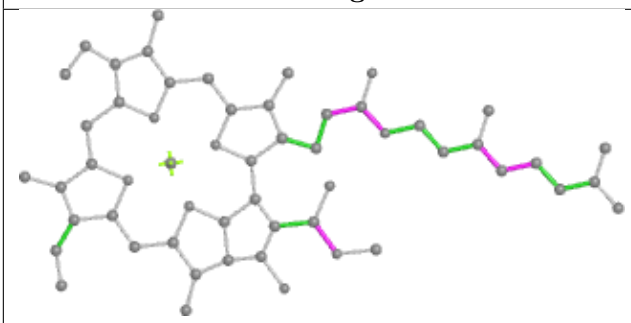
Ligand CLA c5 417



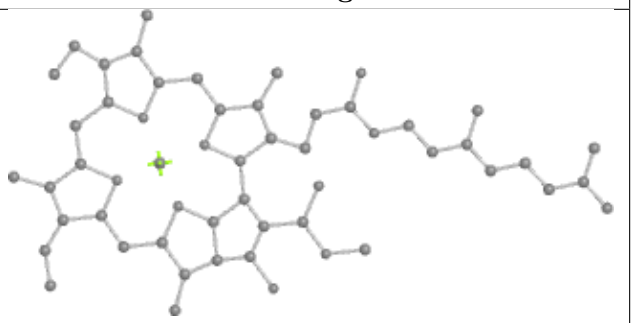
Bond lengths



Bond angles

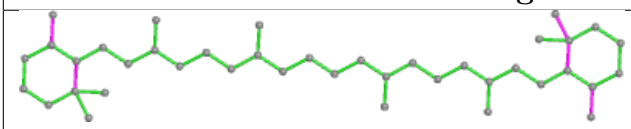


Torsions

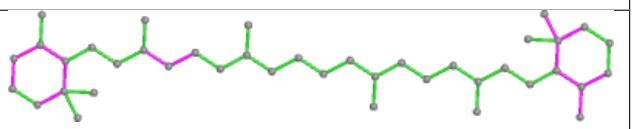


Rings

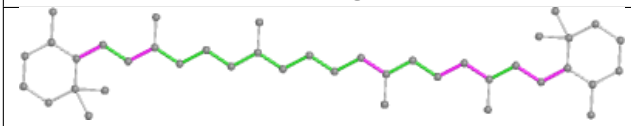
Ligand BCR b2 419



Bond lengths



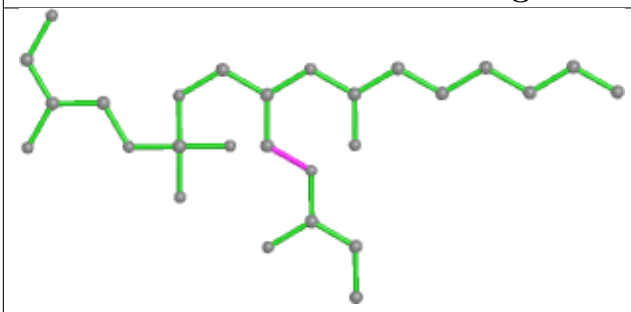
Bond angles



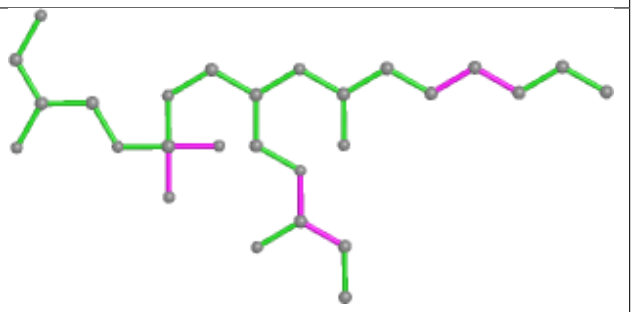
Torsions

Rings

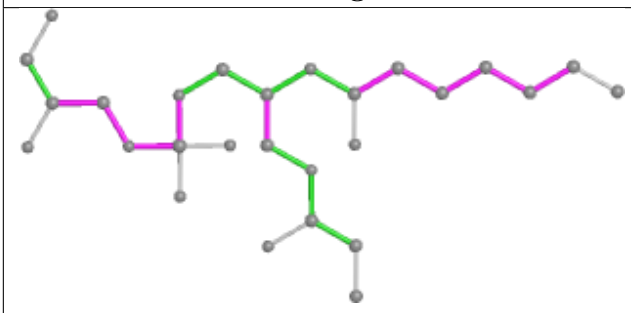
Ligand LHG bA 855



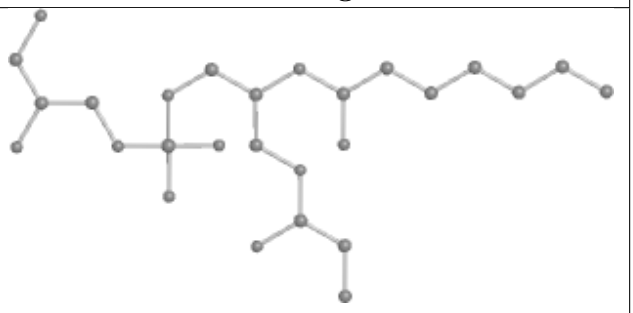
Bond lengths



Bond angles

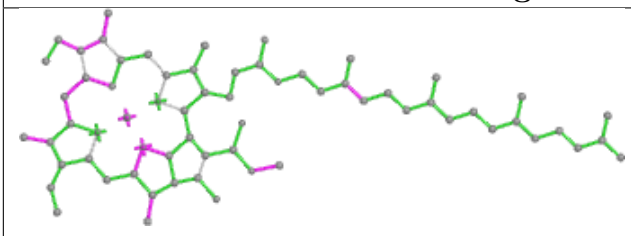


Torsions

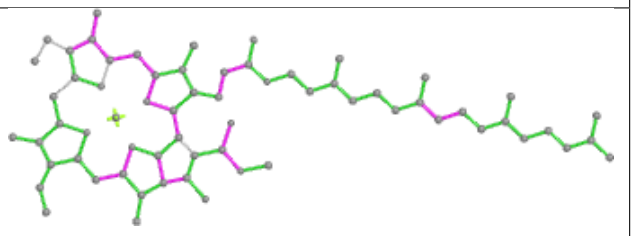


Rings

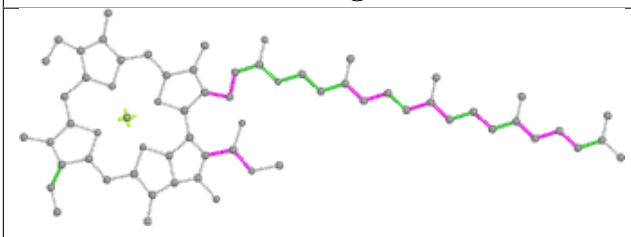
Ligand CLA bA 802



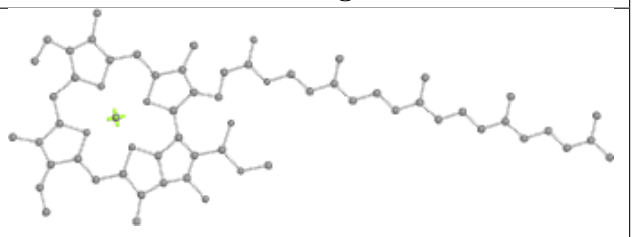
Bond lengths



Bond angles

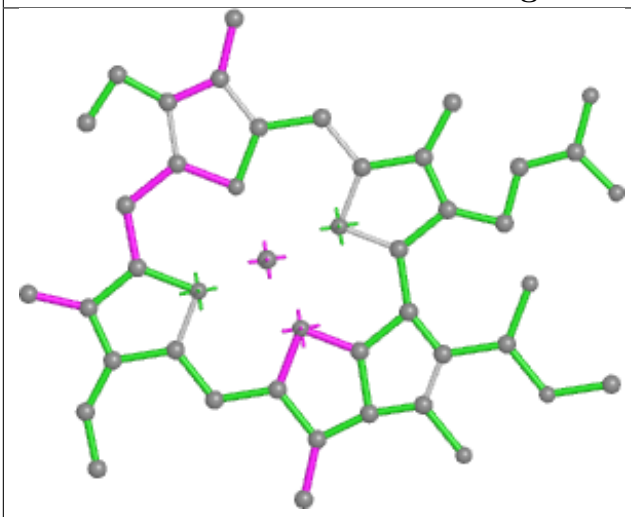


Torsions

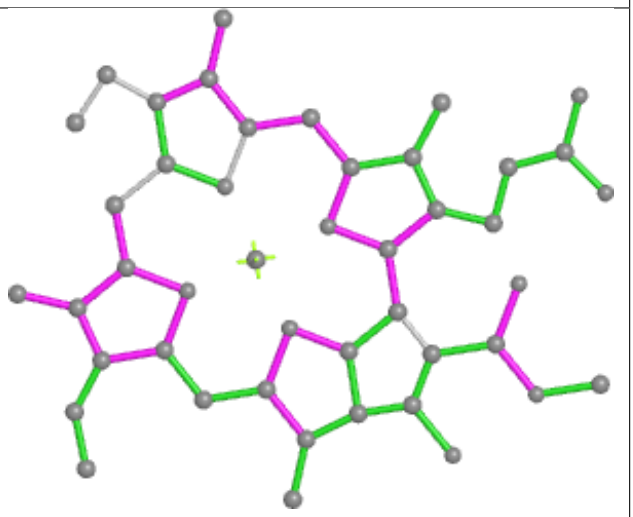


Rings

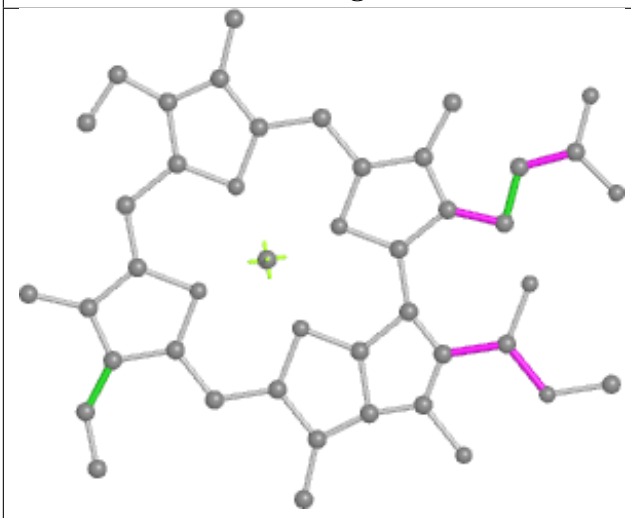
Ligand CLA c3 412



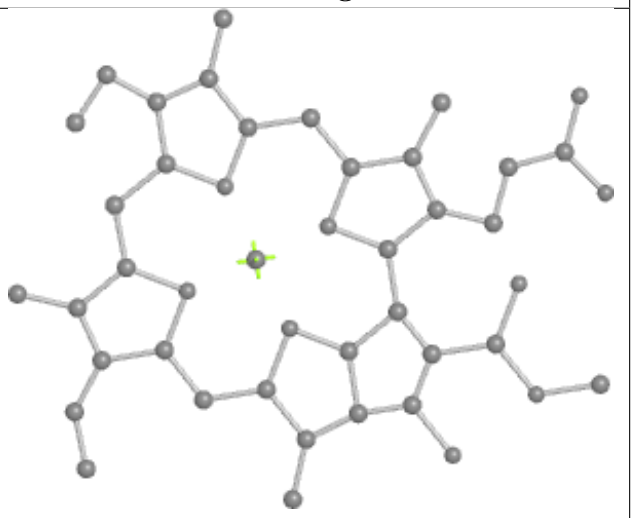
Bond lengths



Bond angles

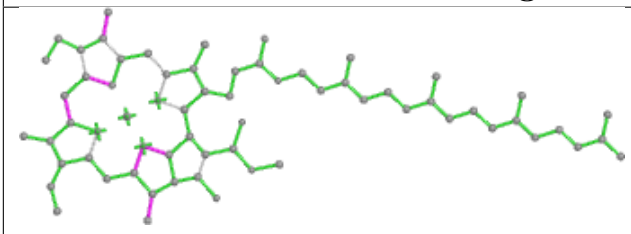


Torsions

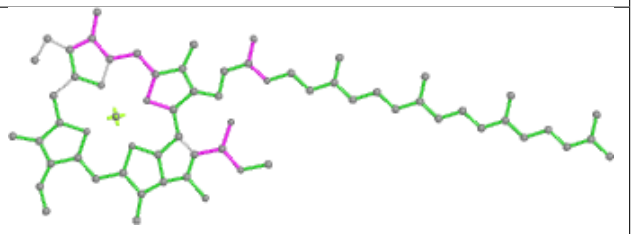


Rings

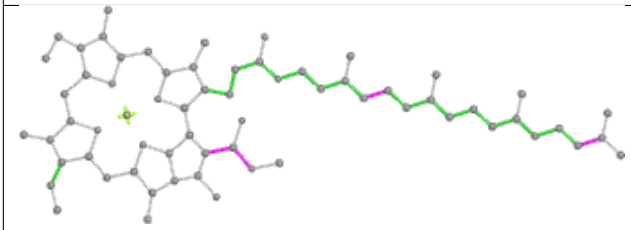
Ligand CLA b4 409



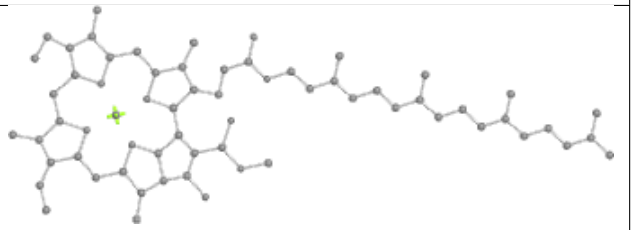
Bond lengths



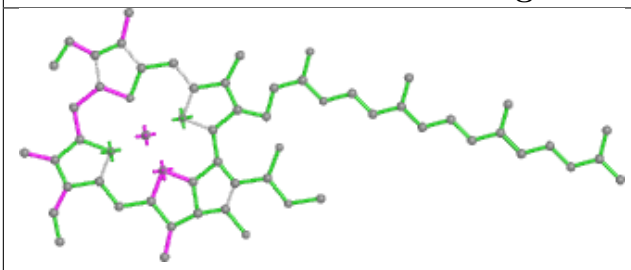
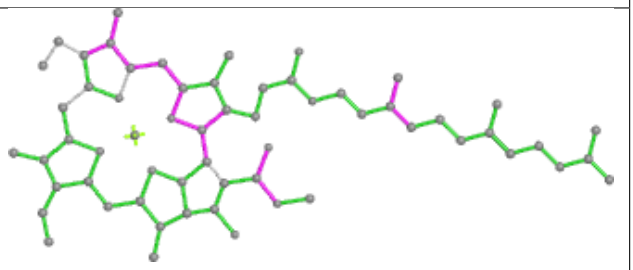
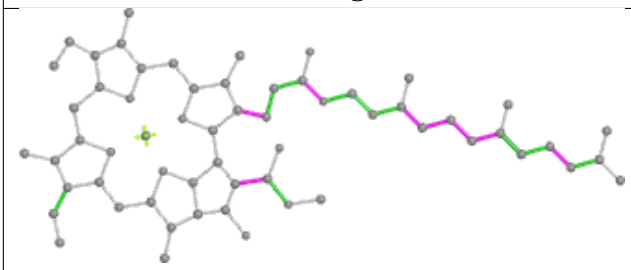
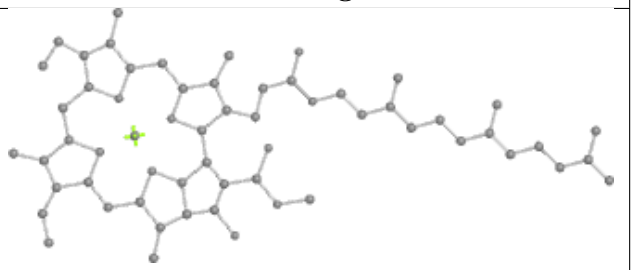
Bond angles

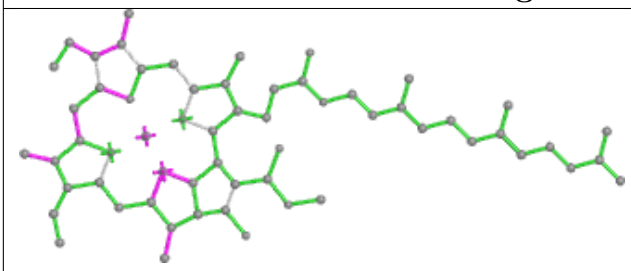
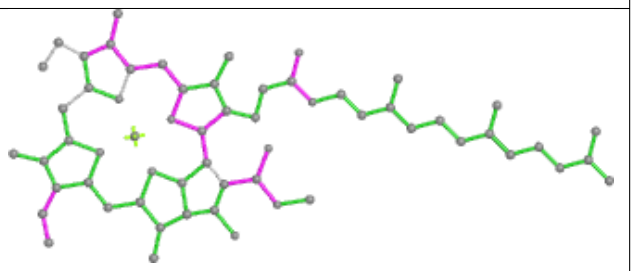
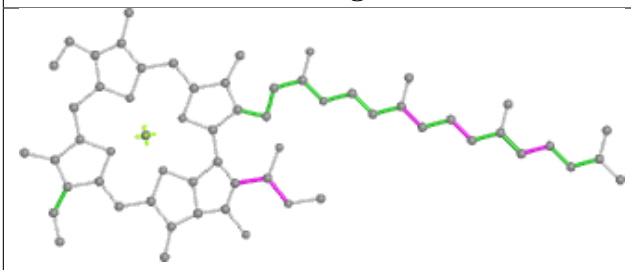
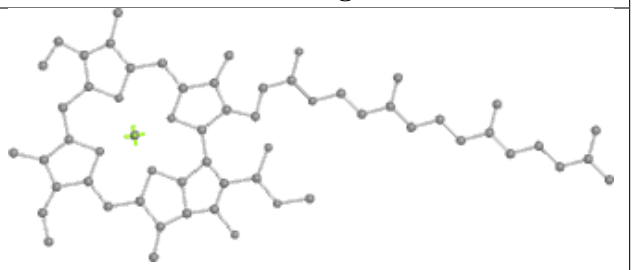


Torsions

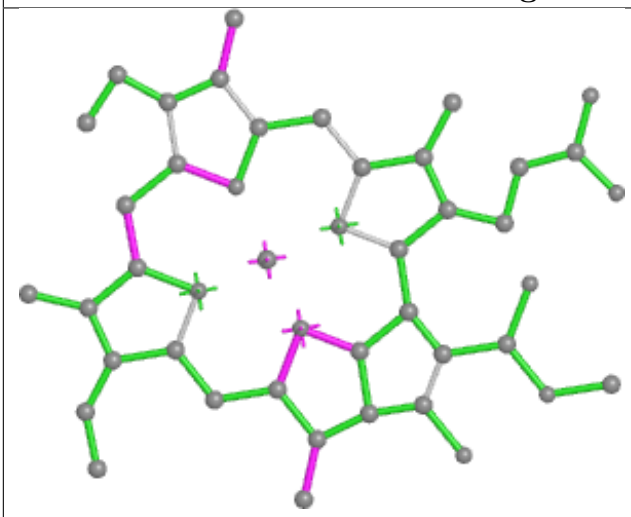


Rings

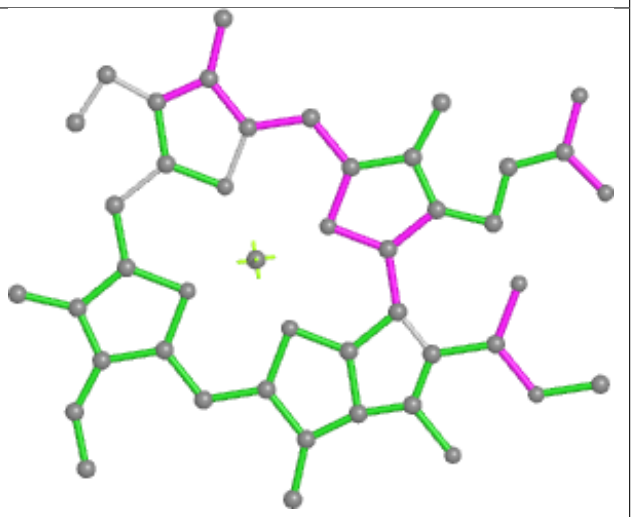
Ligand CLA aB 819	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA aB 836	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

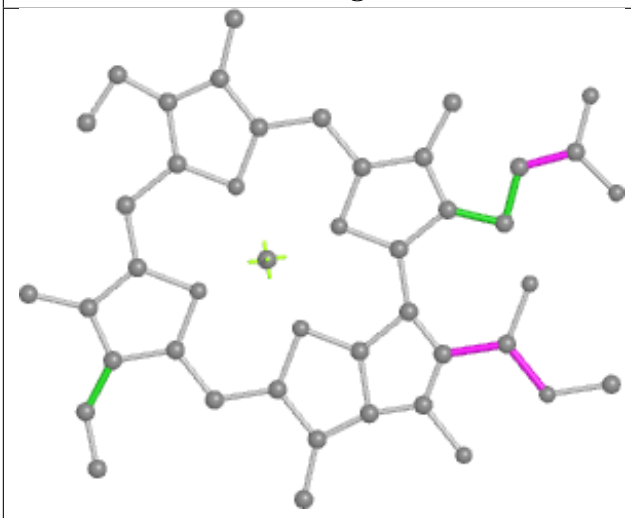
Ligand CLA a6 408



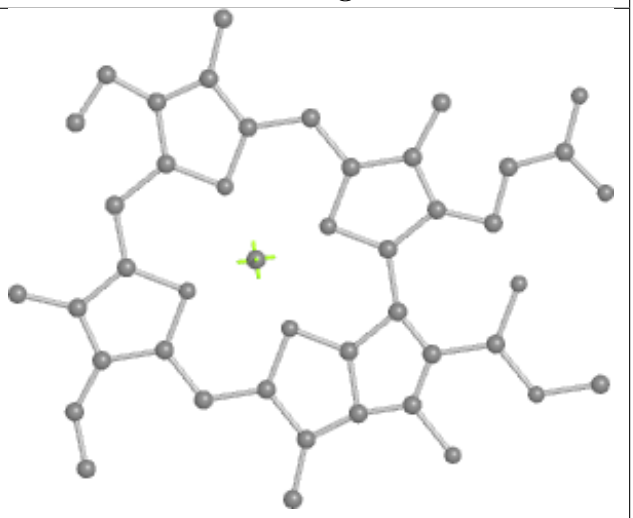
Bond lengths



Bond angles

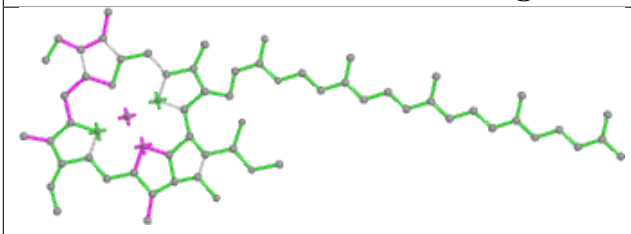


Torsions

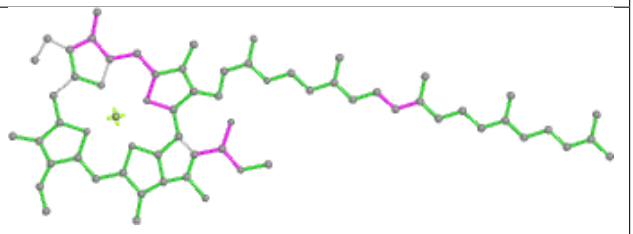


Rings

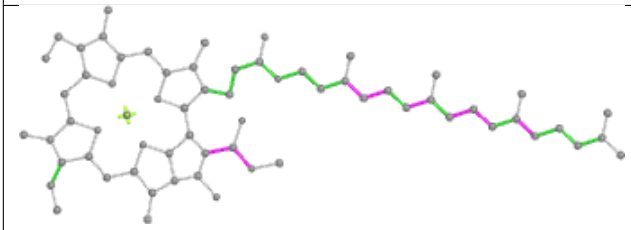
Ligand CLA aA 839



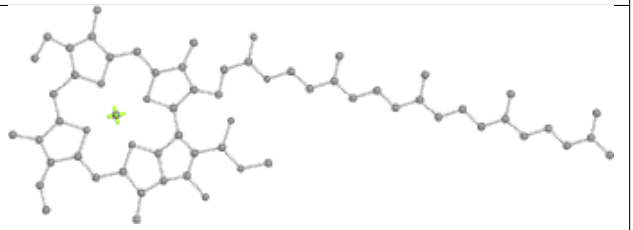
Bond lengths



Bond angles

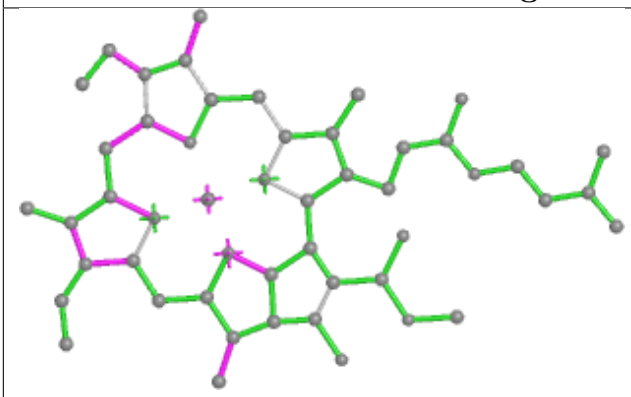


Torsions

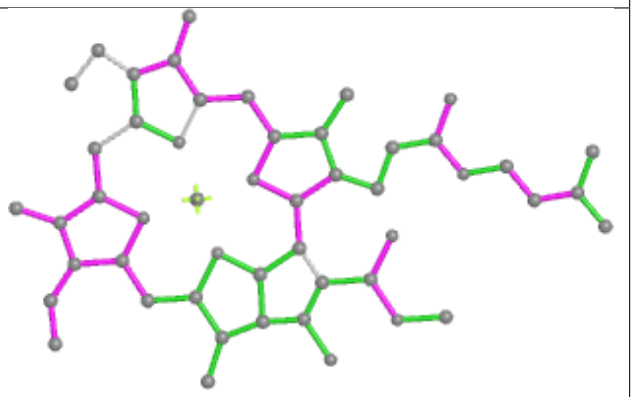


Rings

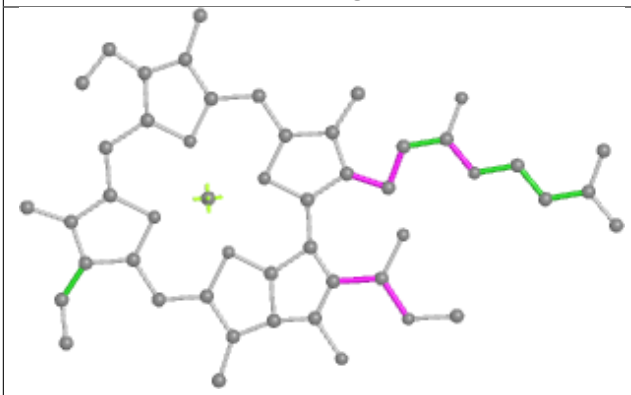
Ligand CLA c1 416



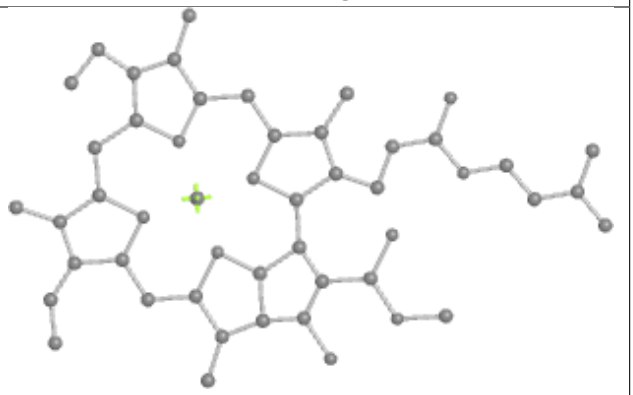
Bond lengths



Bond angles

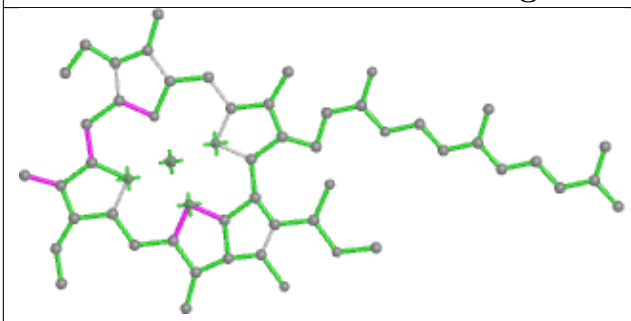


Torsions

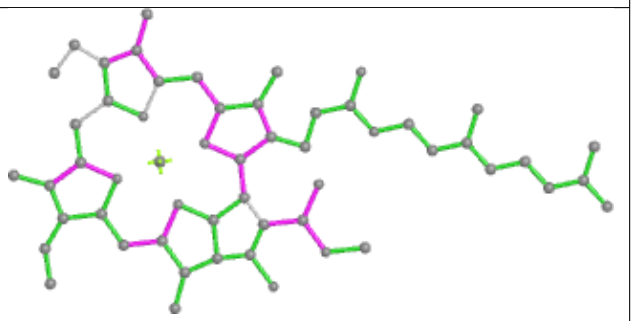


Rings

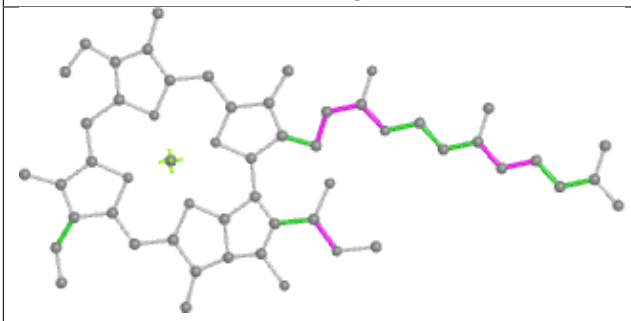
Ligand CLA a6 418



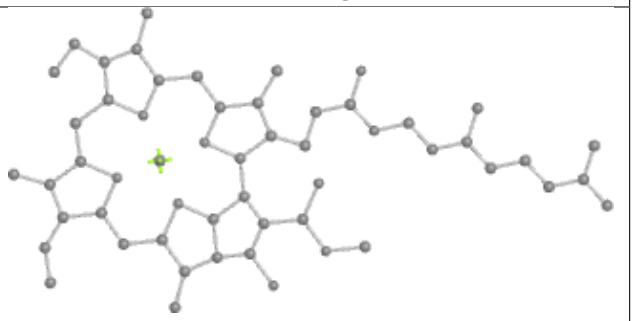
Bond lengths



Bond angles

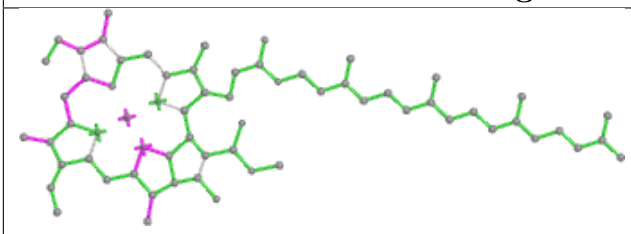


Torsions

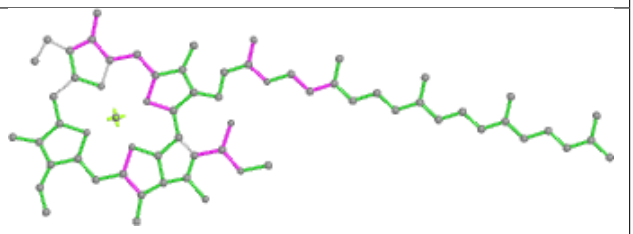


Rings

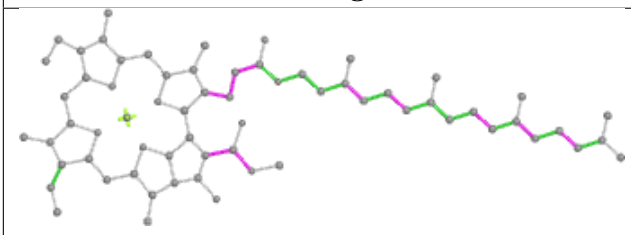
Ligand CLA cA 830



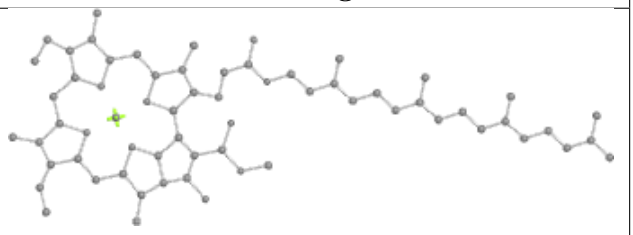
Bond lengths



Bond angles

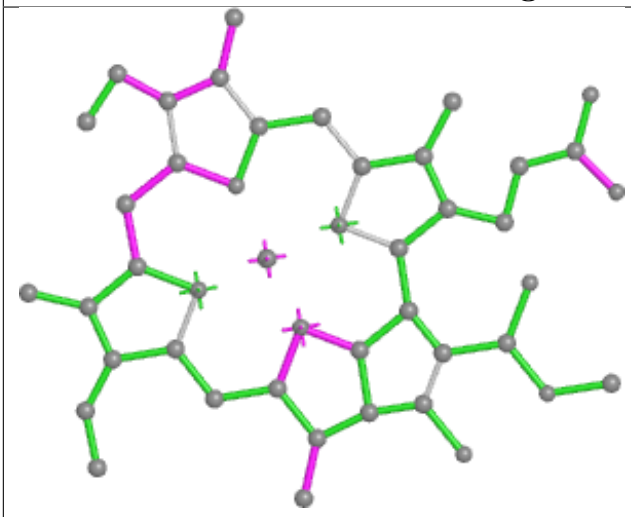


Torsions

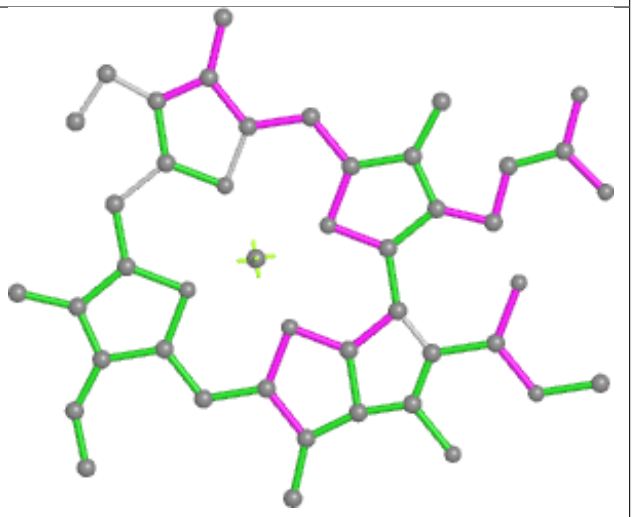


Rings

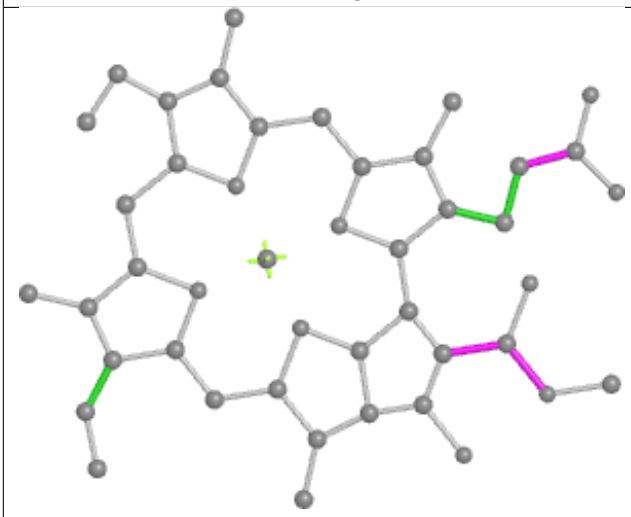
Ligand CLA a3 415



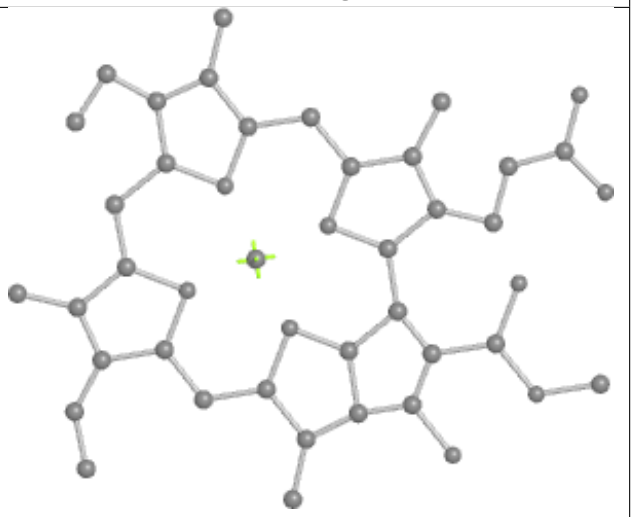
Bond lengths



Bond angles

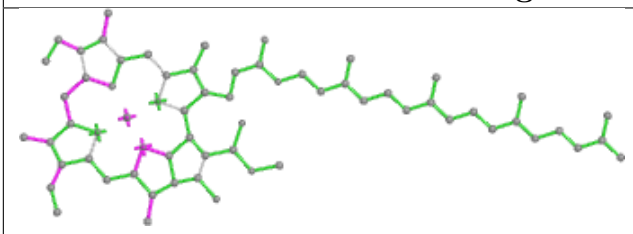


Torsions

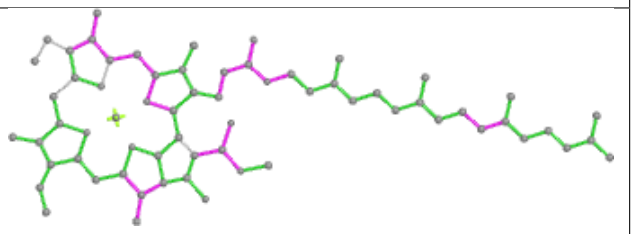


Rings

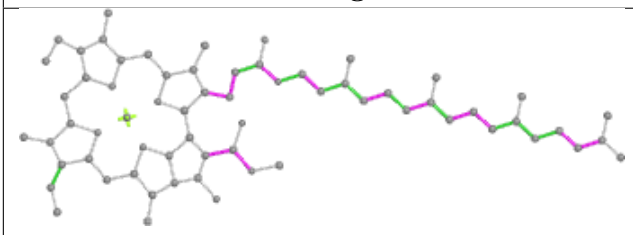
Ligand CLA cA 803



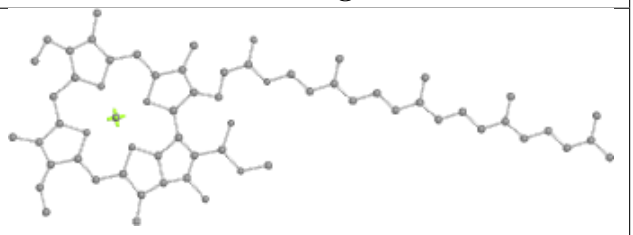
Bond lengths



Bond angles

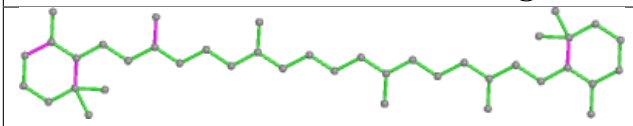


Torsions

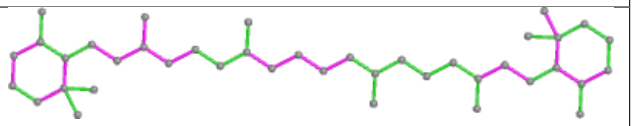


Rings

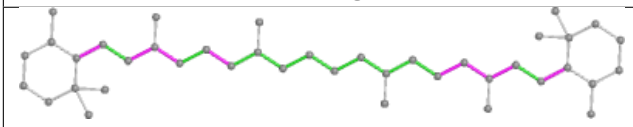
Ligand BCR a6 401



Bond lengths



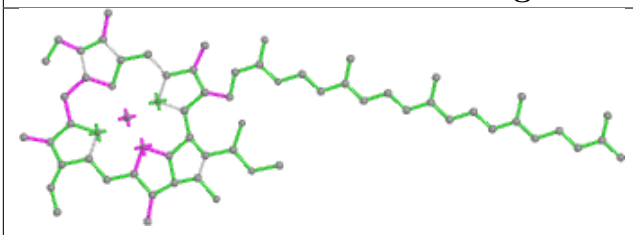
Bond angles



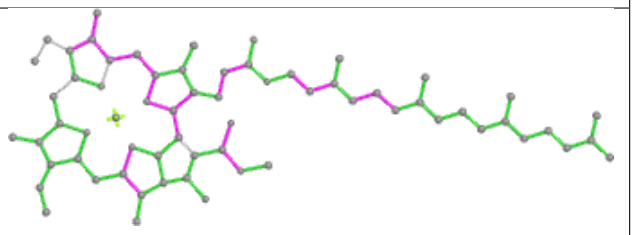
Torsions

Rings

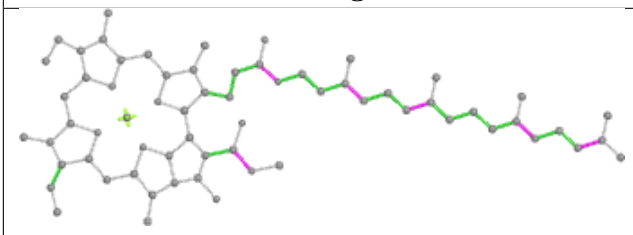
Ligand CLA bA 834



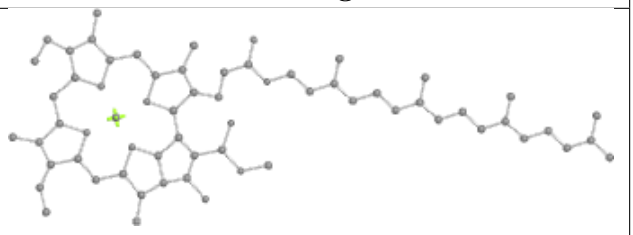
Bond lengths



Bond angles

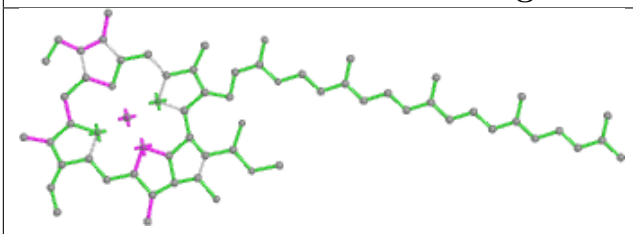


Torsions

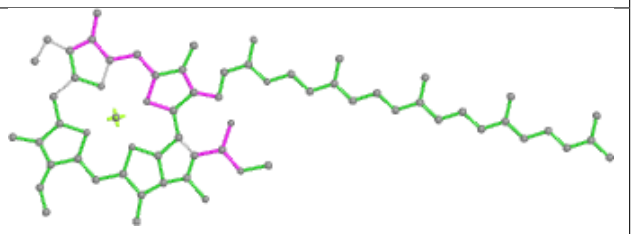


Rings

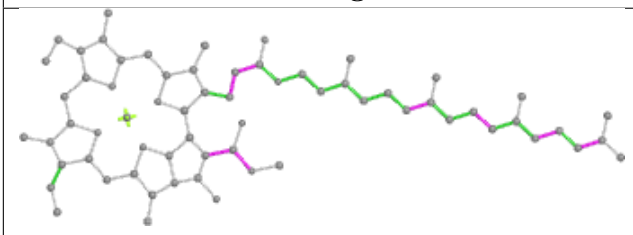
Ligand CLA bL 204



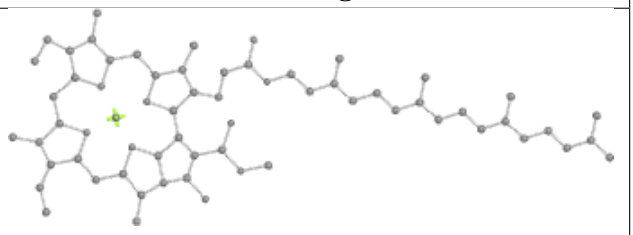
Bond lengths



Bond angles

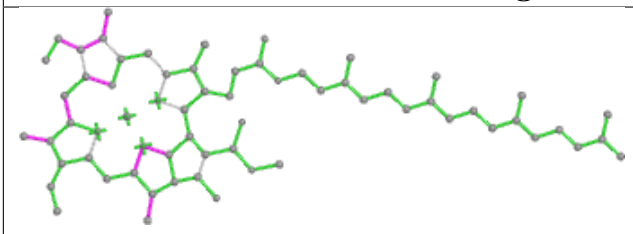


Torsions

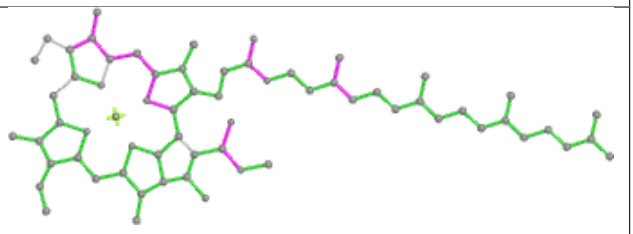


Rings

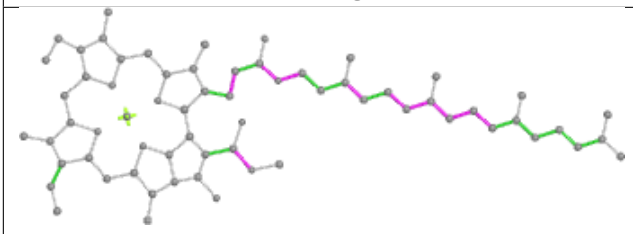
Ligand CLA aA 841



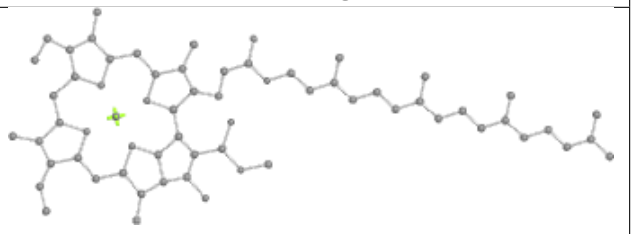
Bond lengths



Bond angles

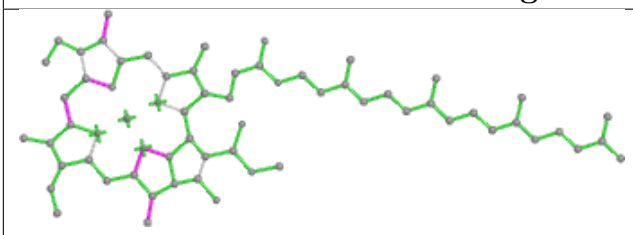


Torsions

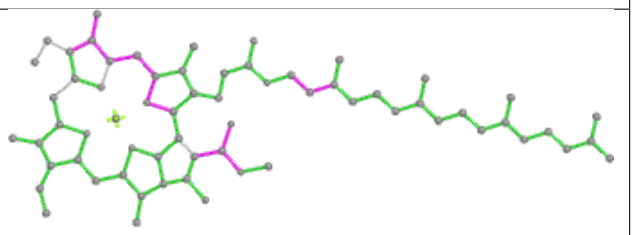


Rings

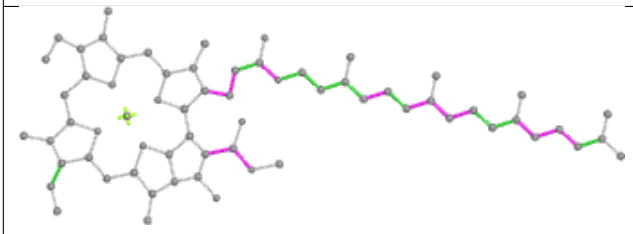
Ligand CLA c4 402



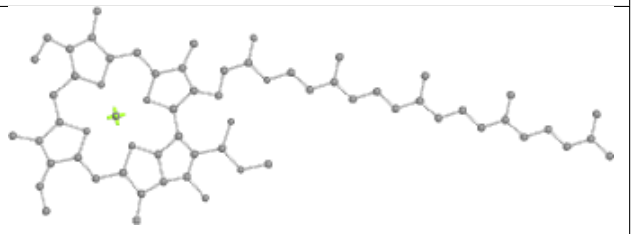
Bond lengths



Bond angles

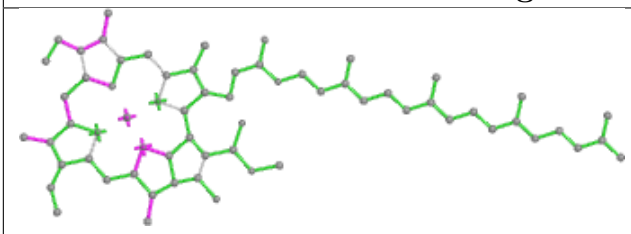


Torsions

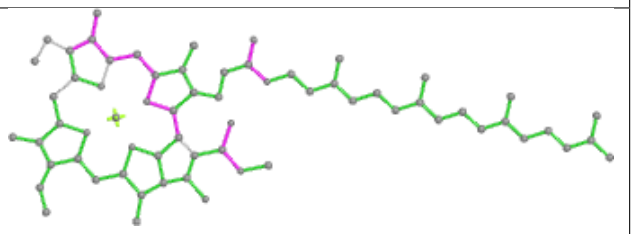


Rings

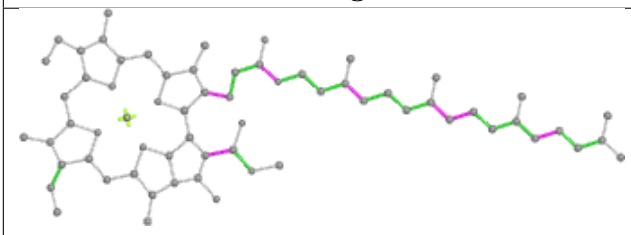
Ligand CLA bL 202



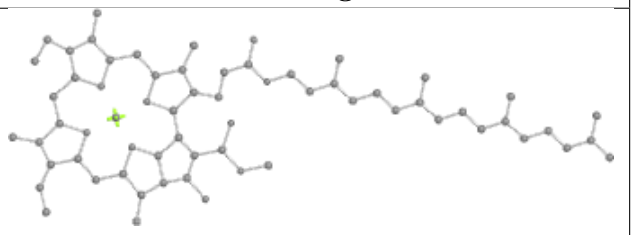
Bond lengths



Bond angles

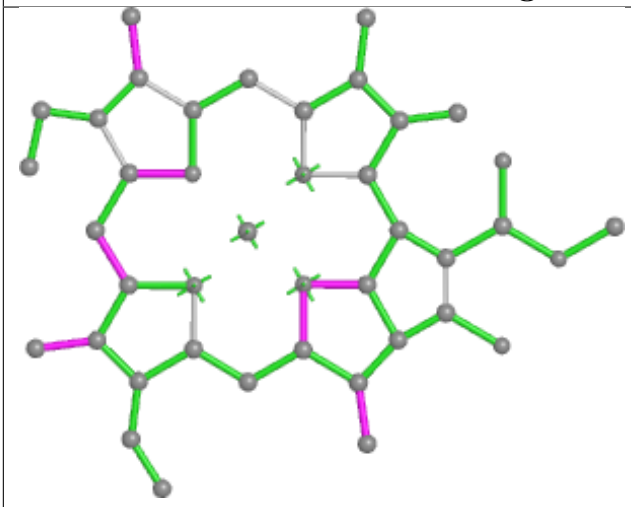


Torsions

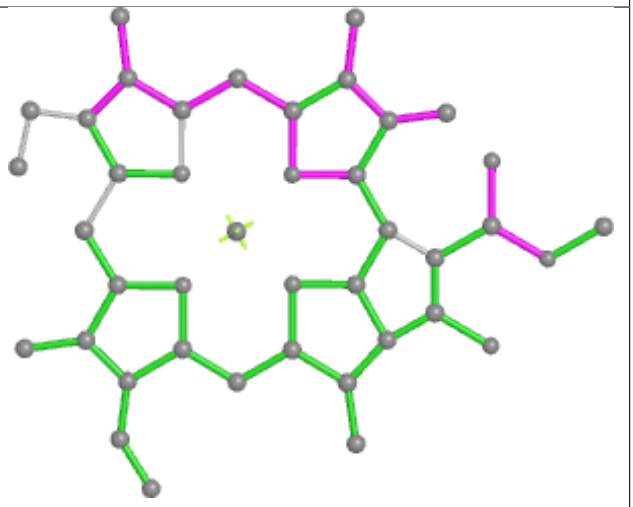


Rings

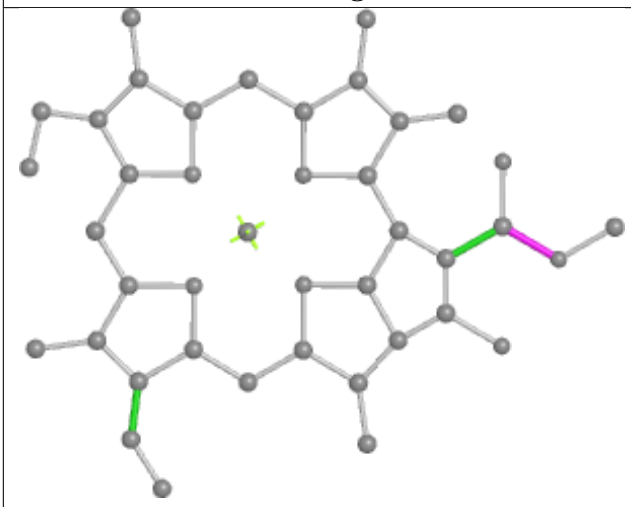
Ligand CLA b1 414



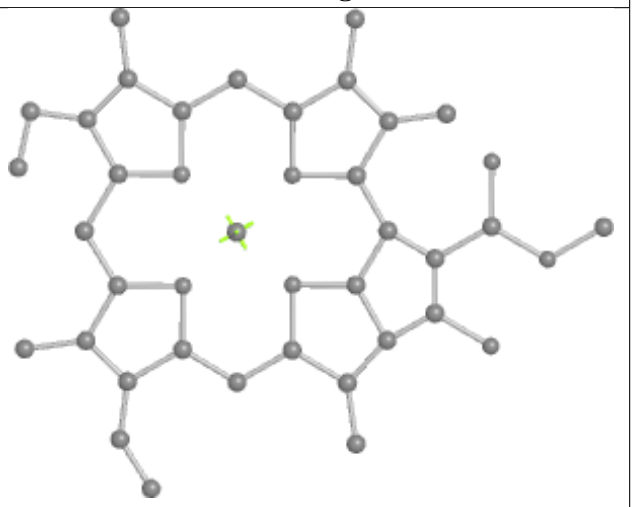
Bond lengths



Bond angles

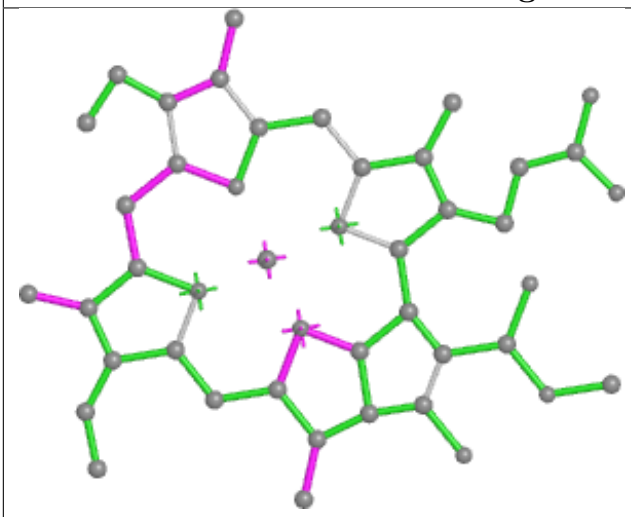


Torsions

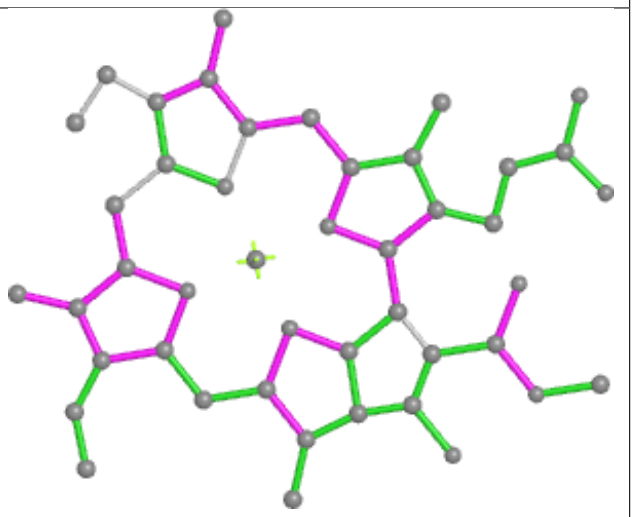


Rings

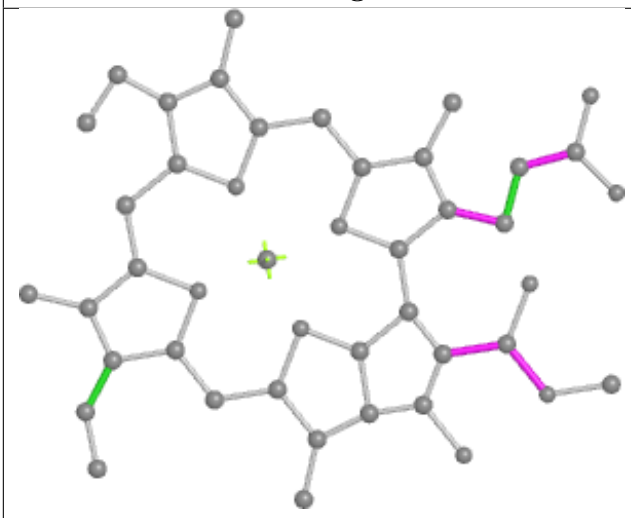
Ligand CLA b4 412



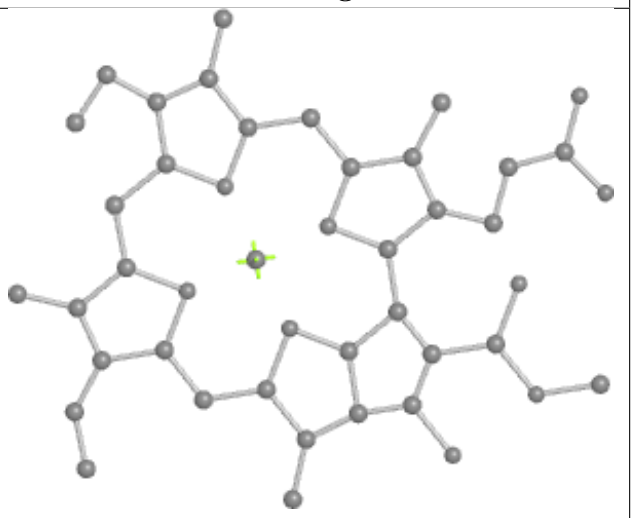
Bond lengths



Bond angles

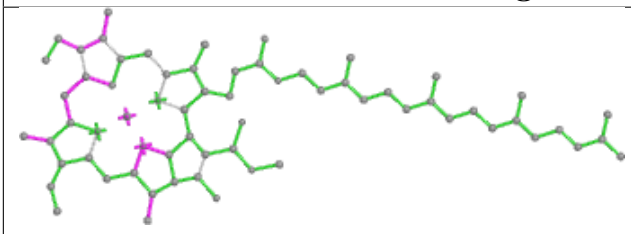


Torsions

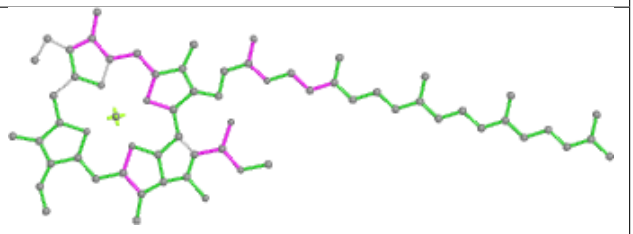


Rings

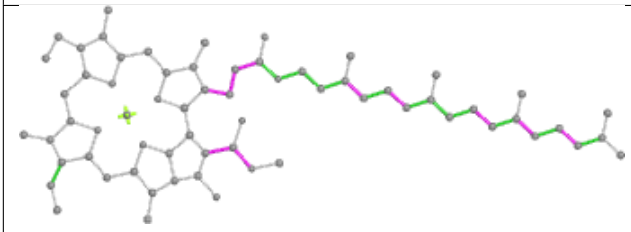
Ligand CLA aA 830



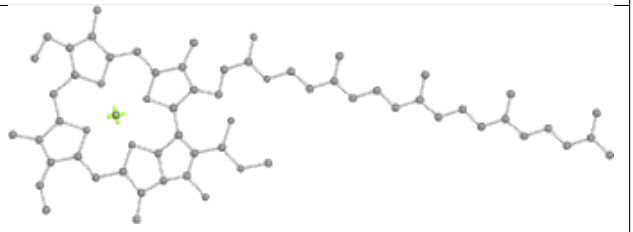
Bond lengths



Bond angles

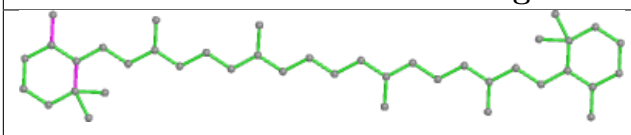


Torsions

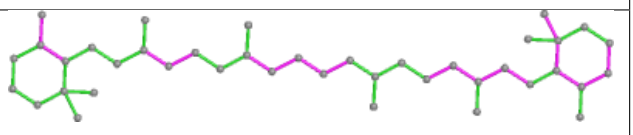


Rings

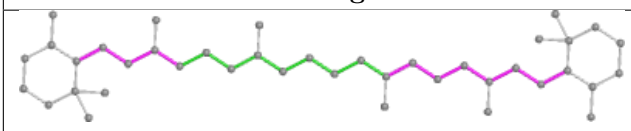
Ligand BCR aA 850



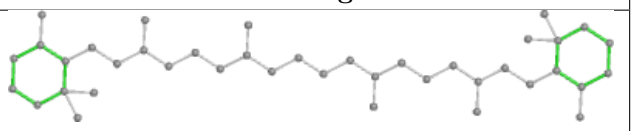
Bond lengths



Bond angles

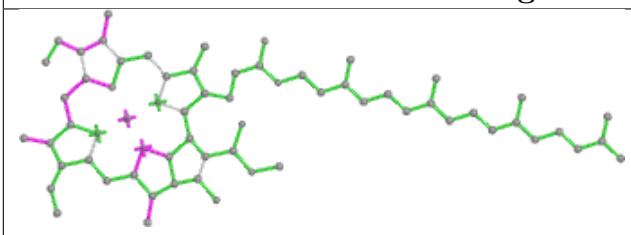


Torsions

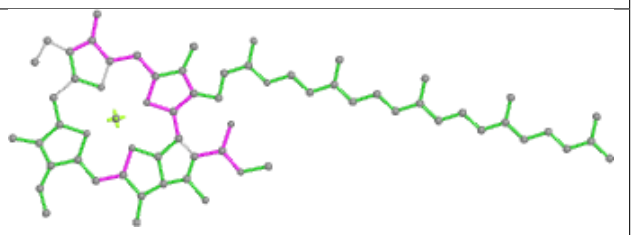


Rings

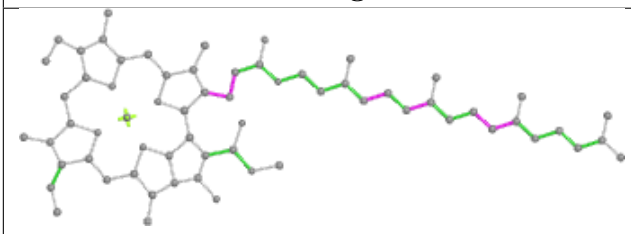
Ligand CLA aL 202



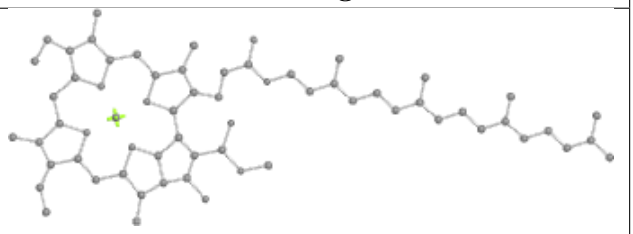
Bond lengths



Bond angles

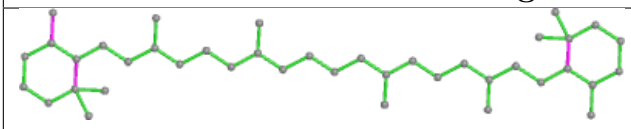


Torsions

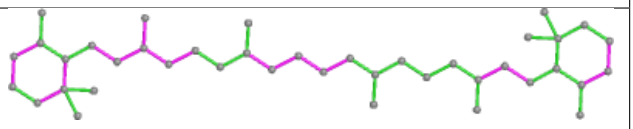


Rings

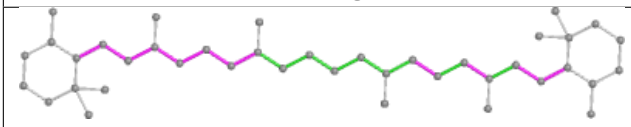
Ligand BCR a1 421



Bond lengths



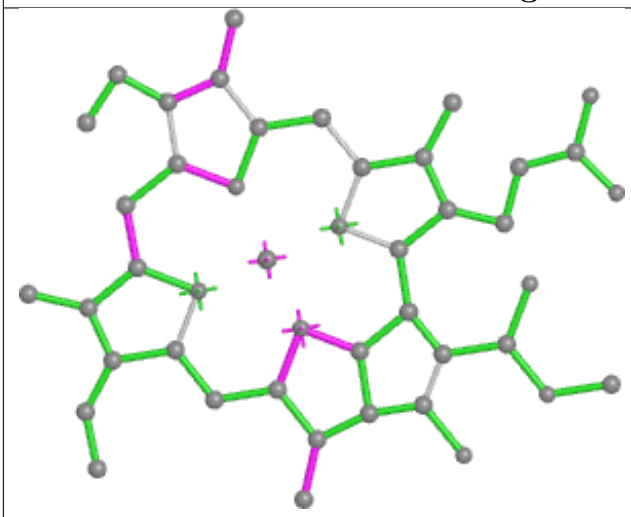
Bond angles



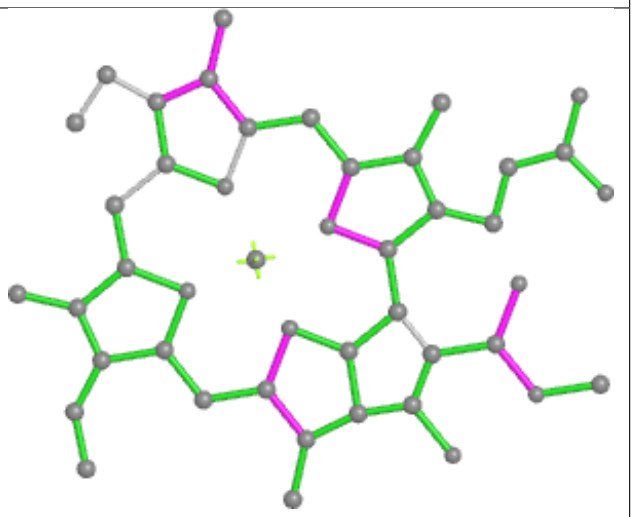
Torsions

Rings

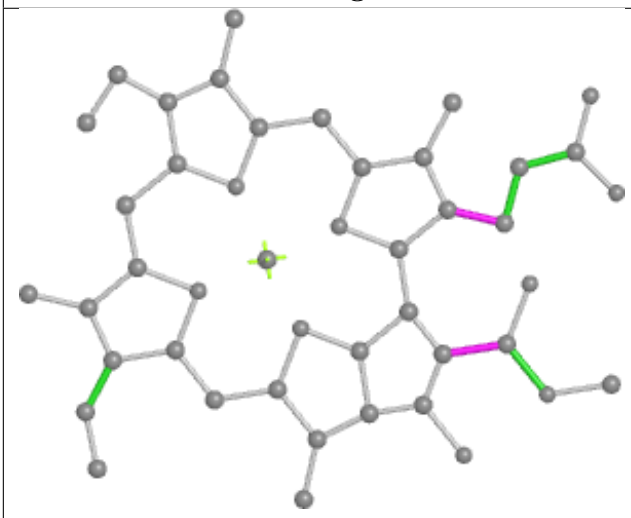
Ligand CLA c1 413



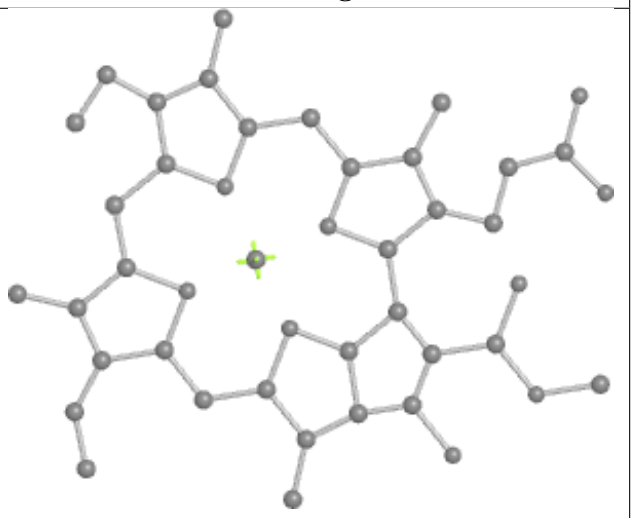
Bond lengths



Bond angles

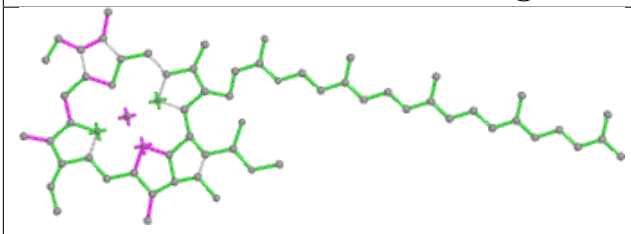


Torsions

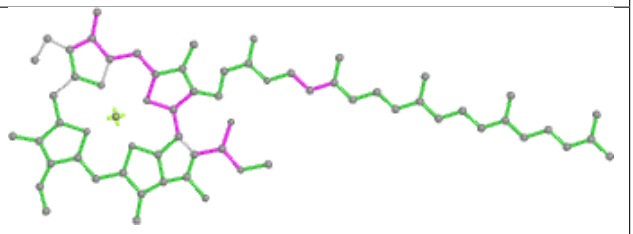


Rings

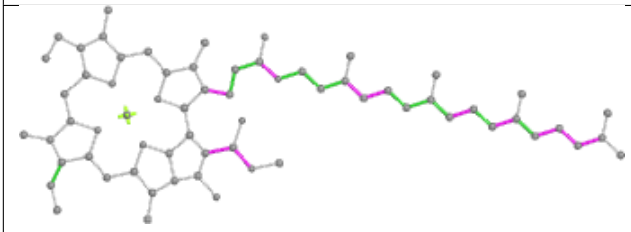
Ligand CLA aA 820



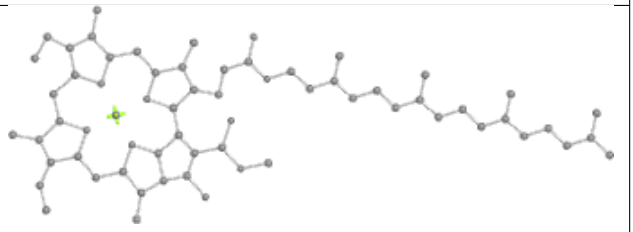
Bond lengths



Bond angles

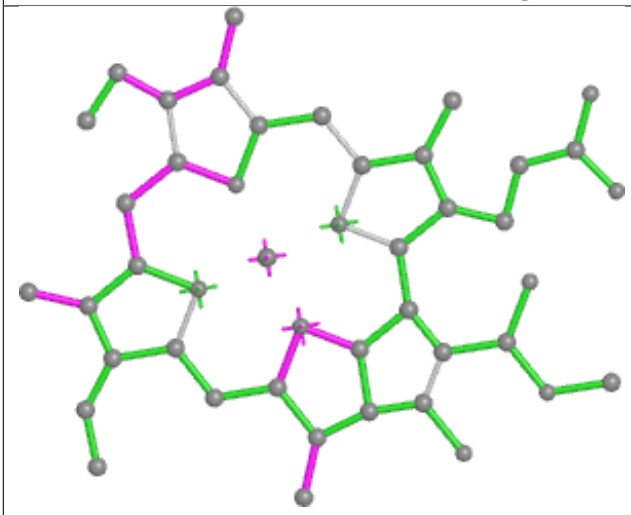


Torsions

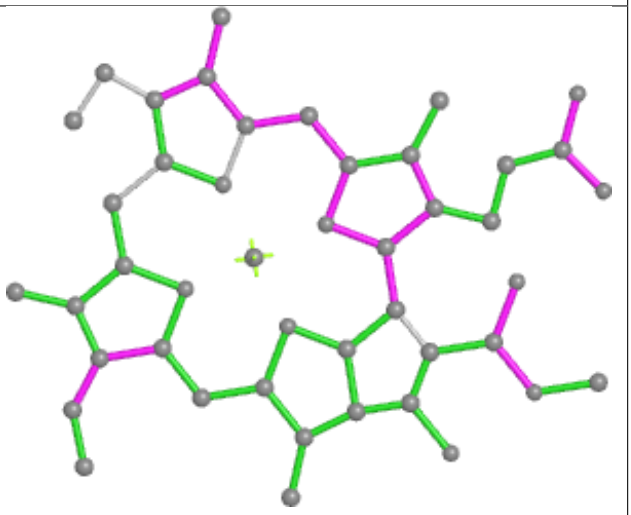


Rings

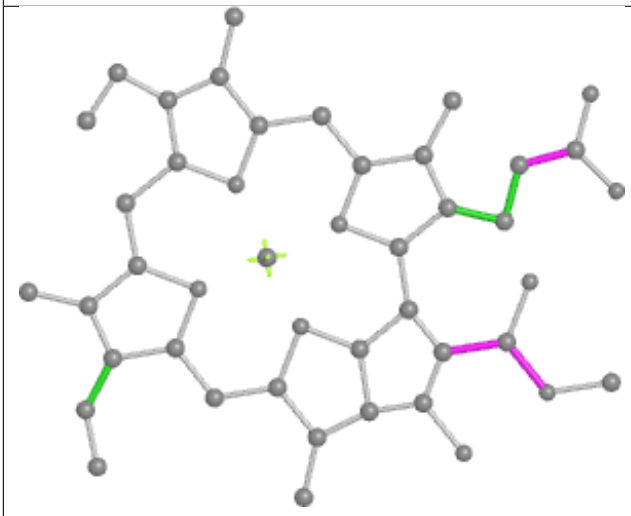
Ligand CLA bF 201



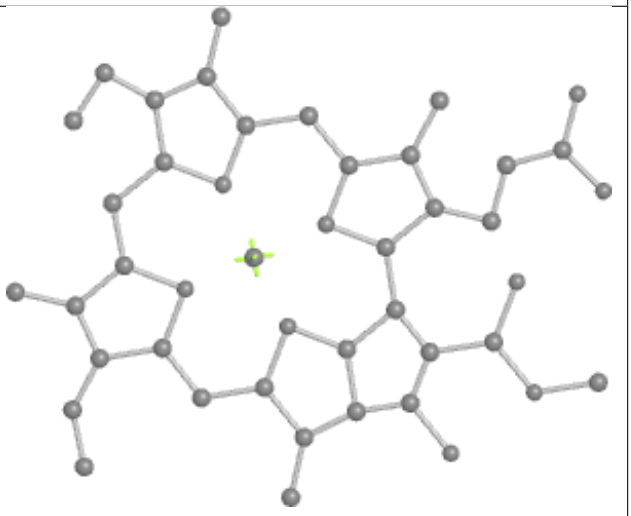
Bond lengths



Bond angles

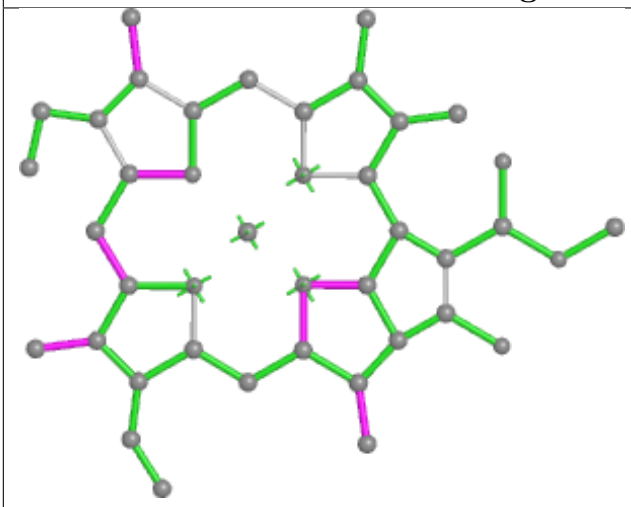


Torsions

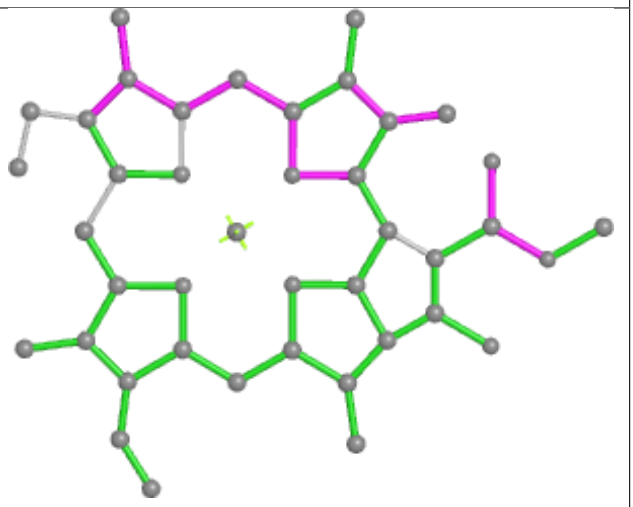


Rings

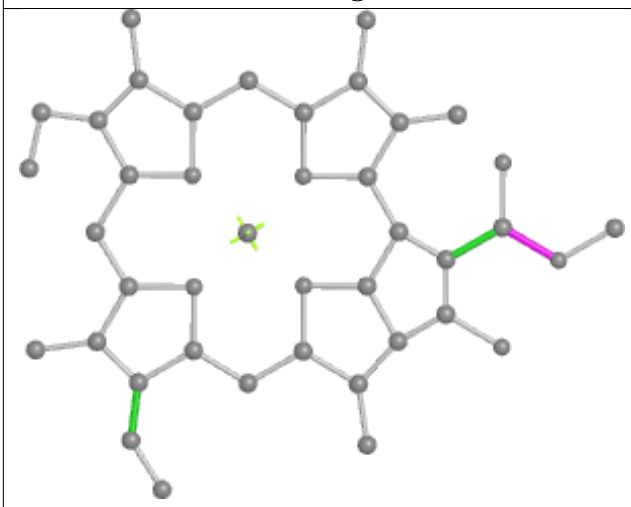
Ligand CLA a2 415



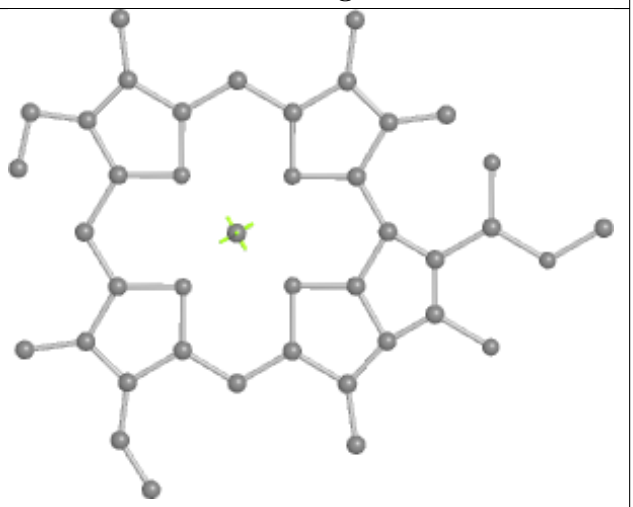
Bond lengths



Bond angles

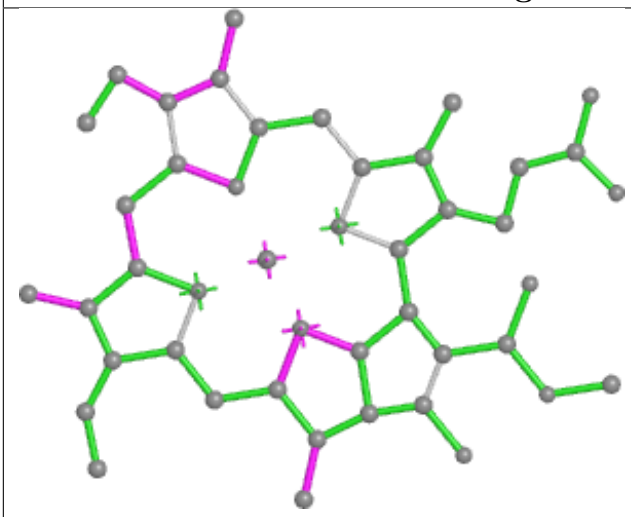


Torsions

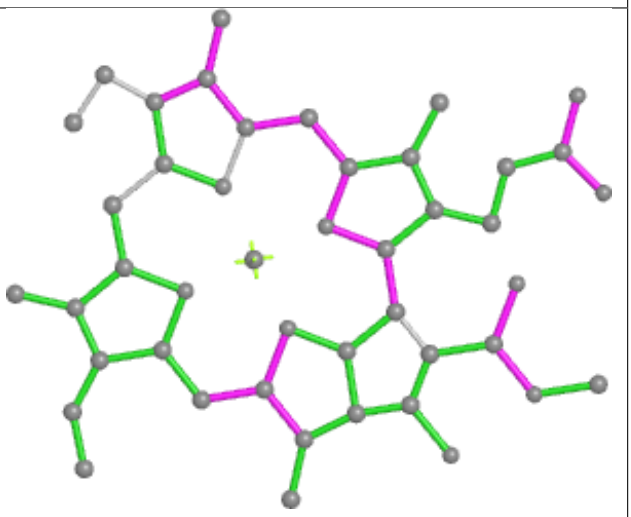


Rings

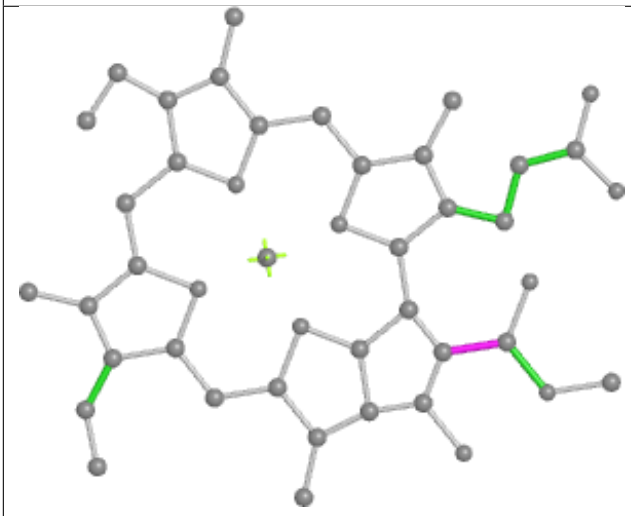
Ligand CLA aA 815



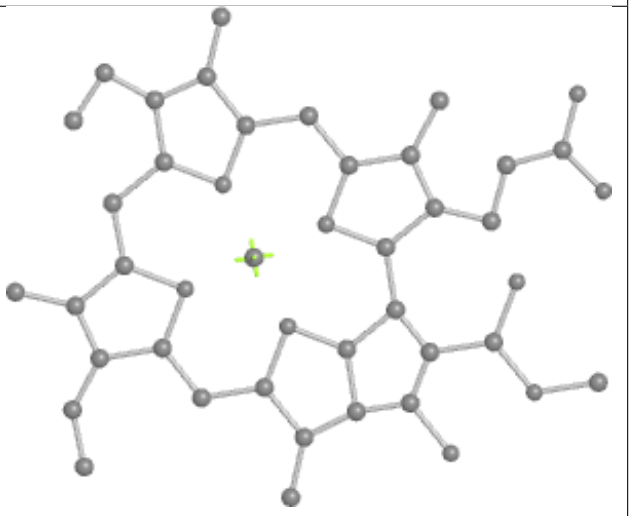
Bond lengths



Bond angles

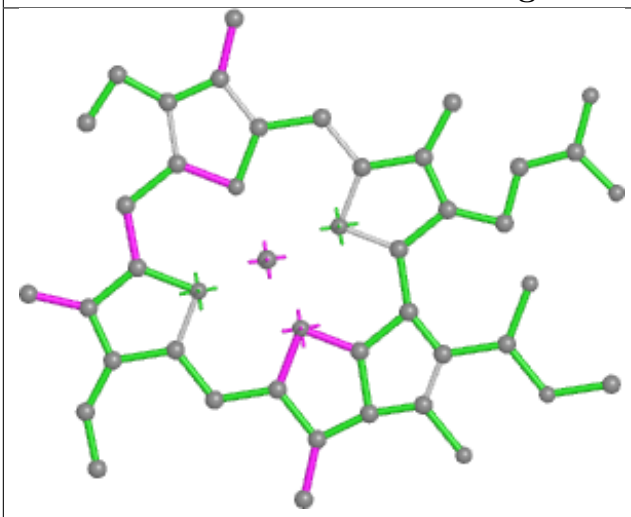


Torsions

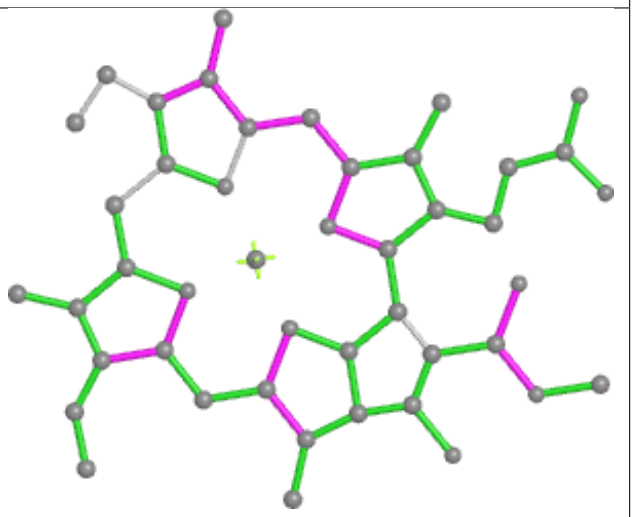


Rings

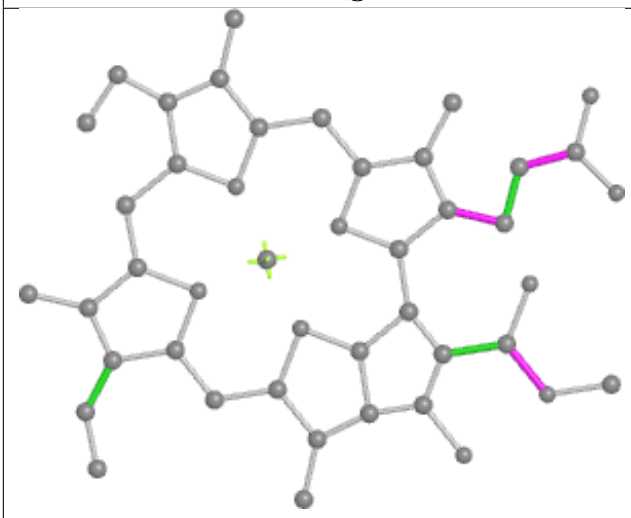
Ligand CLA b6 409



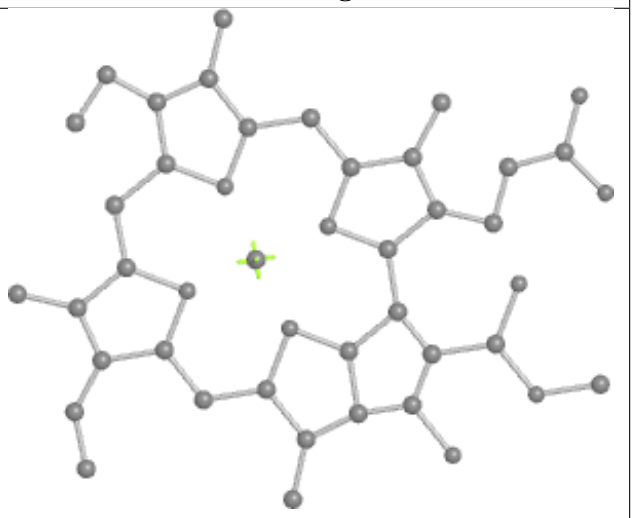
Bond lengths



Bond angles

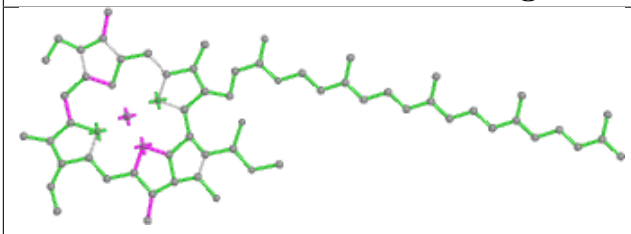


Torsions

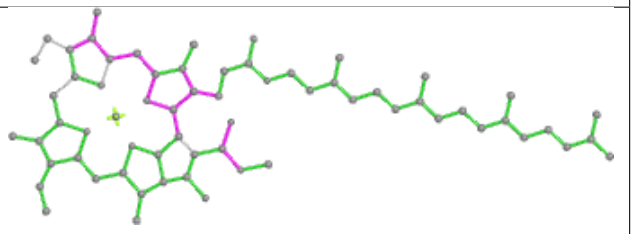


Rings

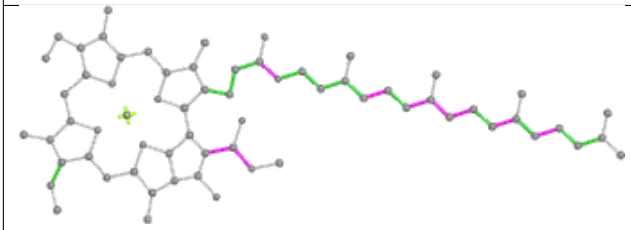
Ligand CLA a6 404



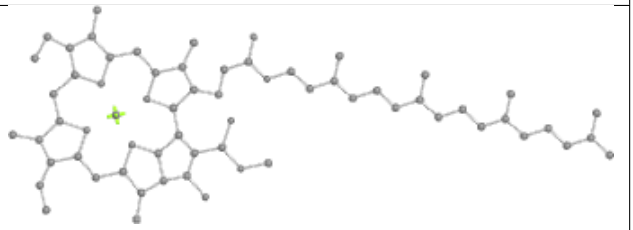
Bond lengths



Bond angles

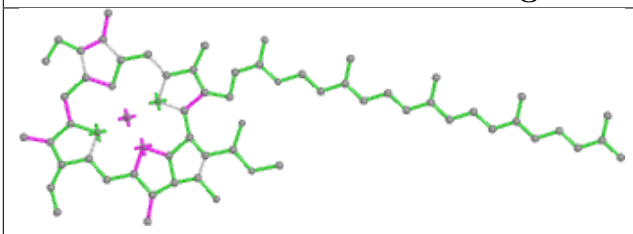


Torsions

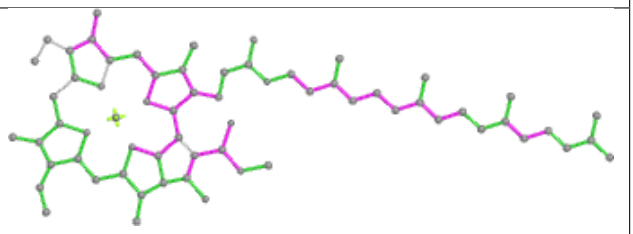


Rings

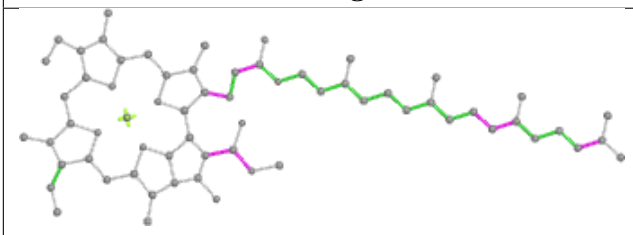
Ligand CLA c5 420



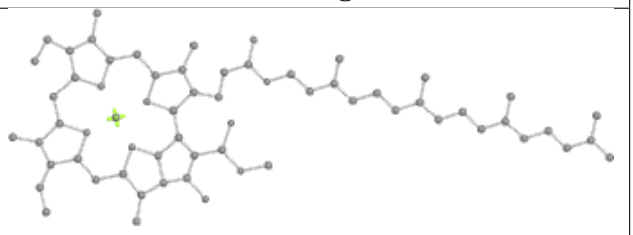
Bond lengths



Bond angles

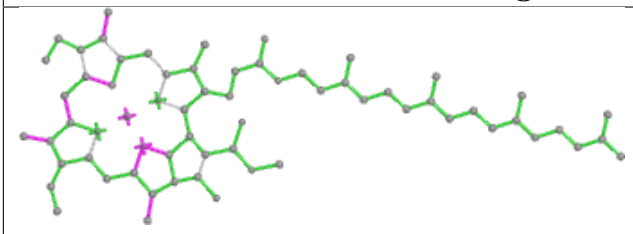


Torsions

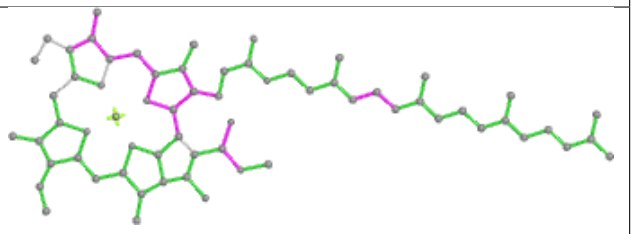


Rings

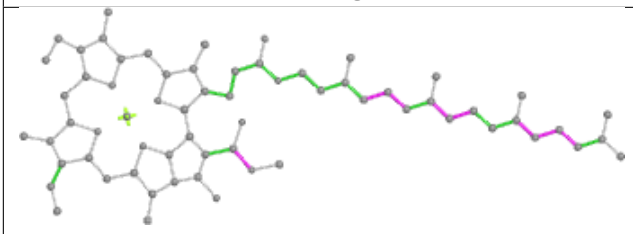
Ligand CLA aA 826



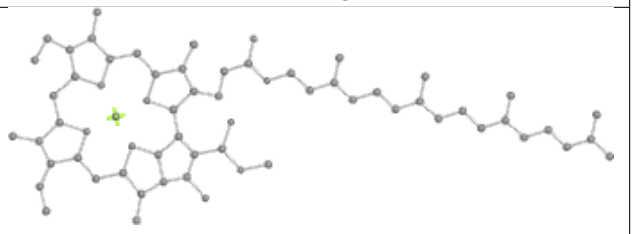
Bond lengths



Bond angles

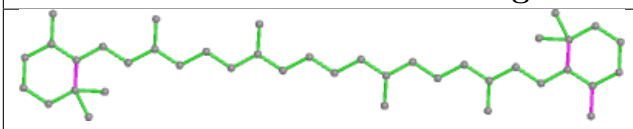


Torsions

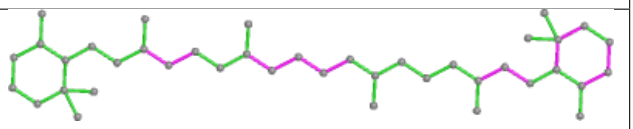


Rings

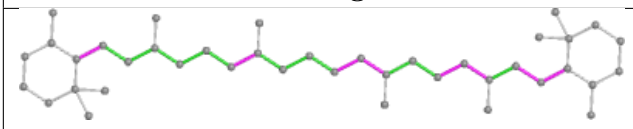
Ligand BCR bA 849



Bond lengths



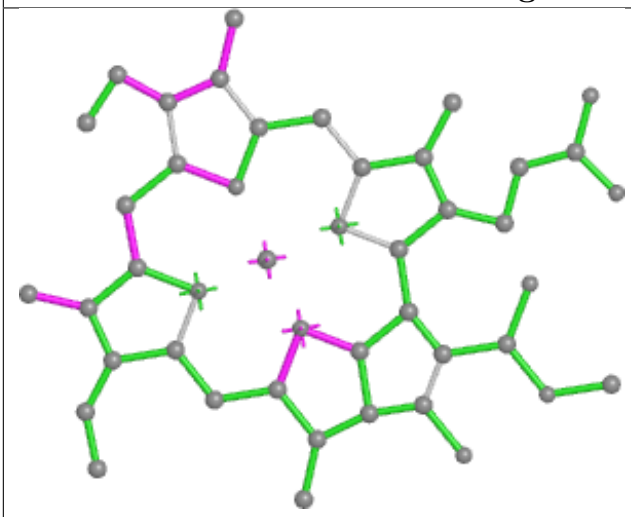
Bond angles



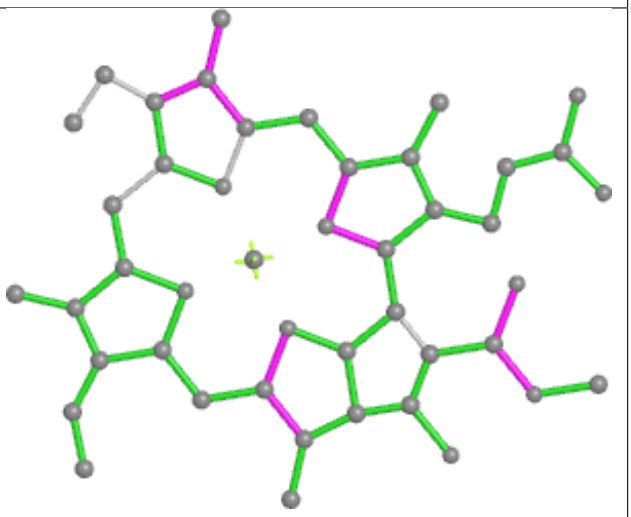
Torsions

Rings

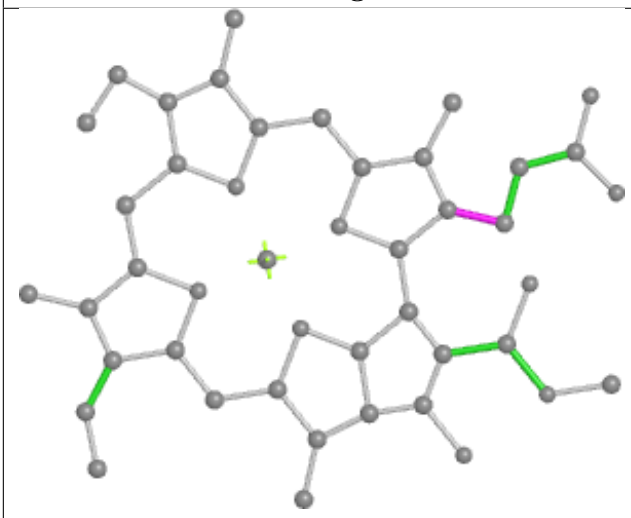
Ligand CLA b5 413



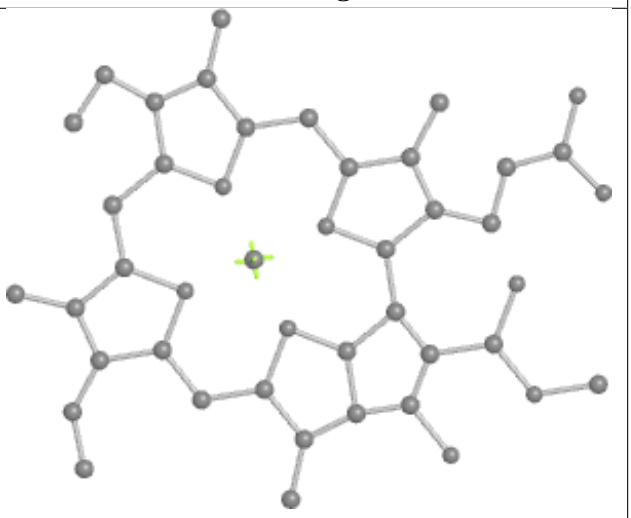
Bond lengths



Bond angles

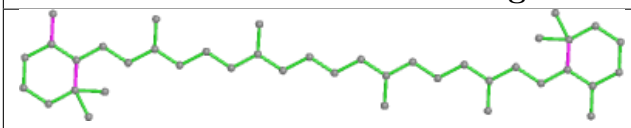


Torsions

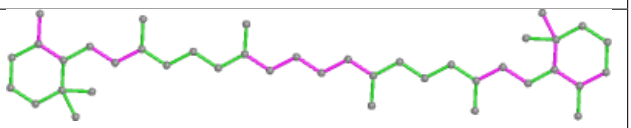


Rings

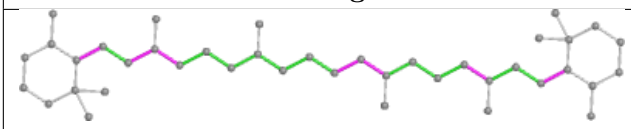
Ligand BCR bM 101



Bond lengths



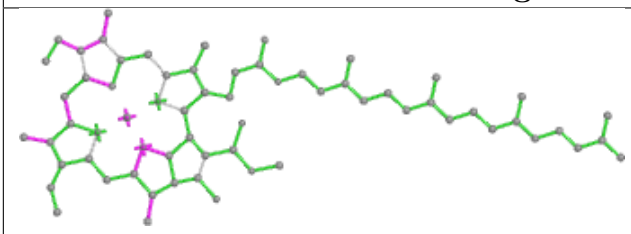
Bond angles



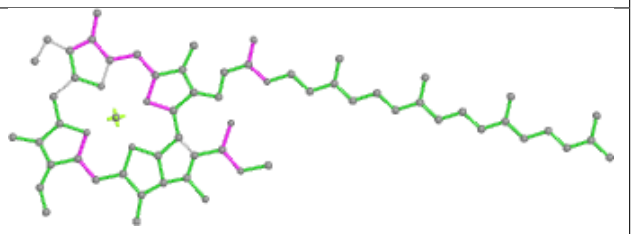
Torsions

Rings

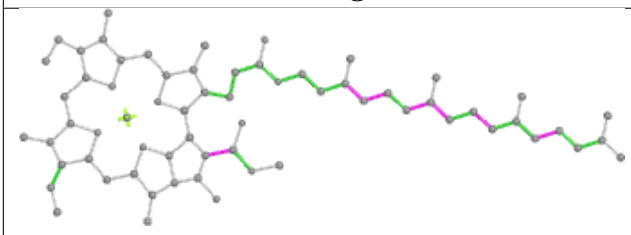
Ligand CLA bA 828



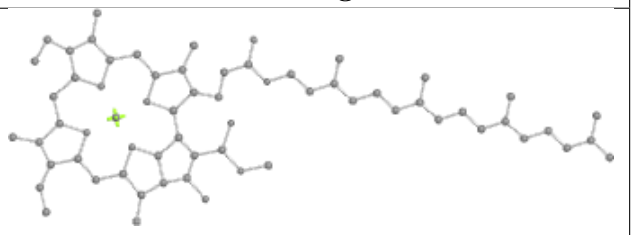
Bond lengths



Bond angles

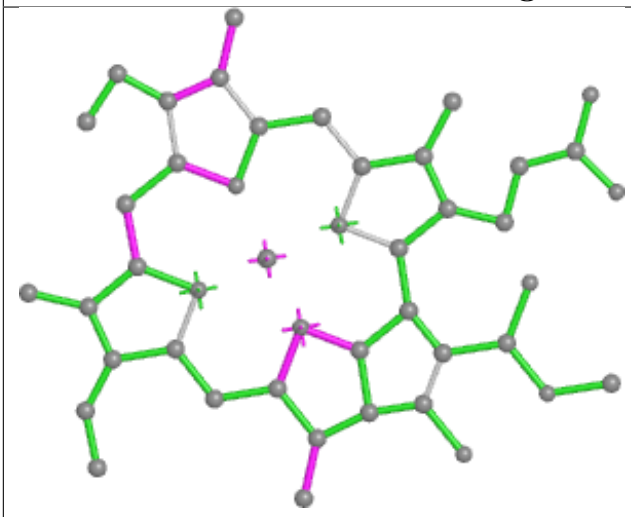


Torsions

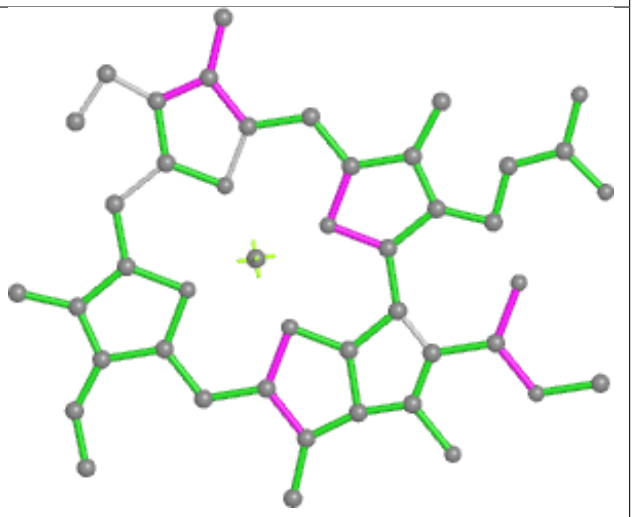


Rings

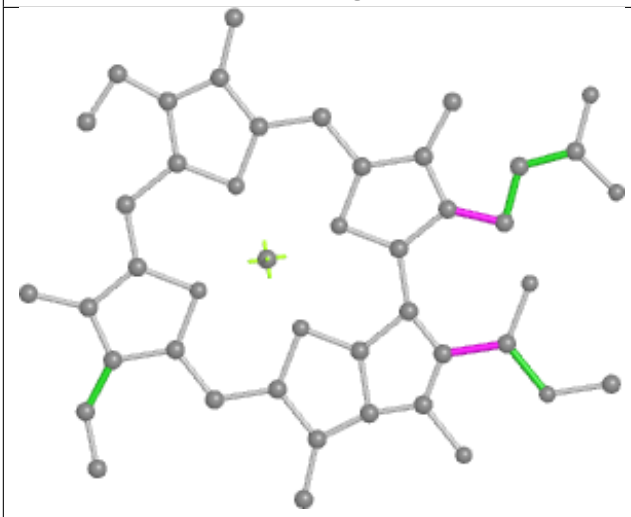
Ligand CLA b4 413



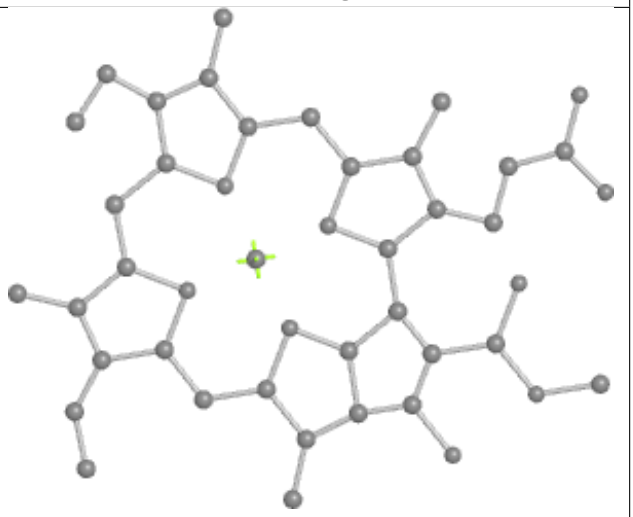
Bond lengths



Bond angles

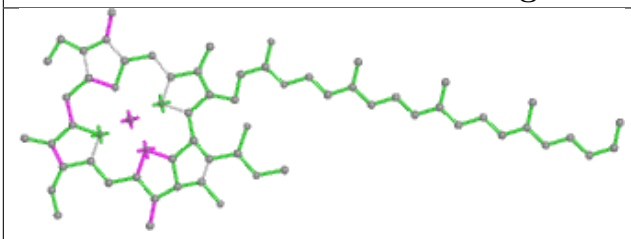


Torsions

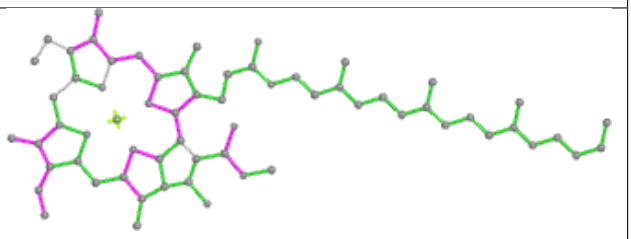


Rings

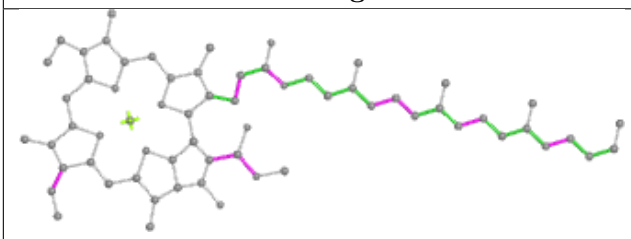
Ligand CLA a5 410



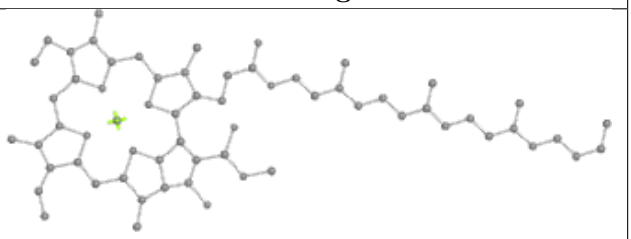
Bond lengths



Bond angles

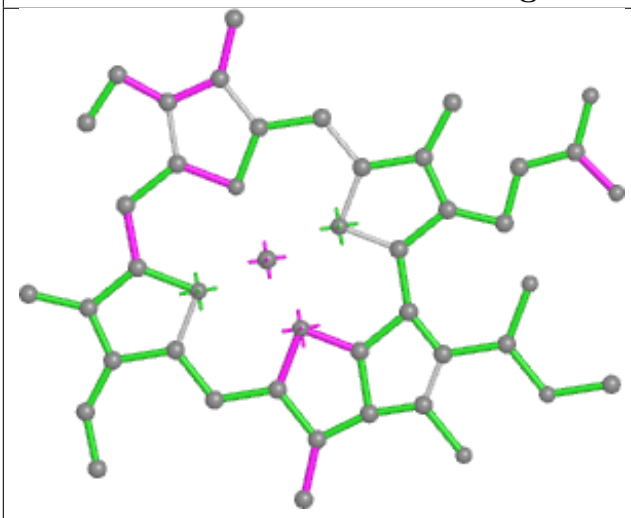


Torsions

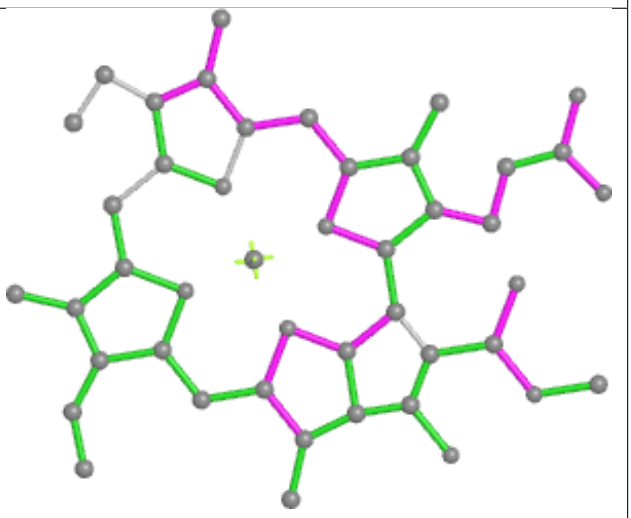


Rings

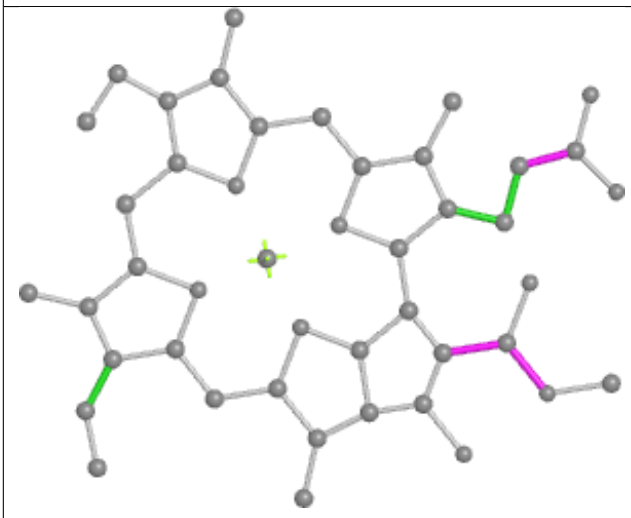
Ligand CLA a1 414



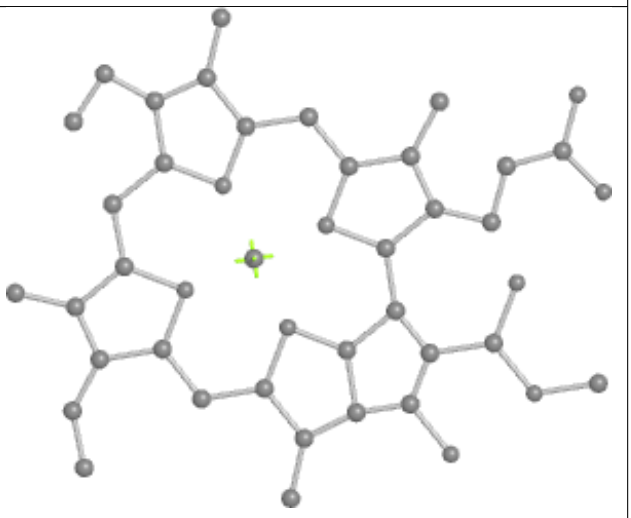
Bond lengths



Bond angles

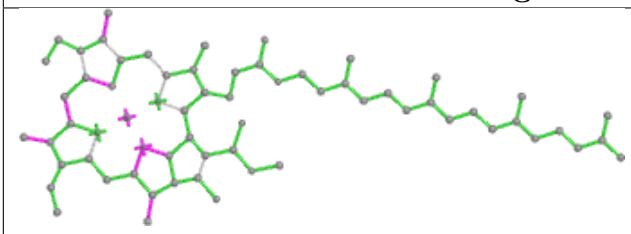


Torsions

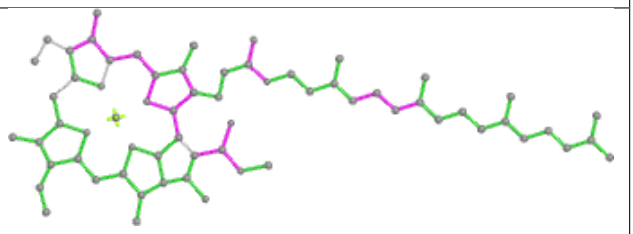


Rings

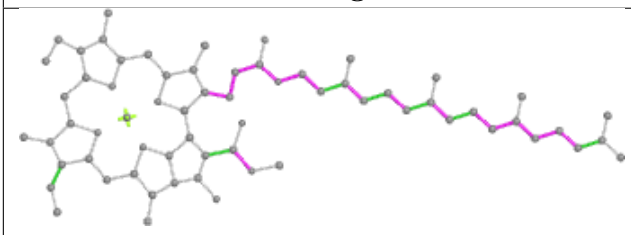
Ligand CLA bA 829



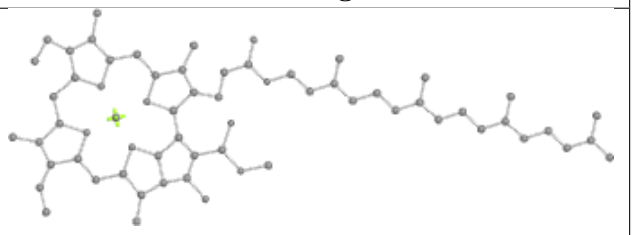
Bond lengths



Bond angles

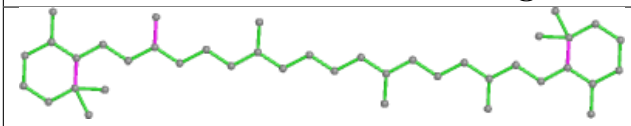


Torsions

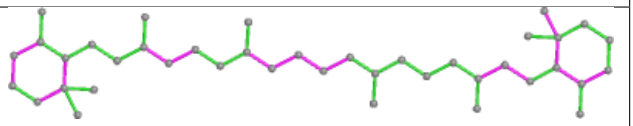


Rings

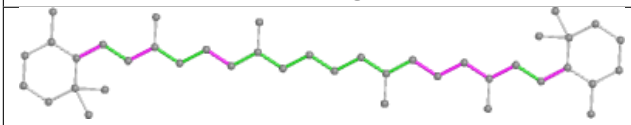
Ligand BCR a2 420



Bond lengths



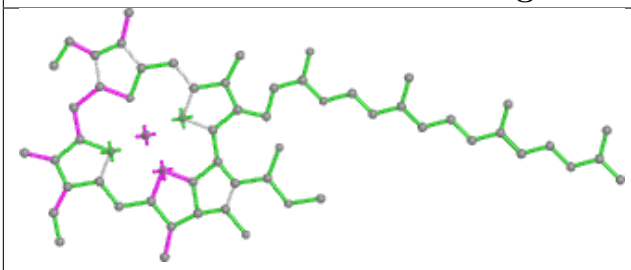
Bond angles



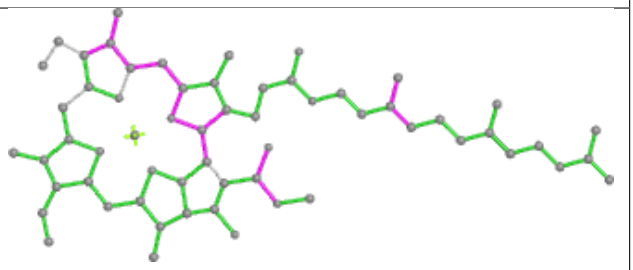
Torsions

Rings

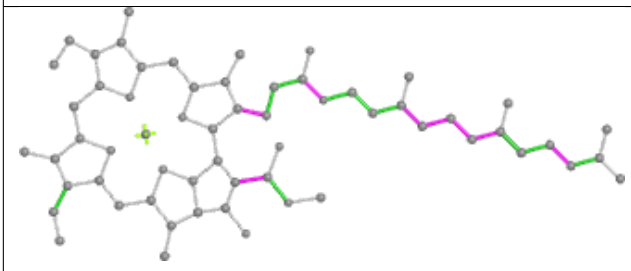
Ligand CLA cB 819



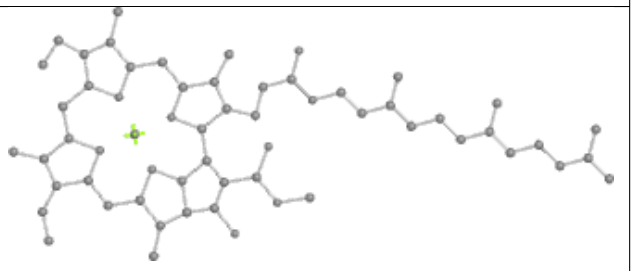
Bond lengths



Bond angles

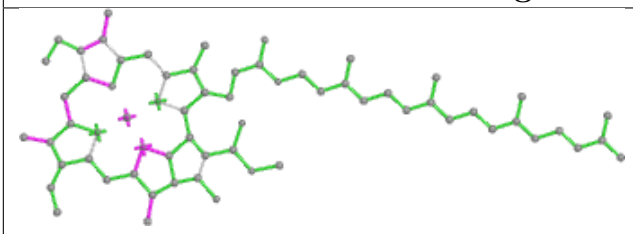


Torsions

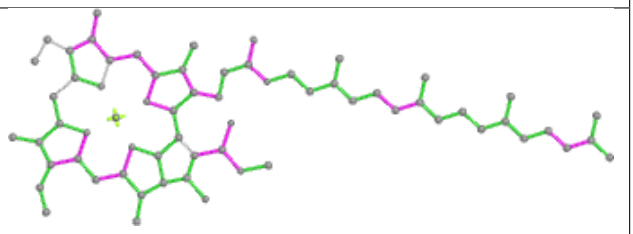


Rings

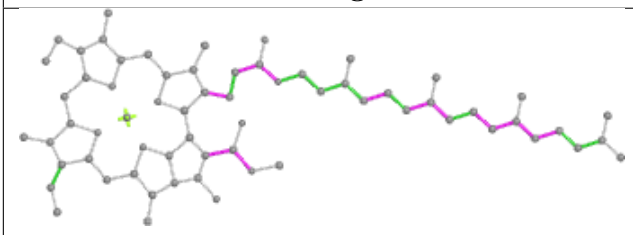
Ligand CLA bB 833



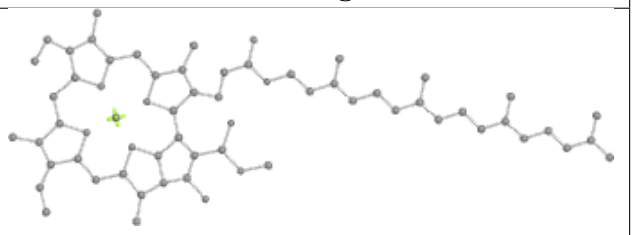
Bond lengths



Bond angles

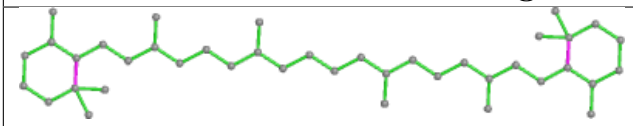


Torsions

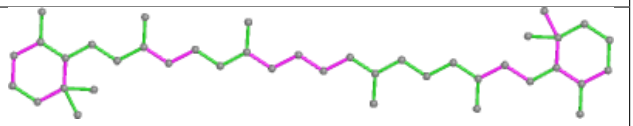


Rings

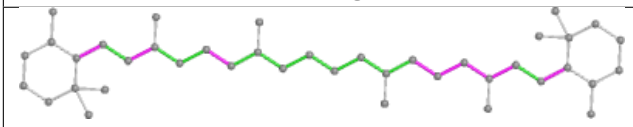
Ligand BCR a3 419



Bond lengths



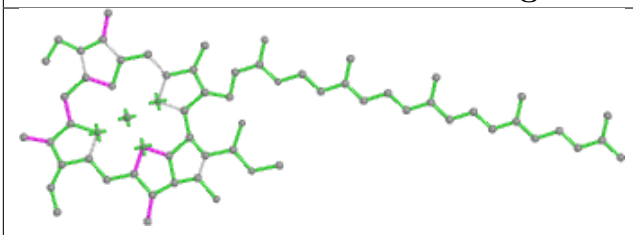
Bond angles



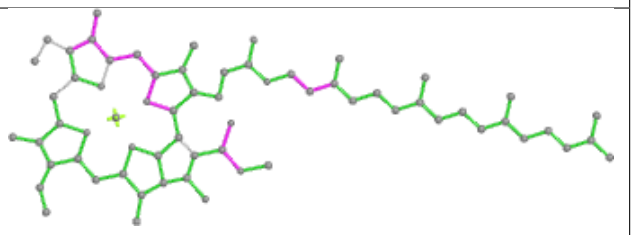
Torsions

Rings

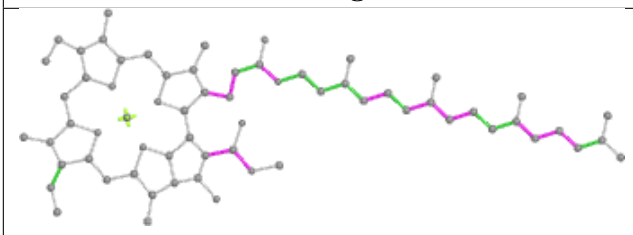
Ligand CLA c5 402



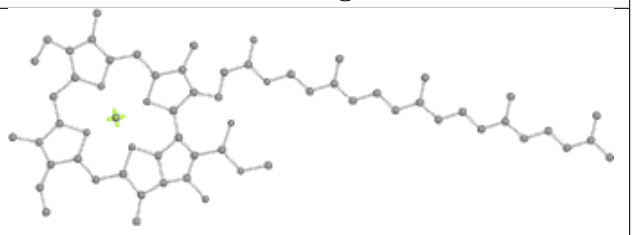
Bond lengths



Bond angles

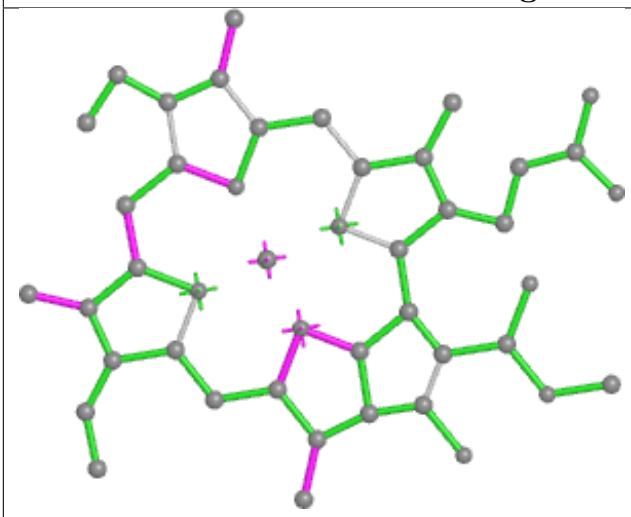


Torsions

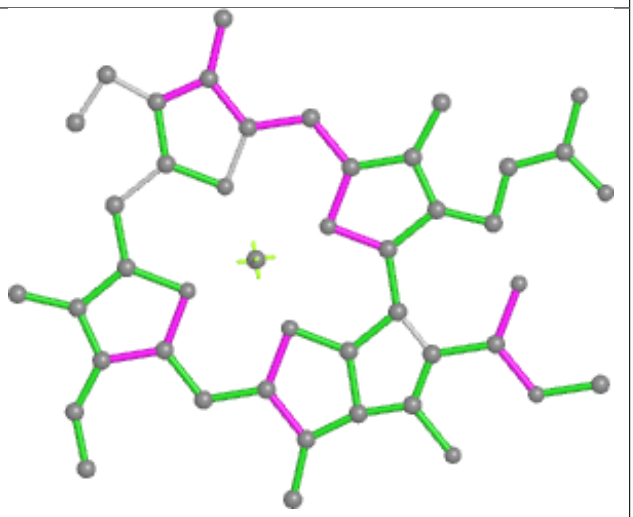


Rings

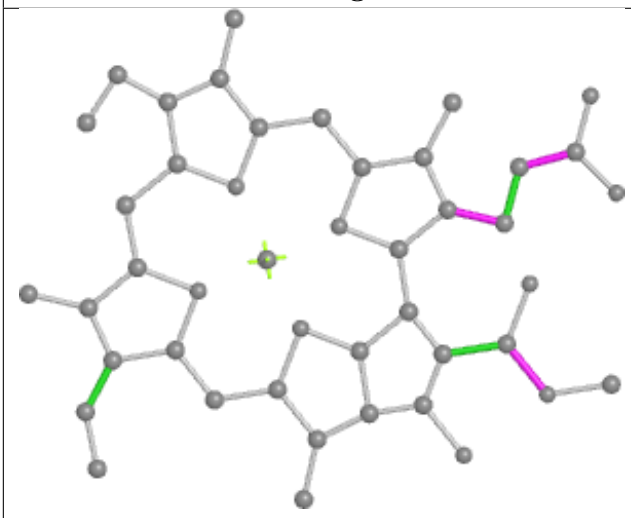
Ligand CLA a1 407



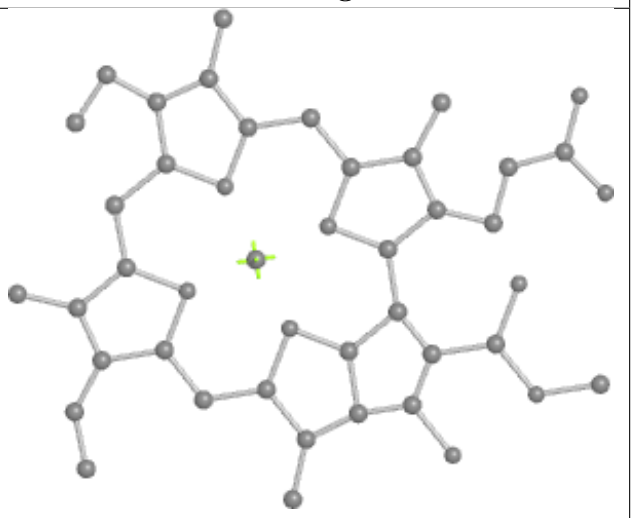
Bond lengths



Bond angles

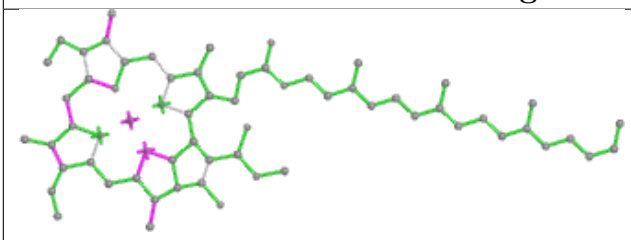


Torsions

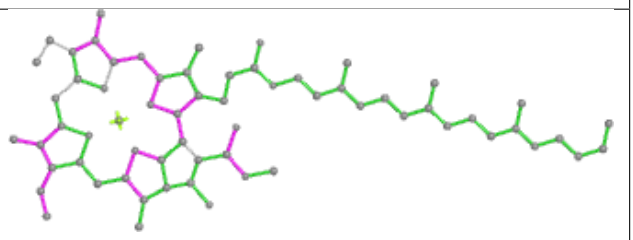


Rings

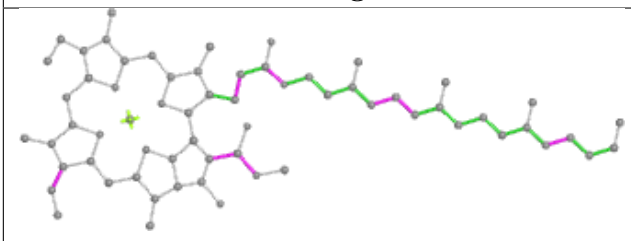
Ligand CLA a6 411



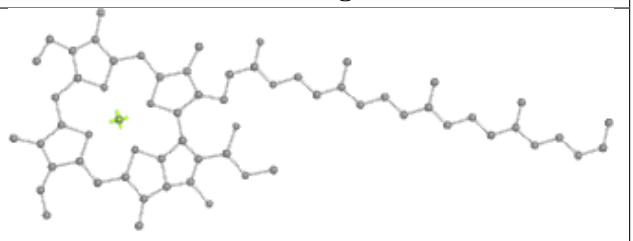
Bond lengths



Bond angles

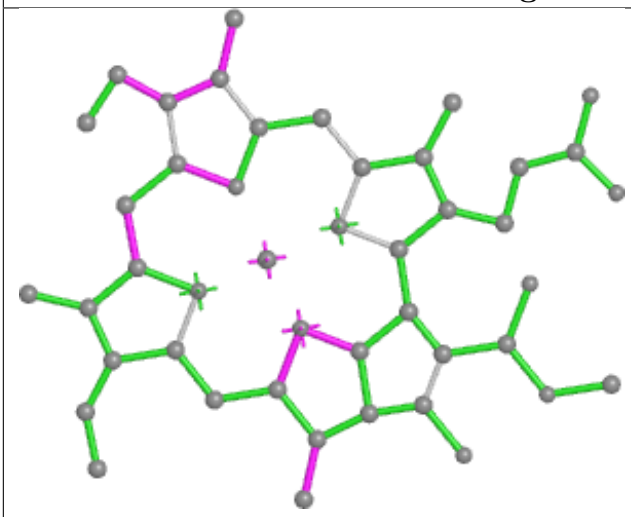


Torsions

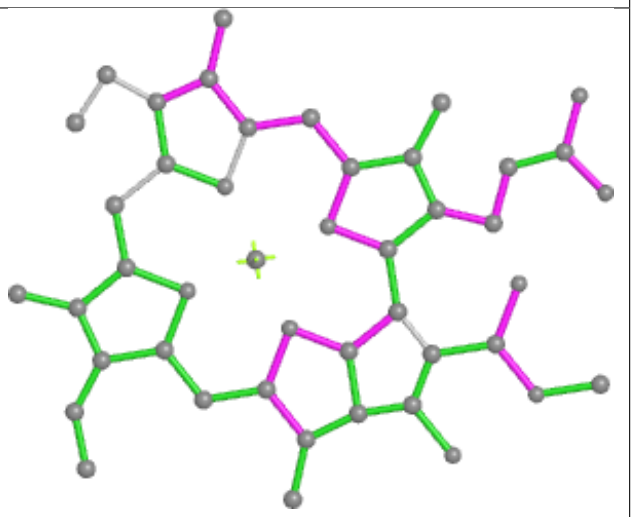


Rings

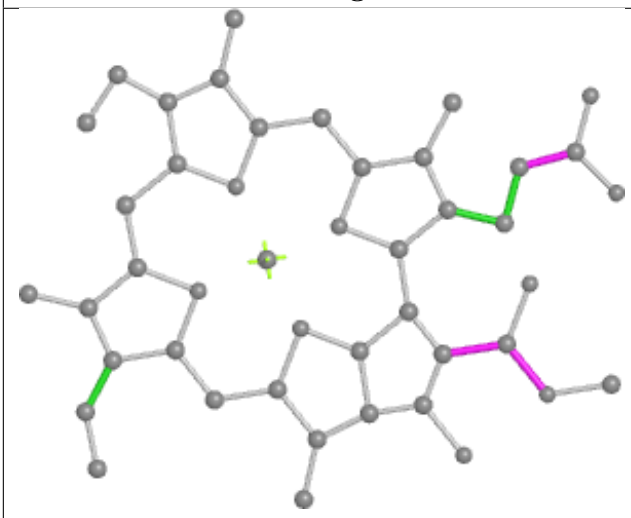
Ligand CLA a6 416



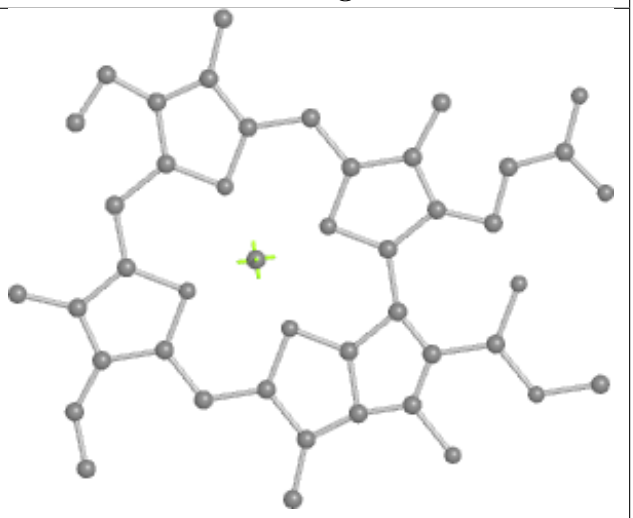
Bond lengths



Bond angles

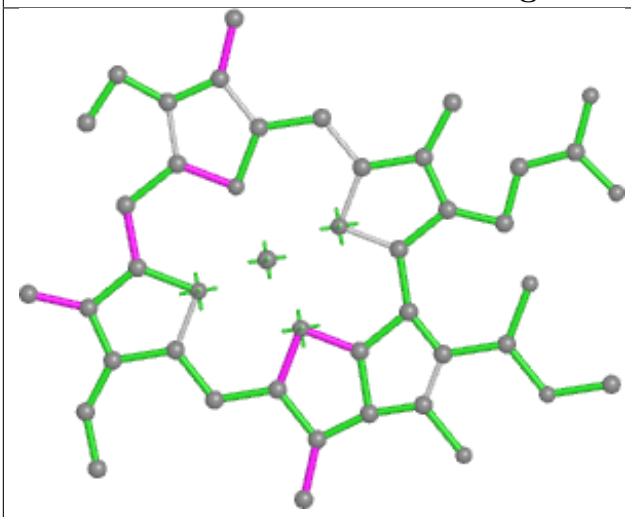


Torsions

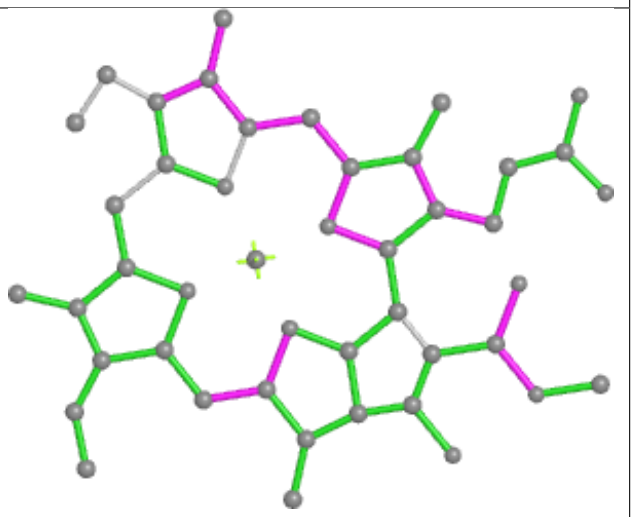


Rings

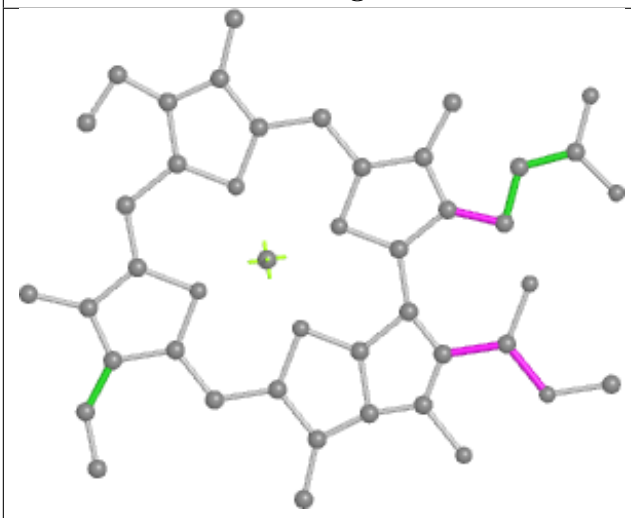
Ligand CLA a4 411



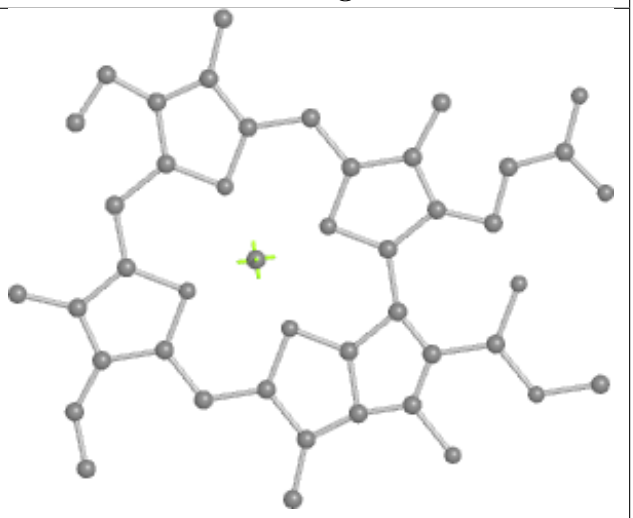
Bond lengths



Bond angles

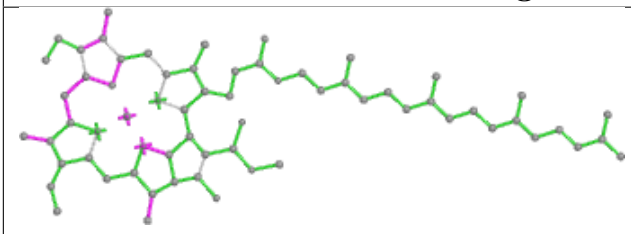


Torsions

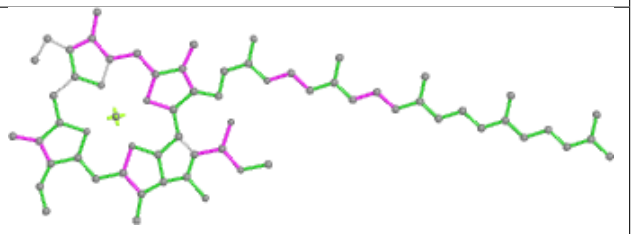


Rings

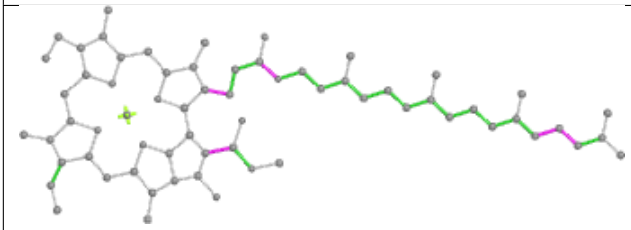
Ligand CLA aB 830



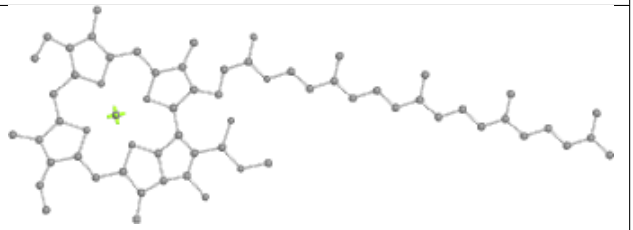
Bond lengths



Bond angles

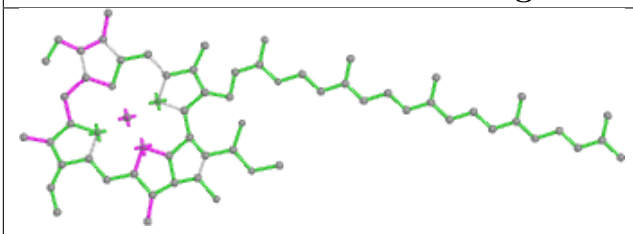


Torsions

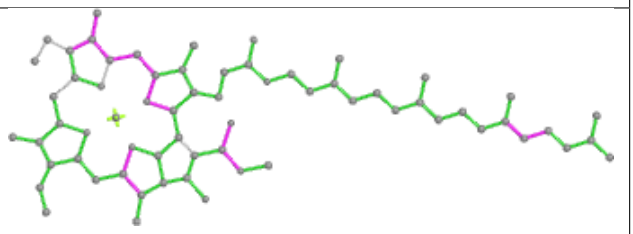


Rings

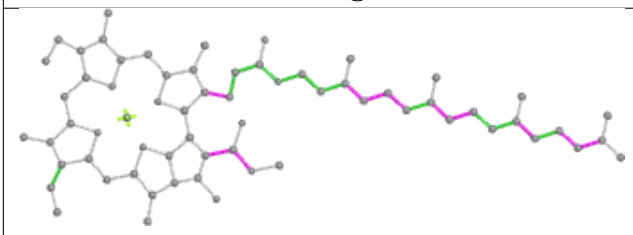
Ligand CLA aA 822



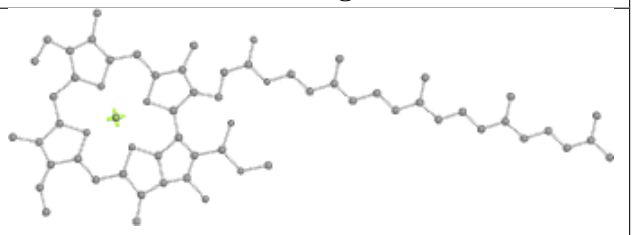
Bond lengths



Bond angles

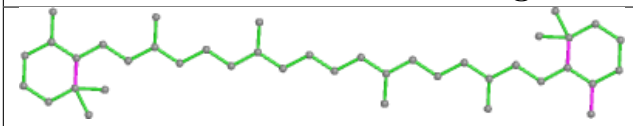


Torsions

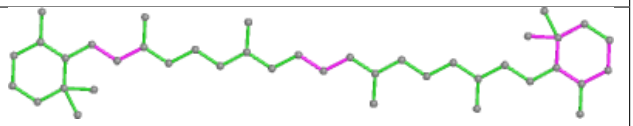


Rings

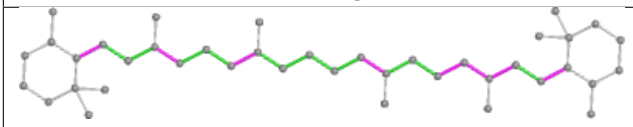
Ligand BCR bB 845



Bond lengths



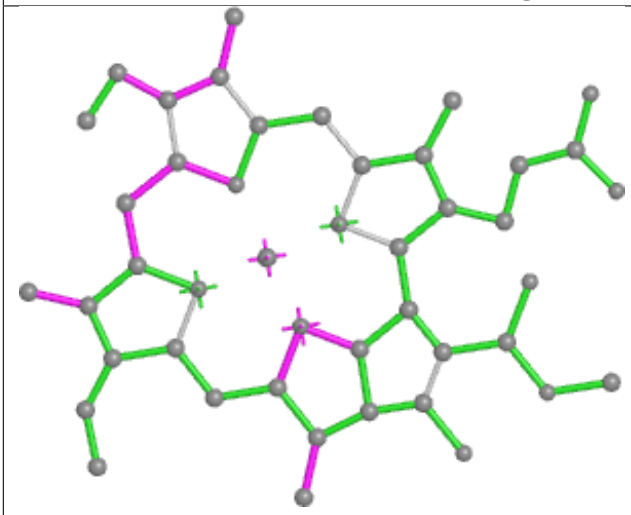
Bond angles



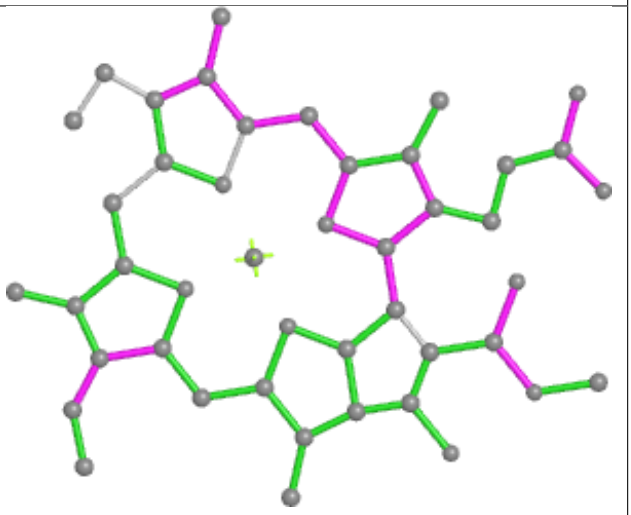
Torsions

Rings

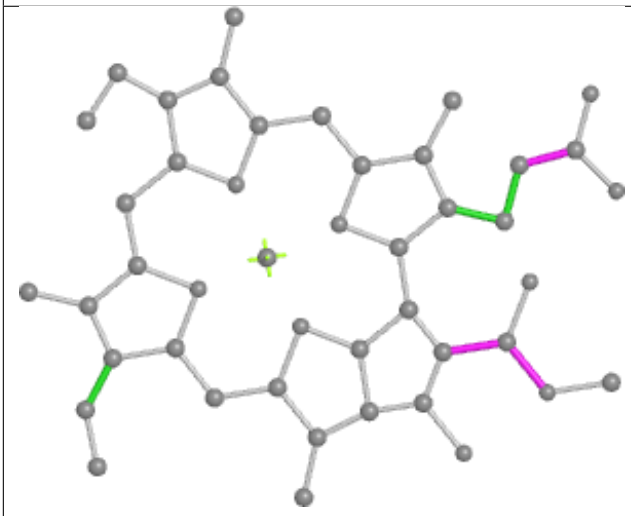
Ligand CLA cF 203



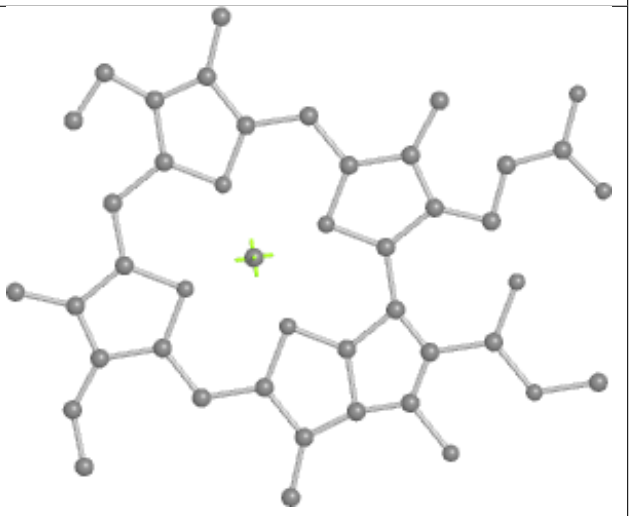
Bond lengths



Bond angles

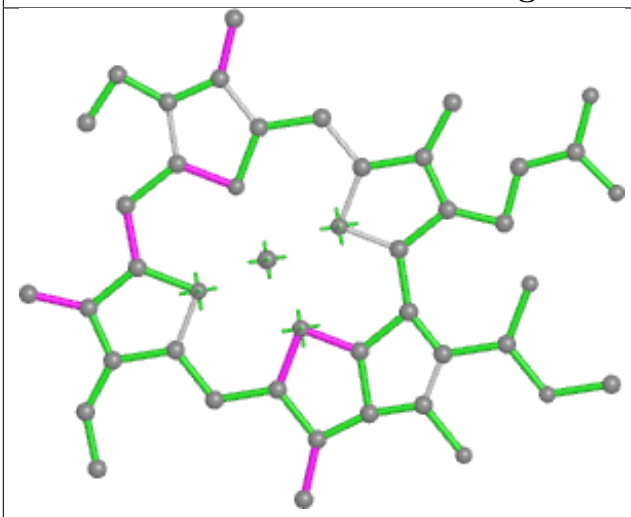


Torsions

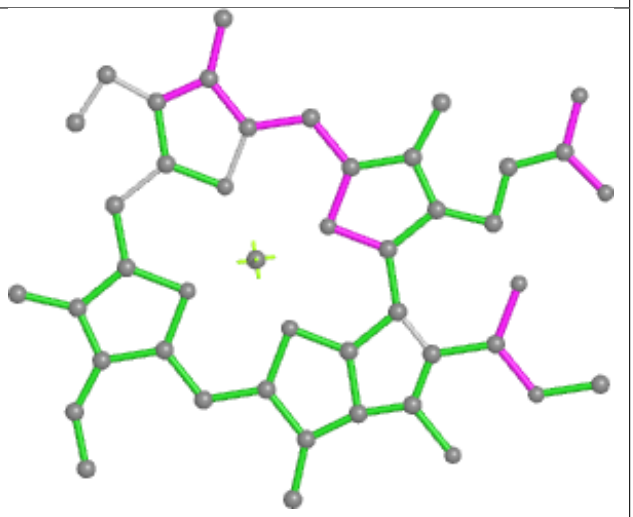


Rings

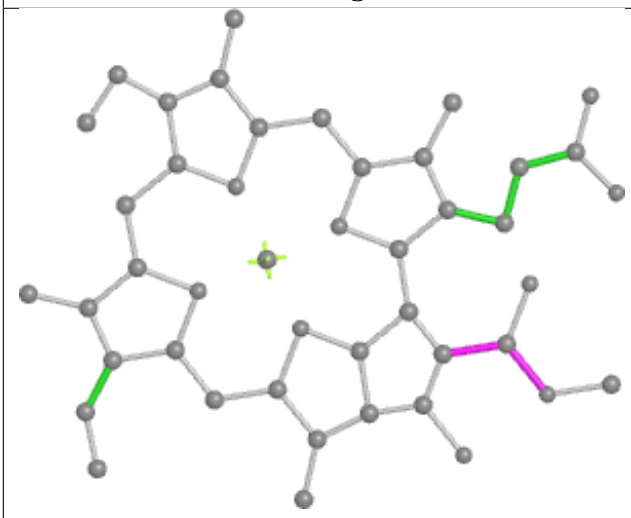
Ligand CLA b1 406



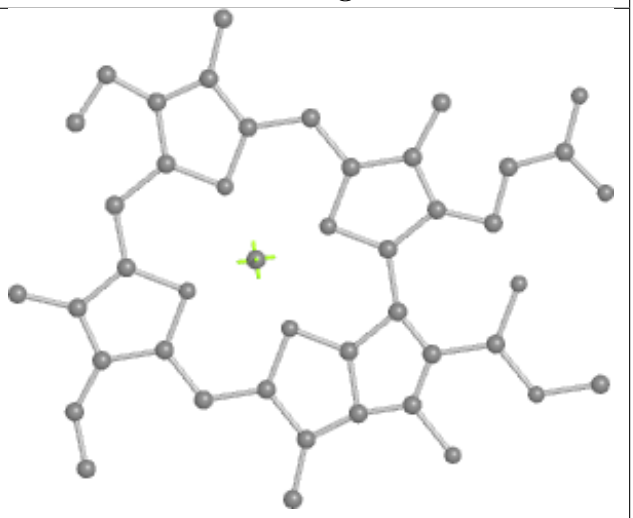
Bond lengths



Bond angles

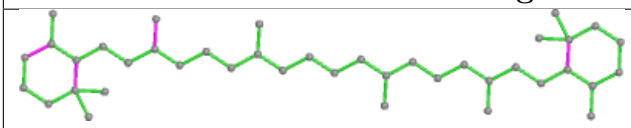


Torsions

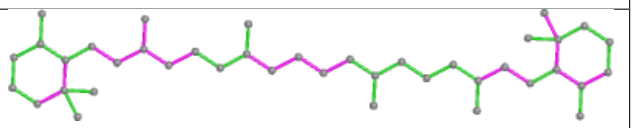


Rings

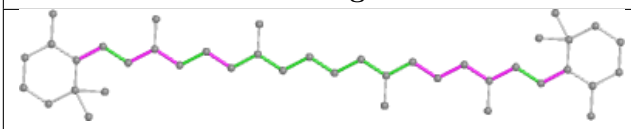
Ligand BCR b1 401



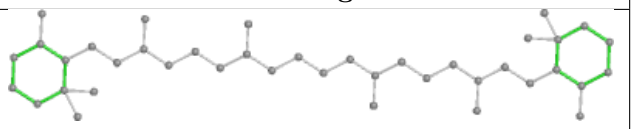
Bond lengths



Bond angles

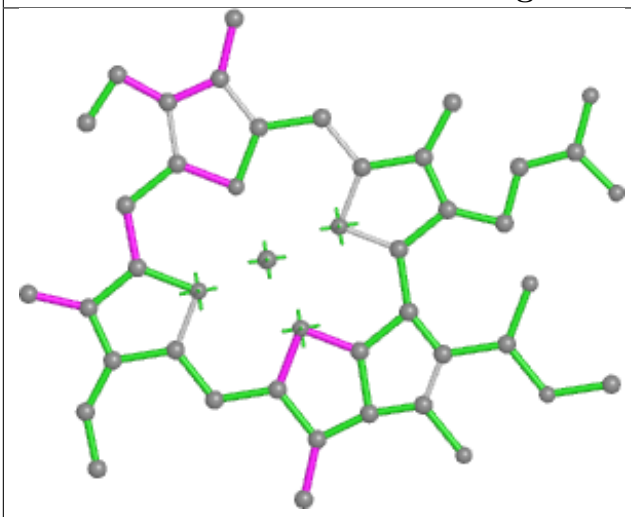


Torsions

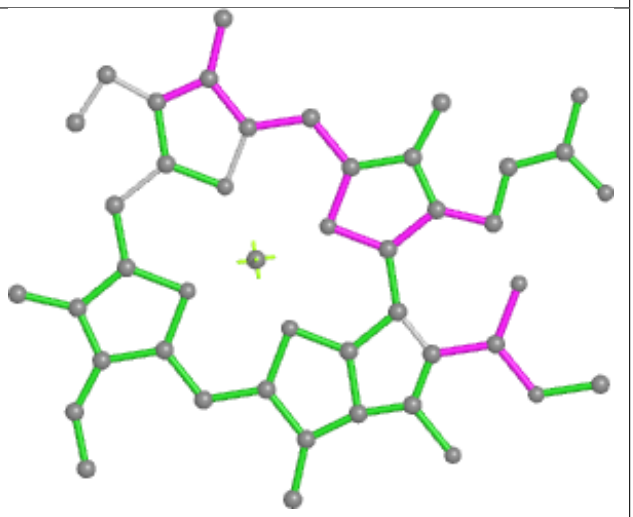


Rings

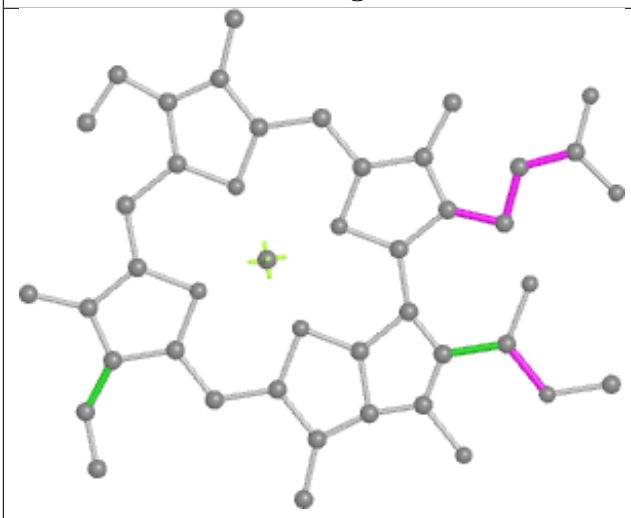
Ligand CLA cB 835



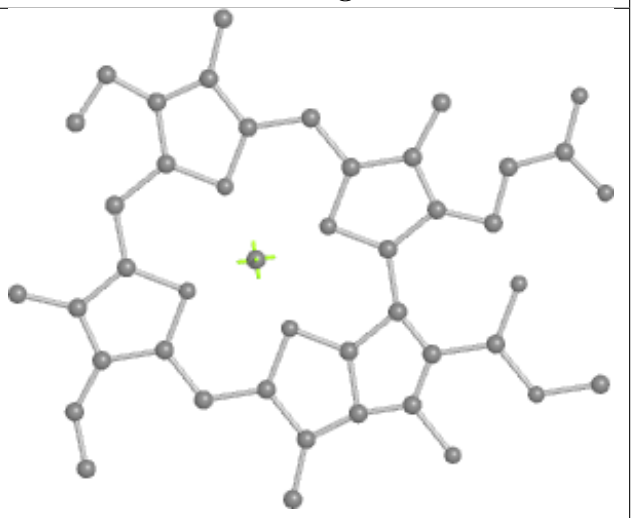
Bond lengths



Bond angles

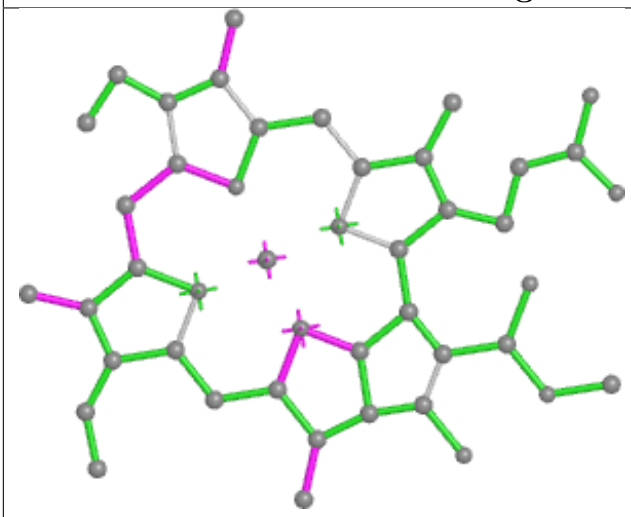


Torsions

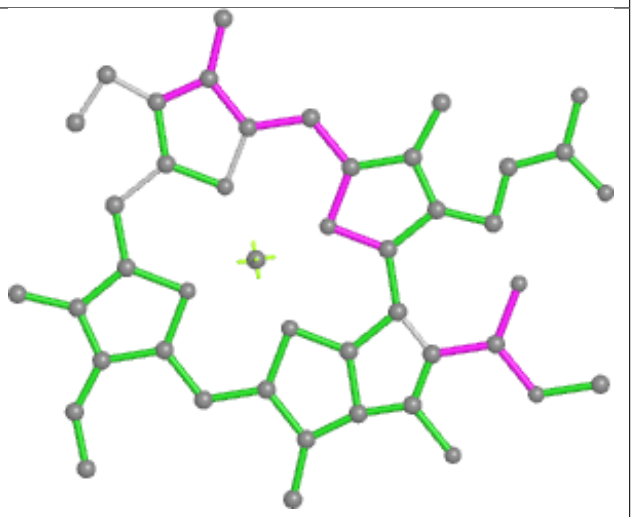


Rings

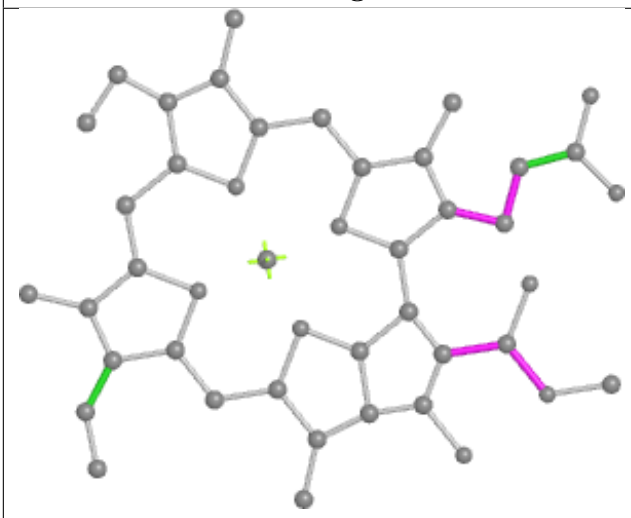
Ligand CLA aB 816



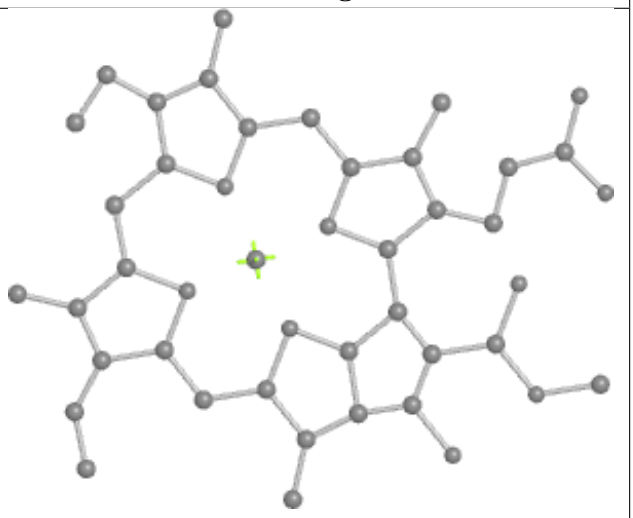
Bond lengths



Bond angles

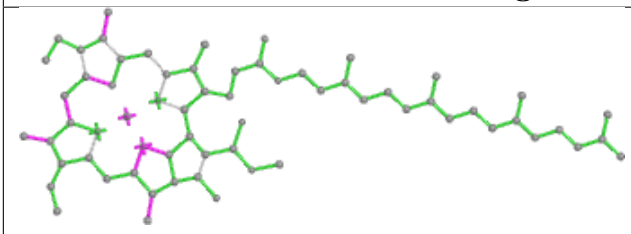


Torsions

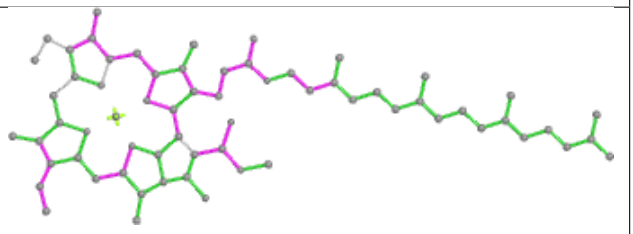


Rings

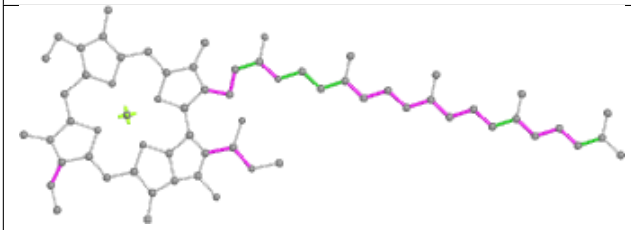
Ligand CLA bB 814



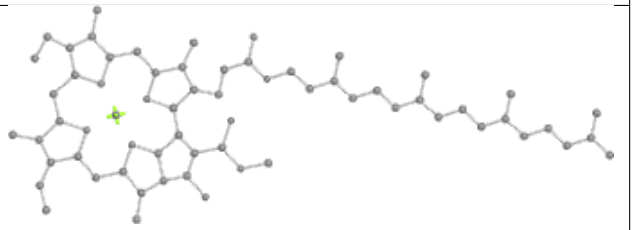
Bond lengths



Bond angles

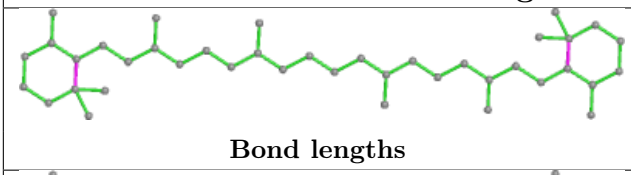


Torsions

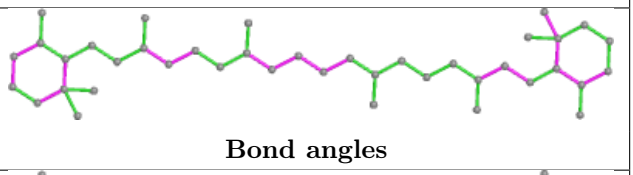


Rings

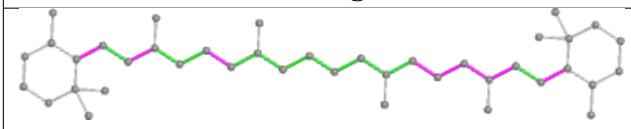
Ligand BCR b3 419



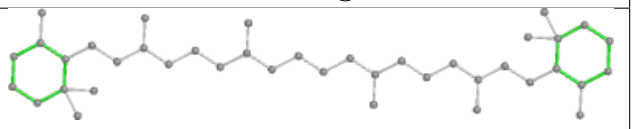
Bond lengths



Bond angles

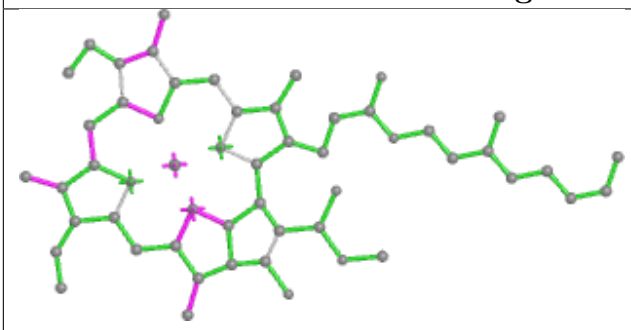


Torsions

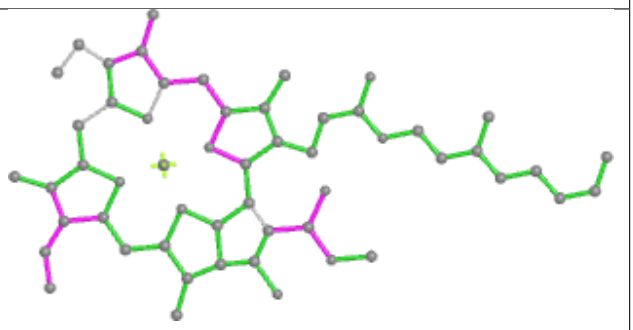


Rings

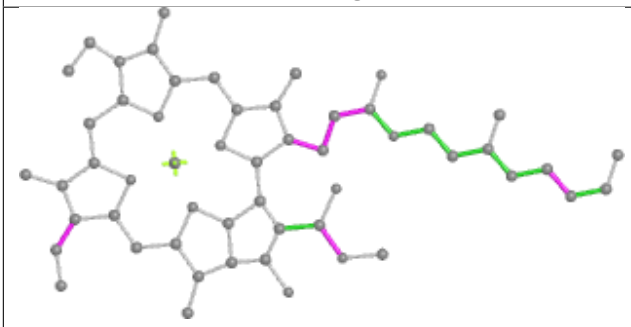
Ligand CLA aA 819



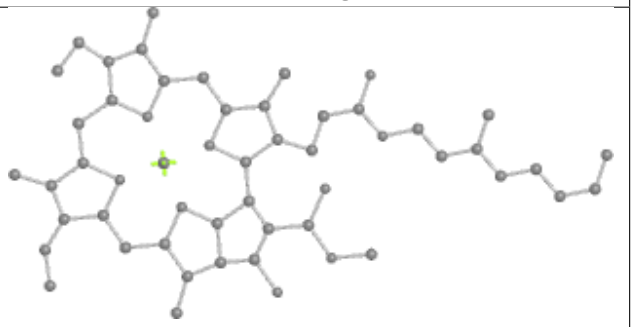
Bond lengths



Bond angles

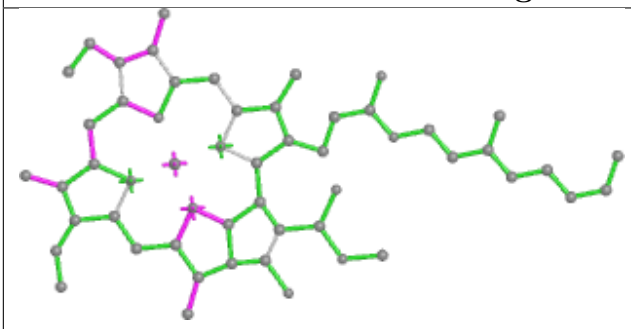


Torsions

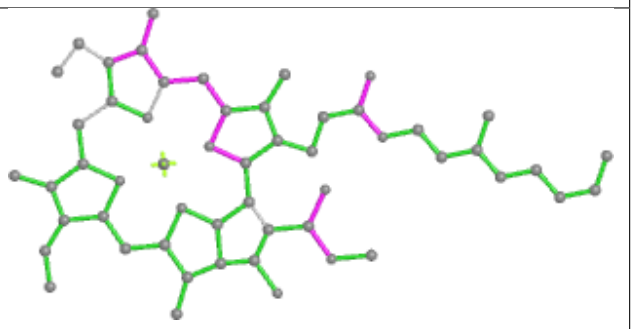


Rings

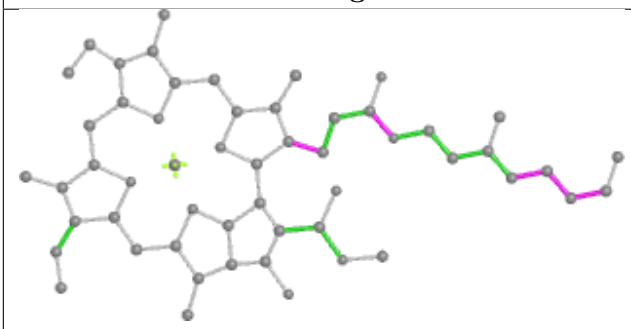
Ligand CLA aA 836



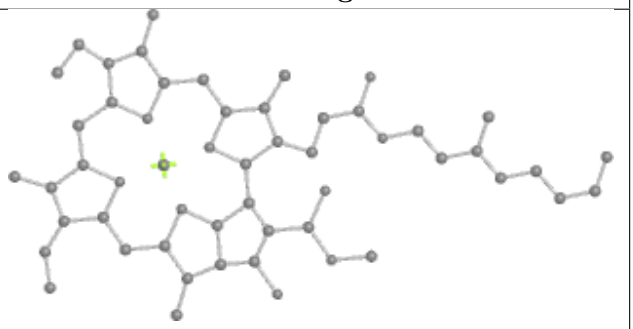
Bond lengths



Bond angles

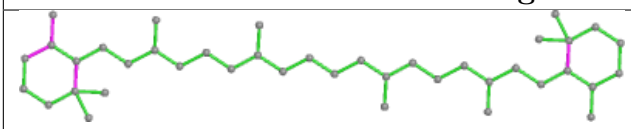


Torsions

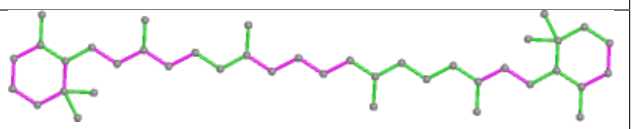


Rings

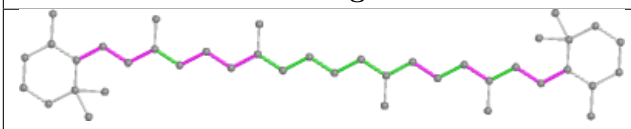
Ligand BCR a6 421



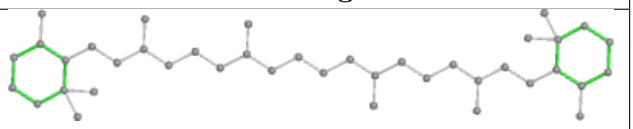
Bond lengths



Bond angles

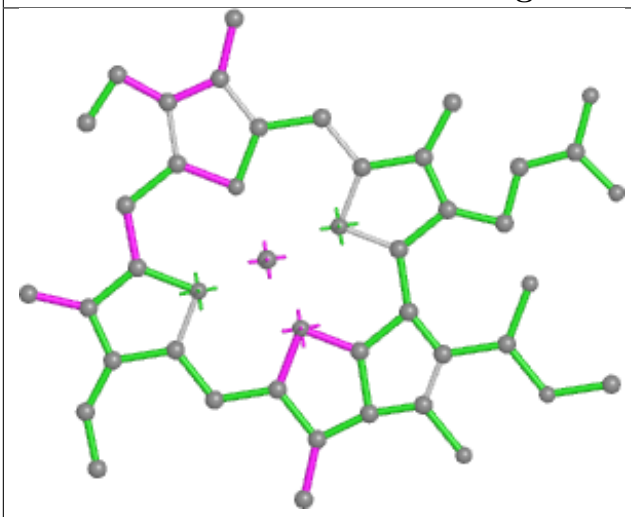


Torsions

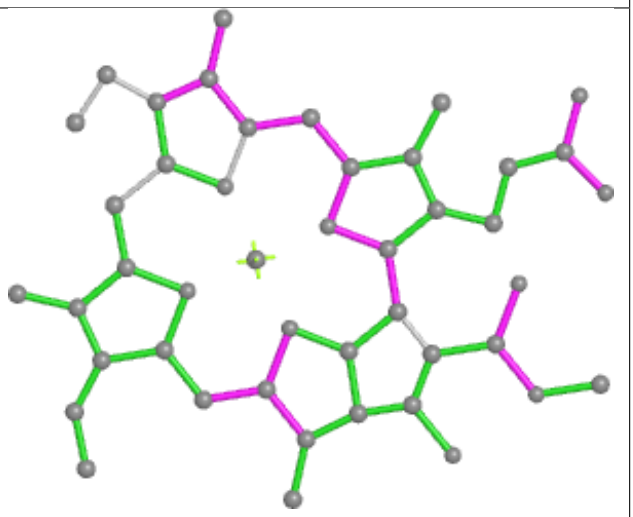


Rings

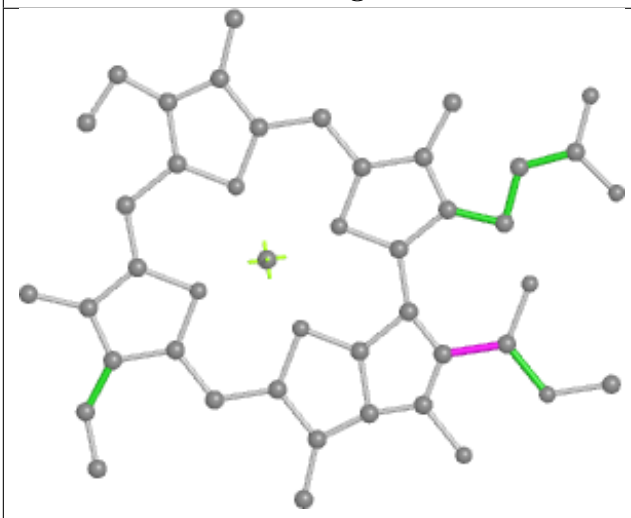
Ligand CLA cA 815



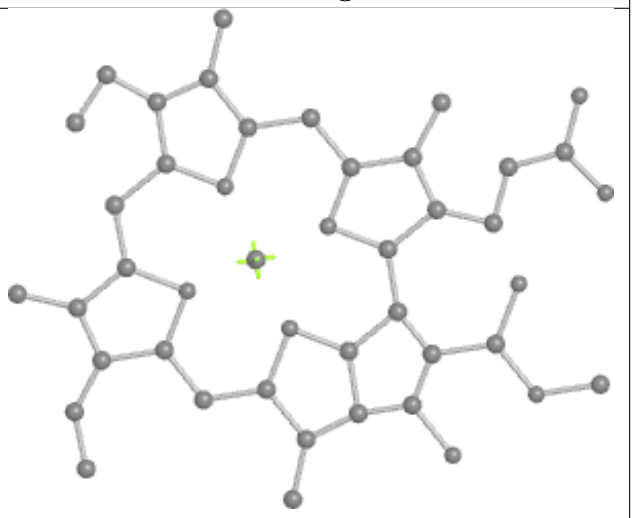
Bond lengths



Bond angles

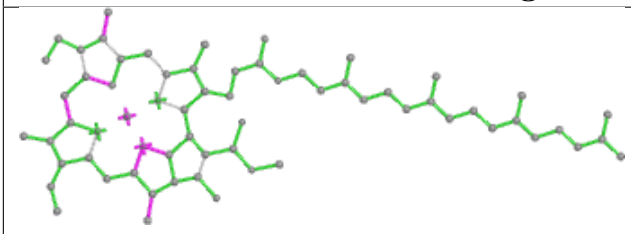


Torsions

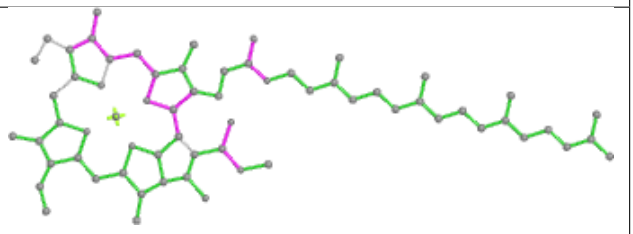


Rings

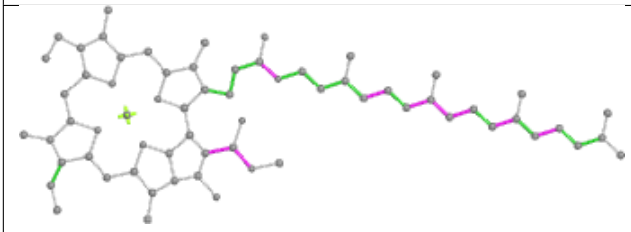
Ligand CLA a4 403



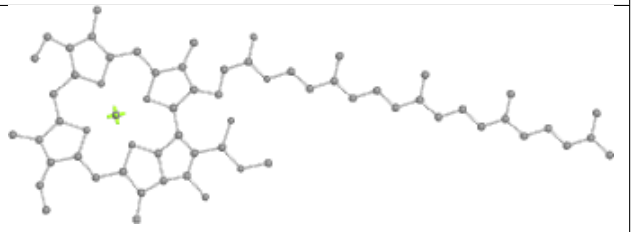
Bond lengths



Bond angles

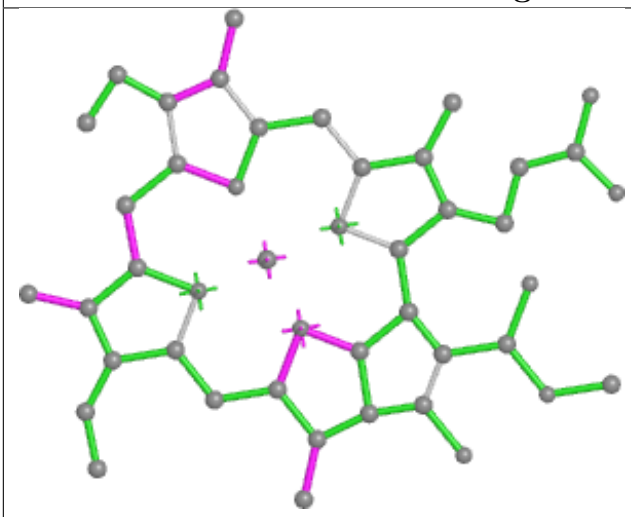


Torsions

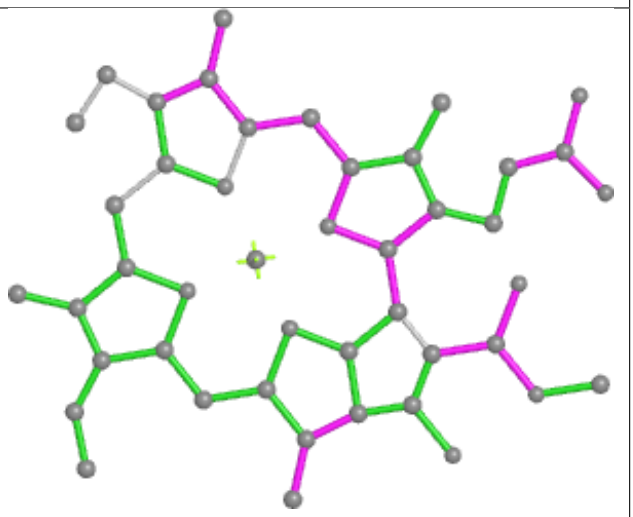


Rings

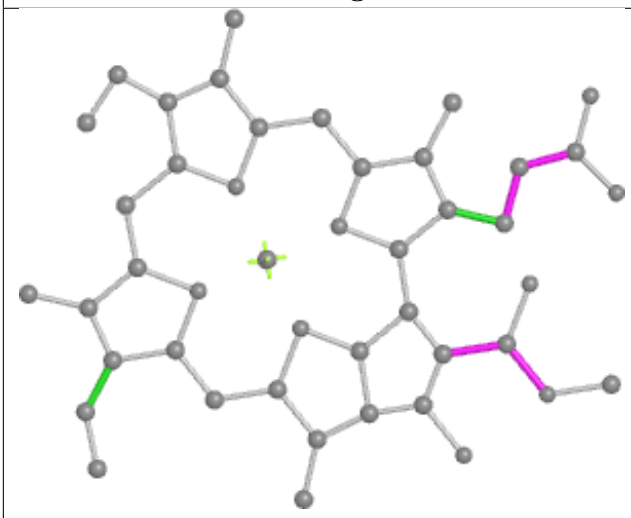
Ligand CLA bX 102



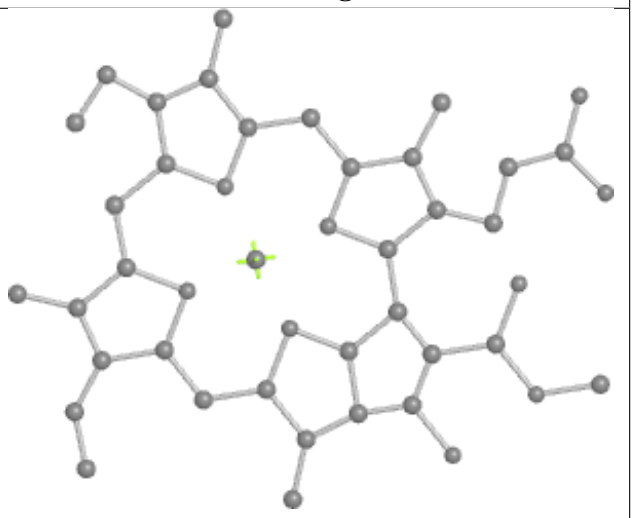
Bond lengths



Bond angles

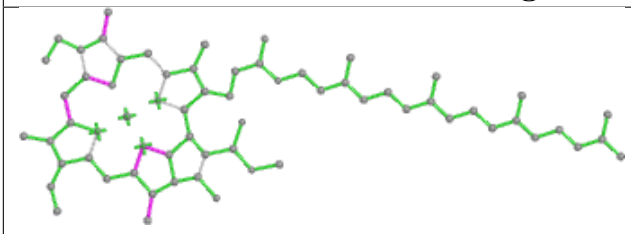


Torsions

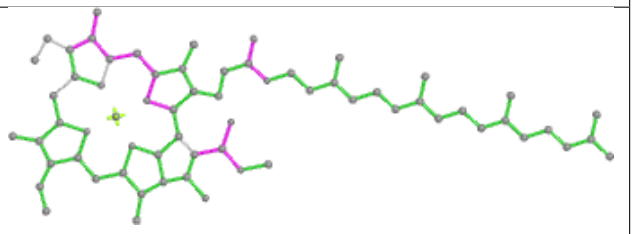


Rings

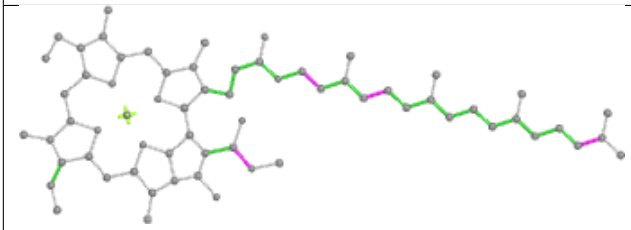
Ligand CLA c4 409



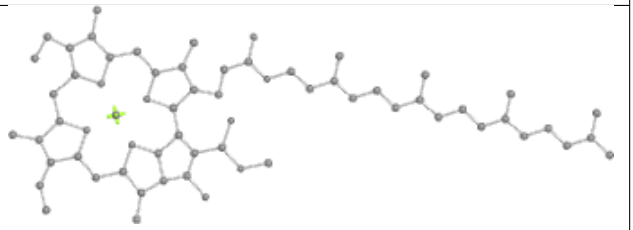
Bond lengths



Bond angles

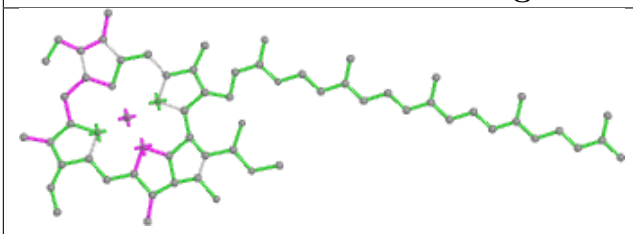


Torsions

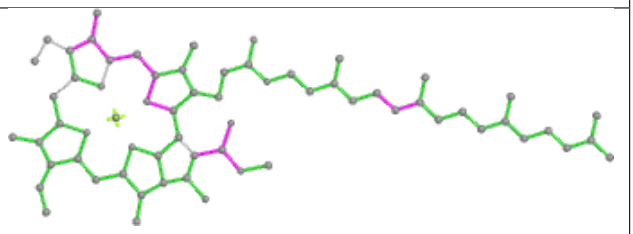


Rings

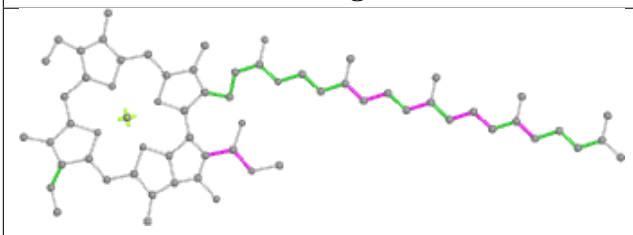
Ligand CLA bA 839



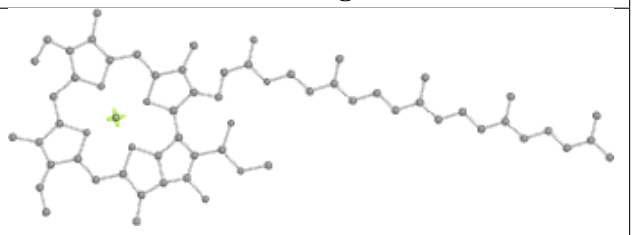
Bond lengths



Bond angles

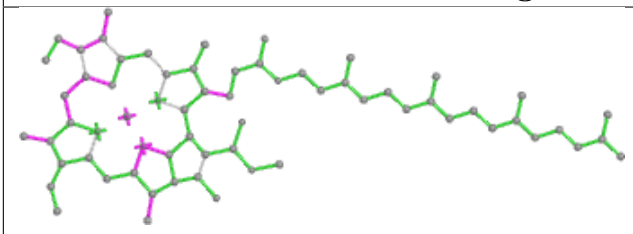


Torsions

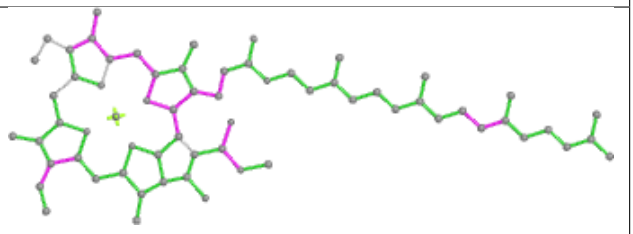


Rings

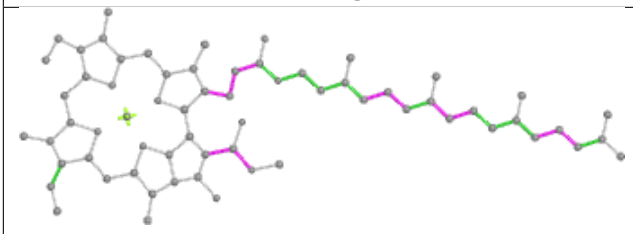
Ligand CLA cB 810



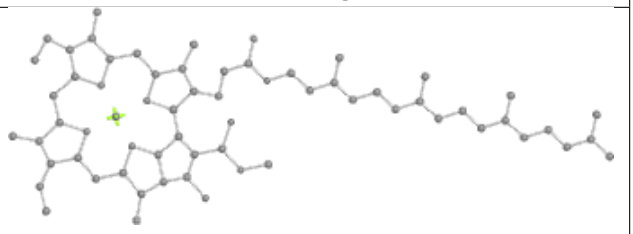
Bond lengths



Bond angles

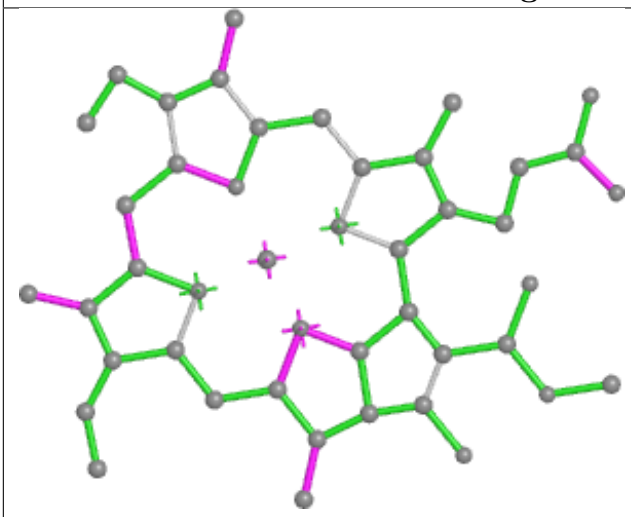


Torsions

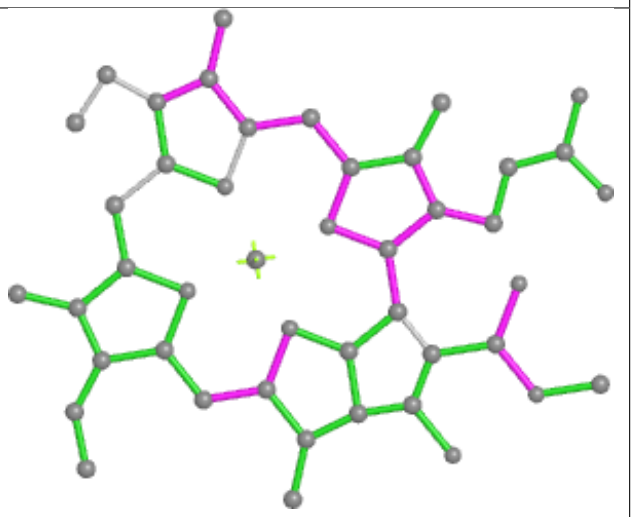


Rings

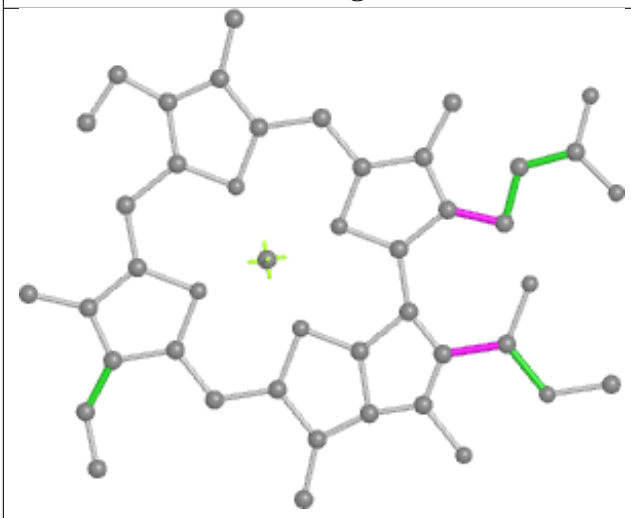
Ligand CLA c2 412



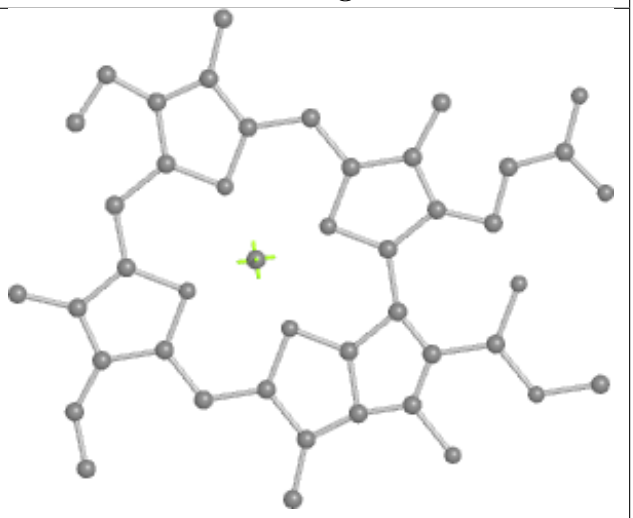
Bond lengths



Bond angles

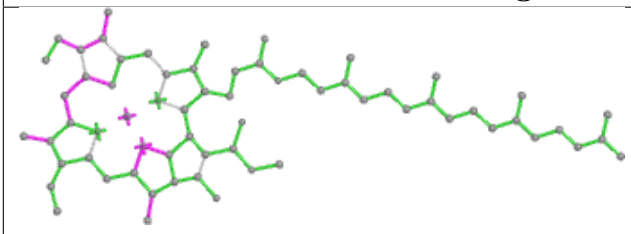


Torsions

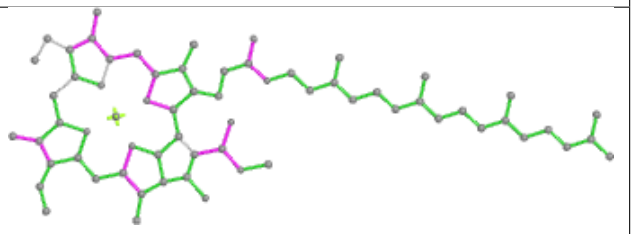


Rings

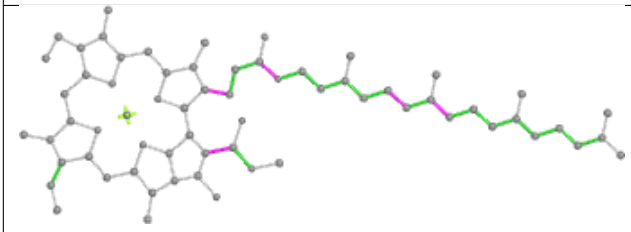
Ligand CLA aA 831



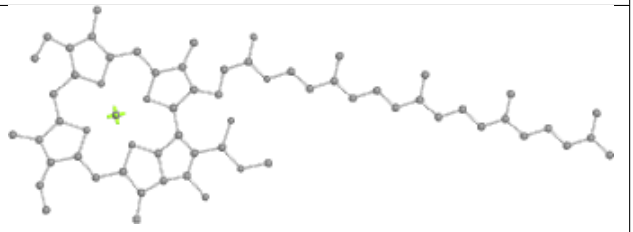
Bond lengths



Bond angles

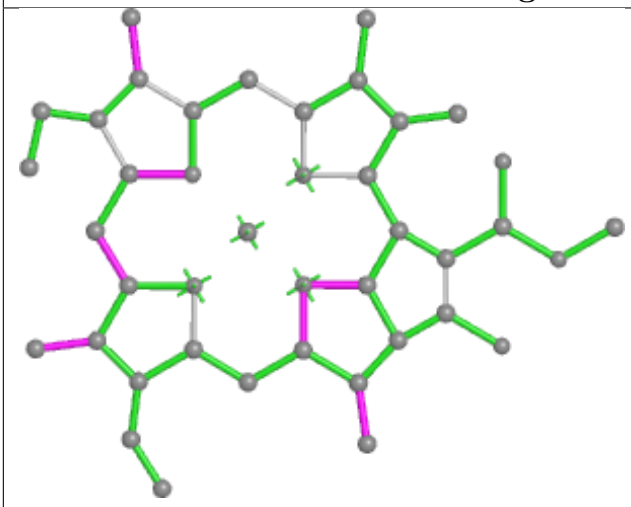


Torsions

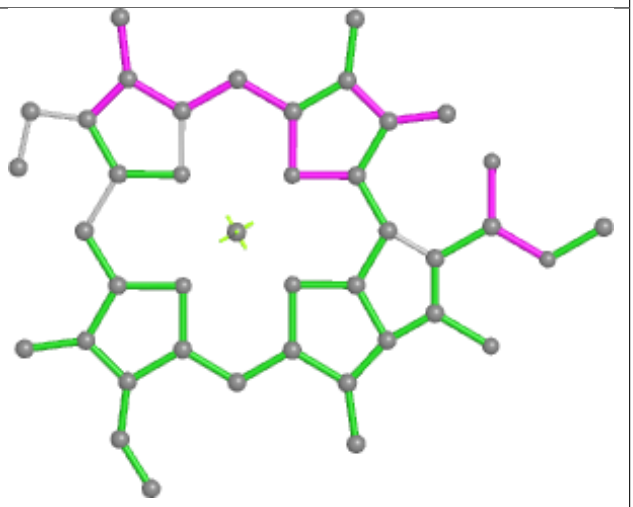


Rings

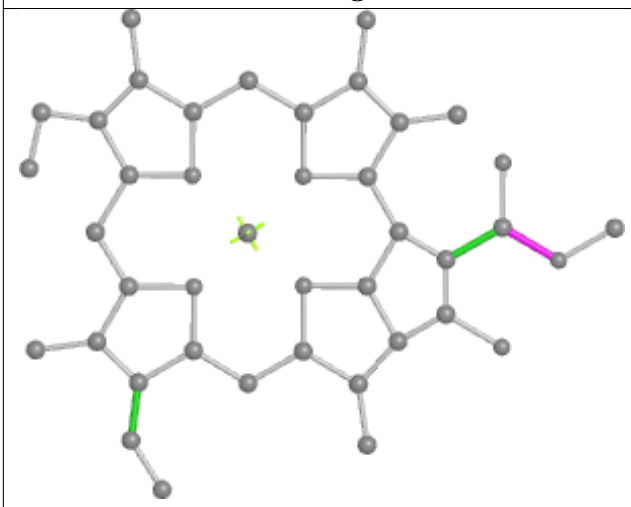
Ligand CLA b2 415



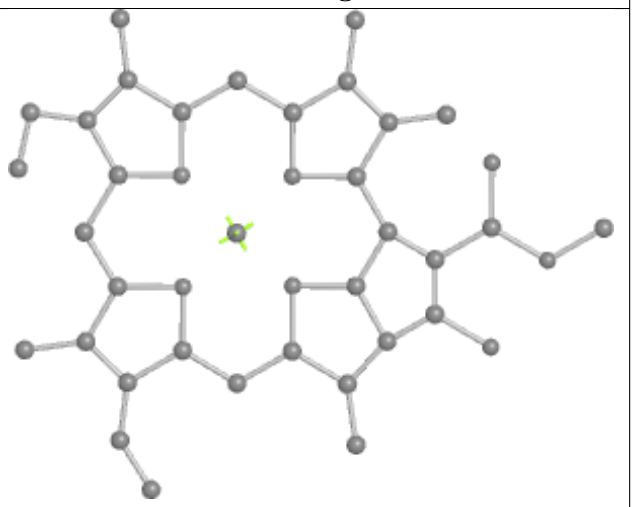
Bond lengths



Bond angles

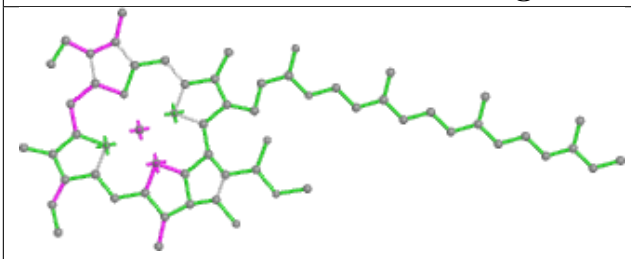


Torsions

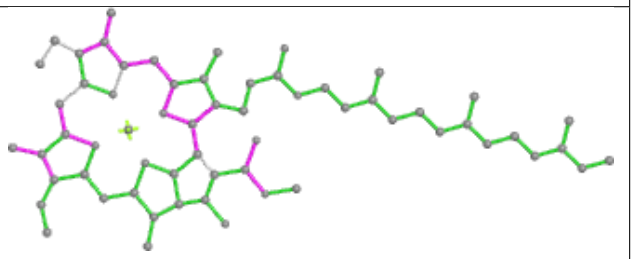


Rings

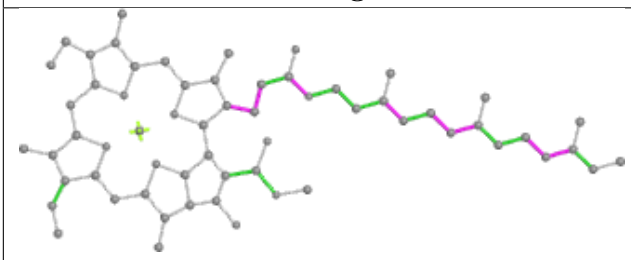
Ligand CLA aA 821



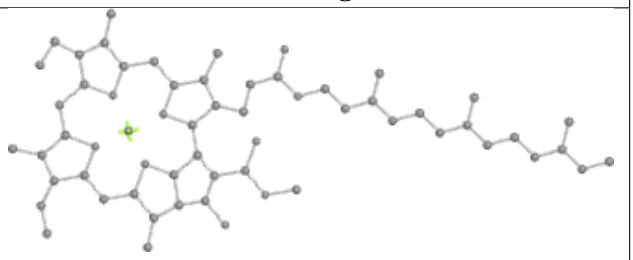
Bond lengths



Bond angles

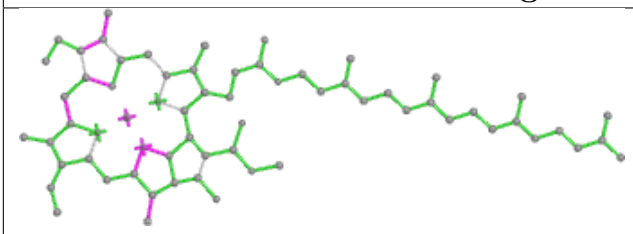


Torsions

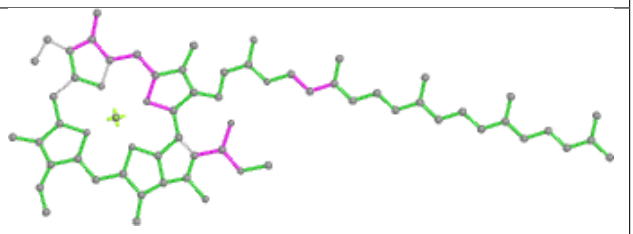


Rings

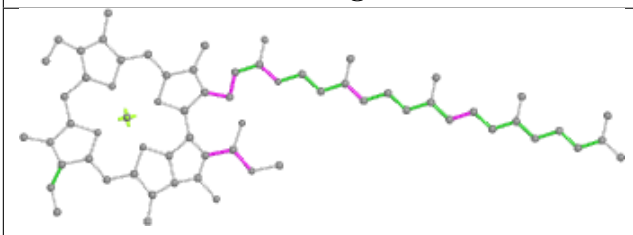
Ligand CLA c1 404



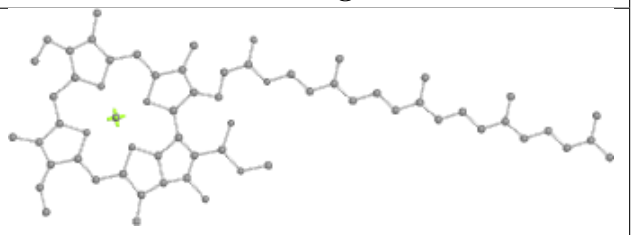
Bond lengths



Bond angles

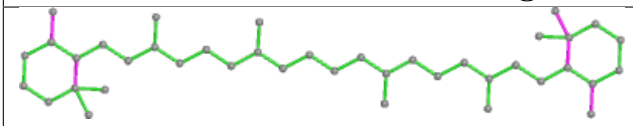


Torsions

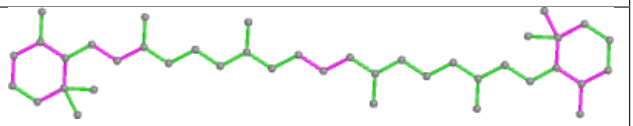


Rings

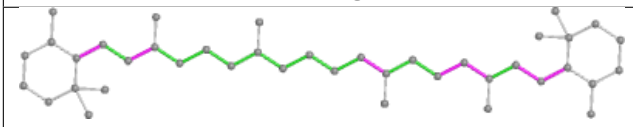
Ligand BCR c6 419



Bond lengths



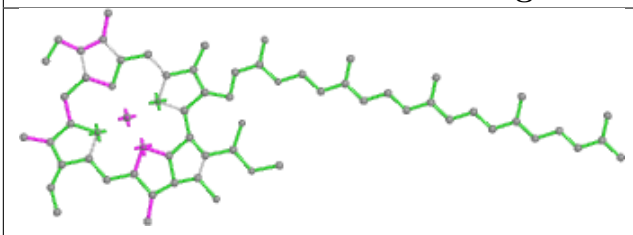
Bond angles



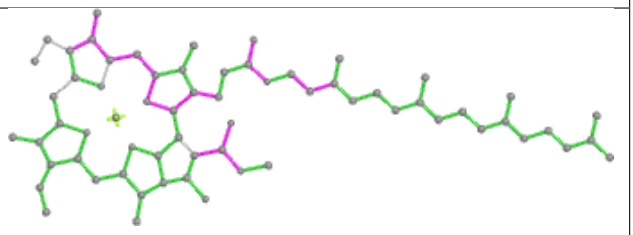
Torsions

Rings

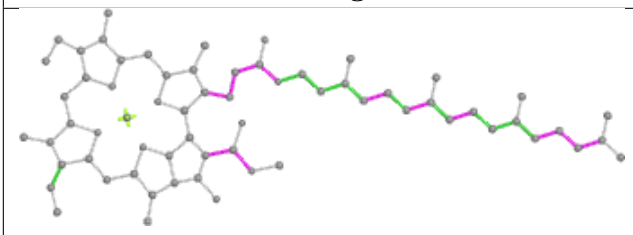
Ligand CLA cA 809



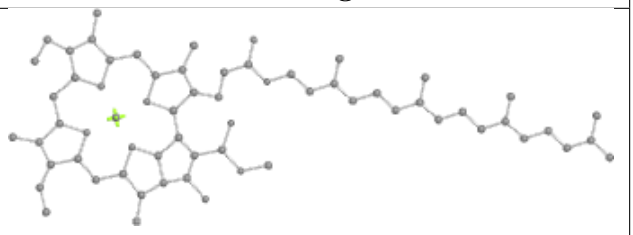
Bond lengths



Bond angles

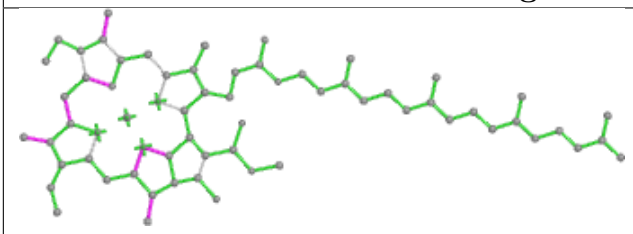


Torsions

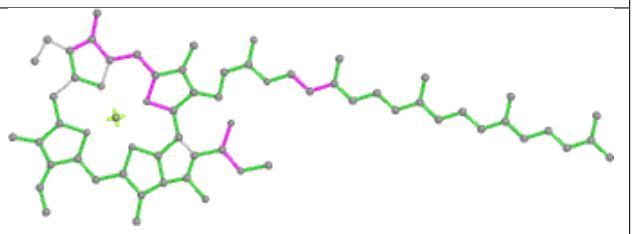


Rings

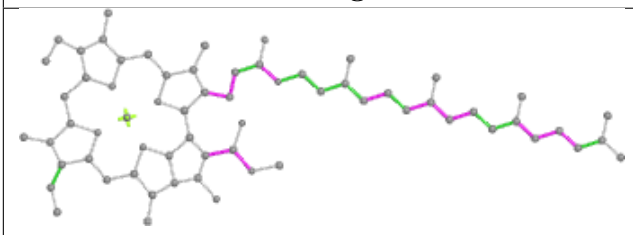
Ligand CLA a5 402



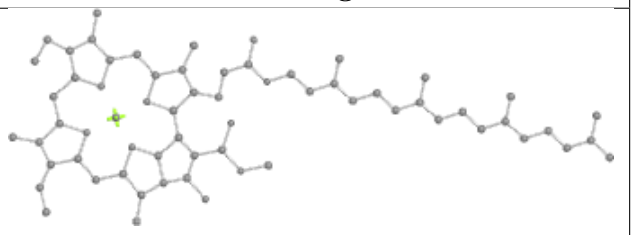
Bond lengths



Bond angles

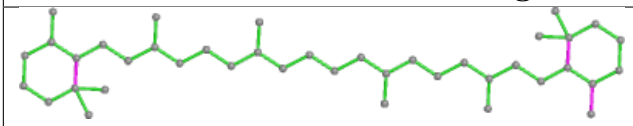


Torsions

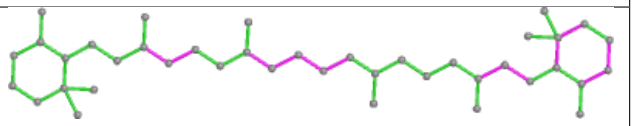


Rings

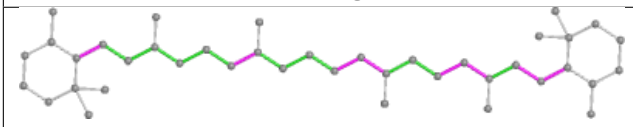
Ligand BCR cA 847



Bond lengths



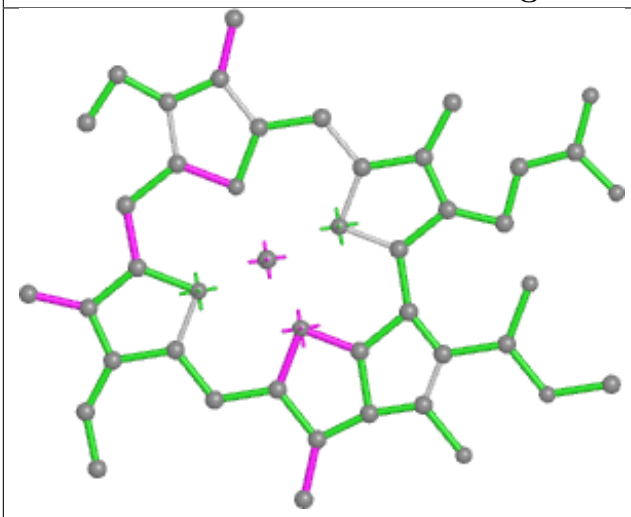
Bond angles



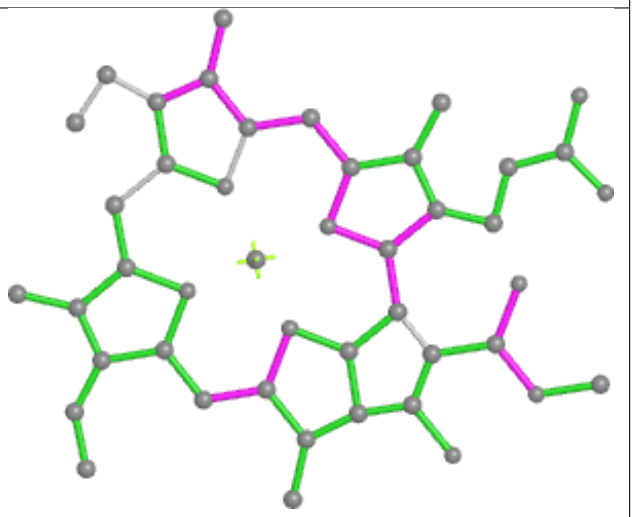
Torsions

Rings

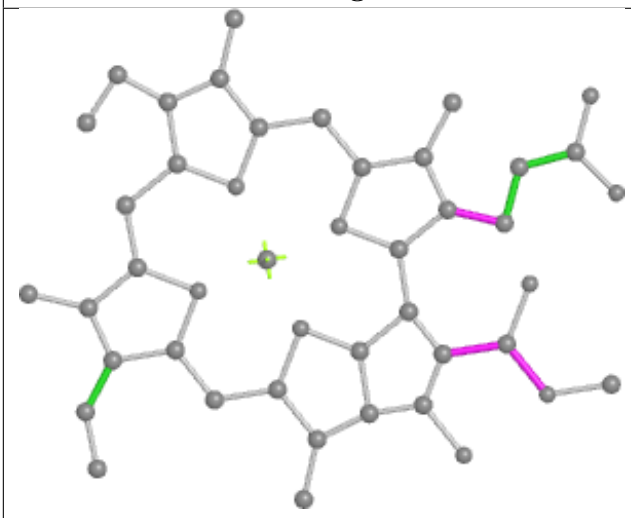
Ligand CLA c1 411



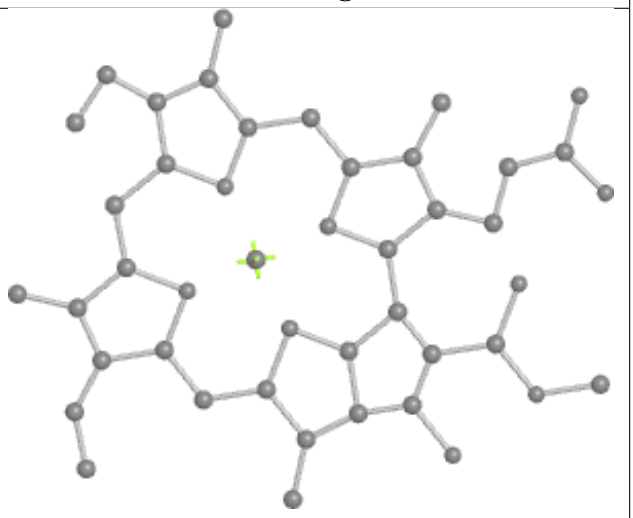
Bond lengths



Bond angles

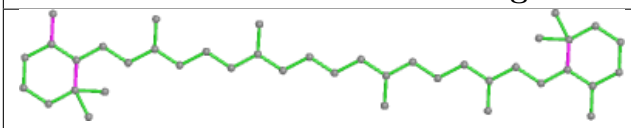


Torsions

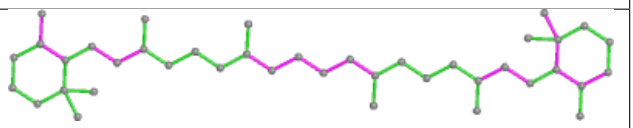


Rings

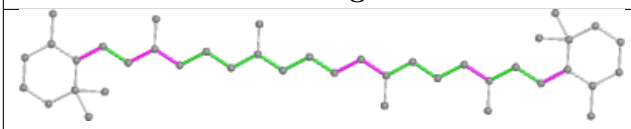
Ligand BCR cM 101



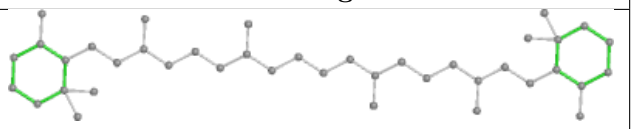
Bond lengths



Bond angles

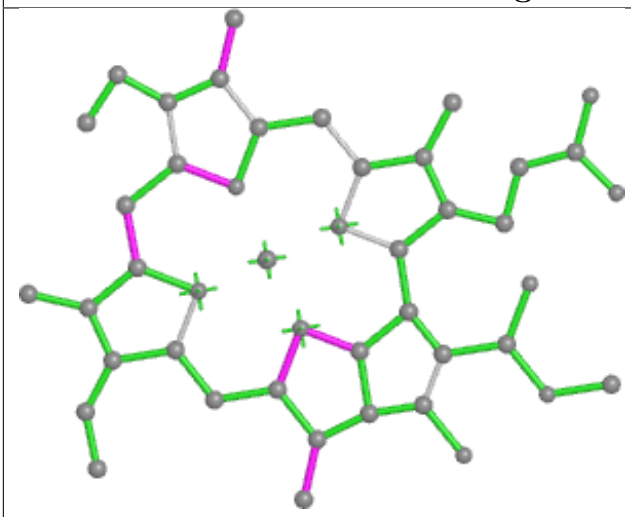


Torsions

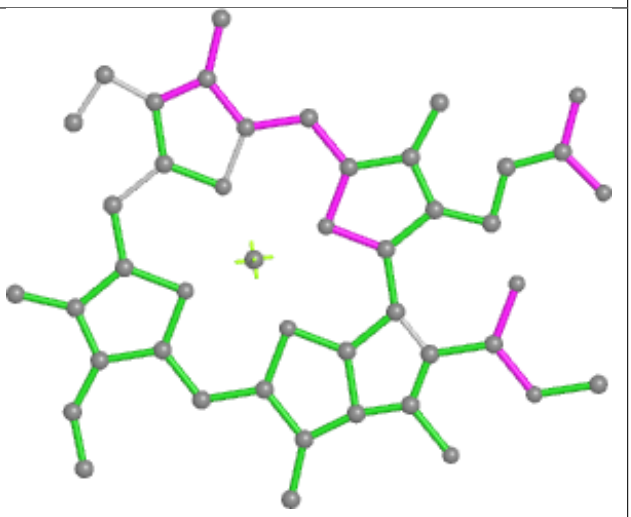


Rings

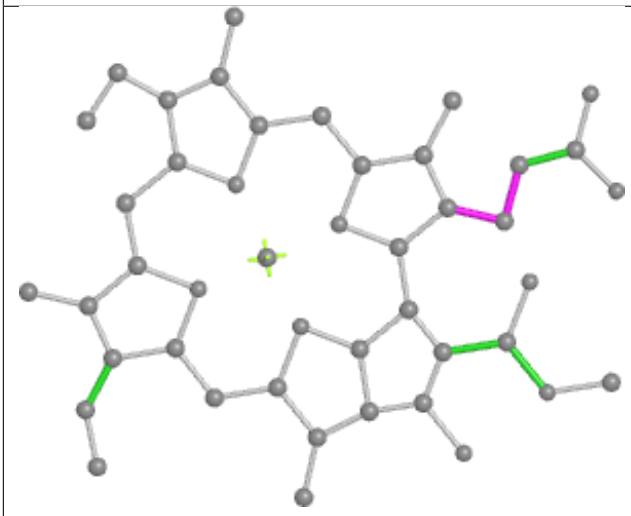
Ligand CLA bB 822



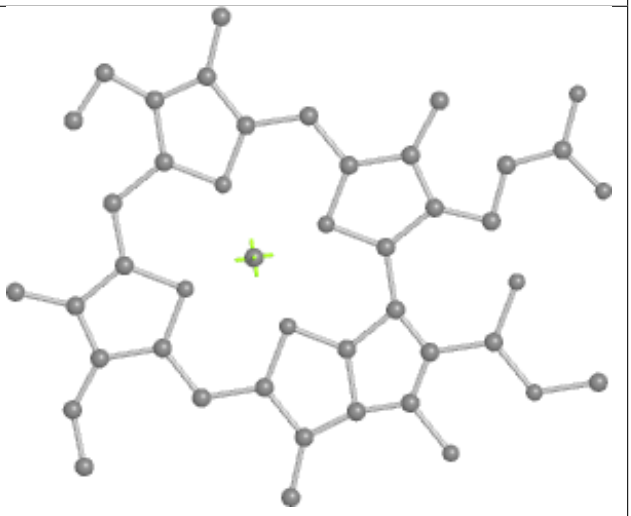
Bond lengths



Bond angles

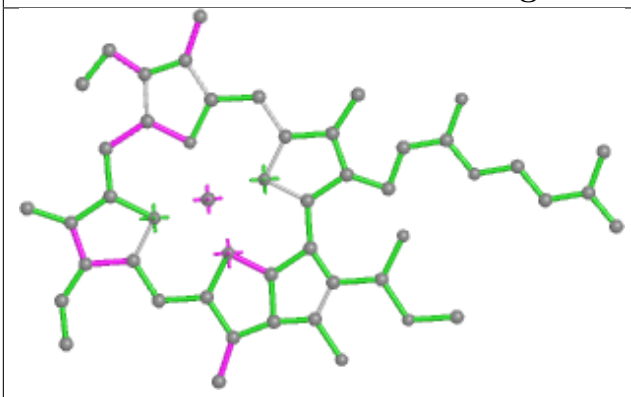


Torsions

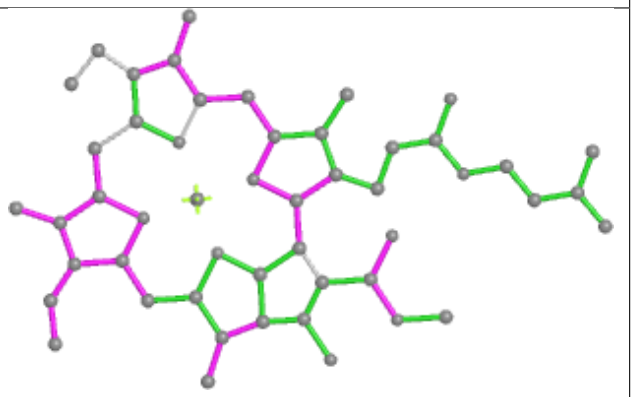


Rings

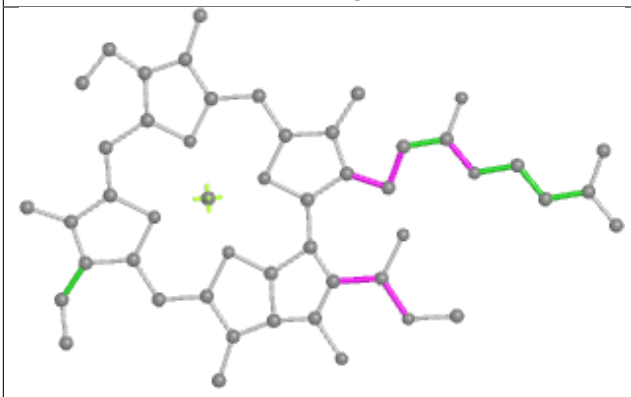
Ligand CLA a5 416



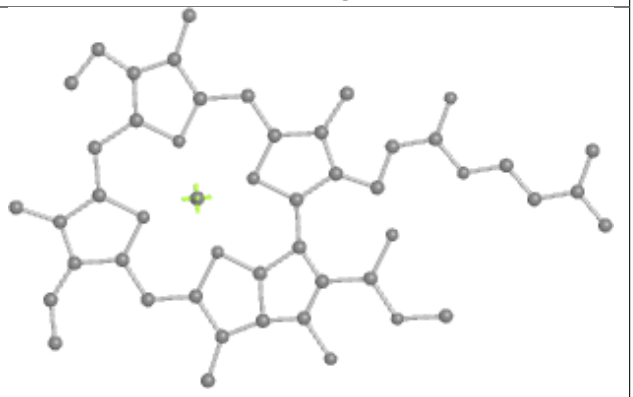
Bond lengths



Bond angles

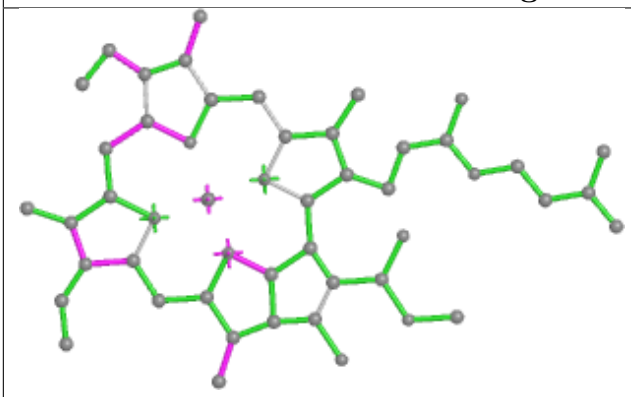


Torsions

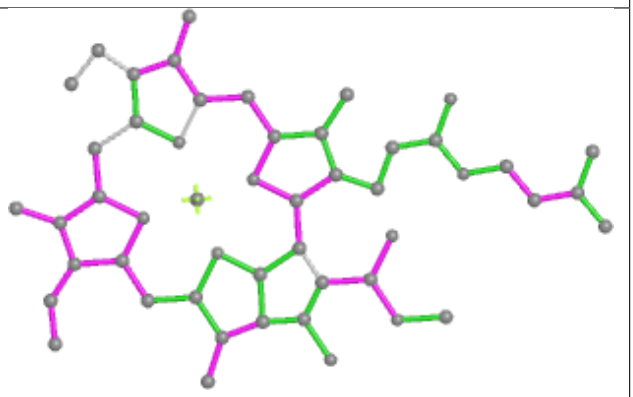


Rings

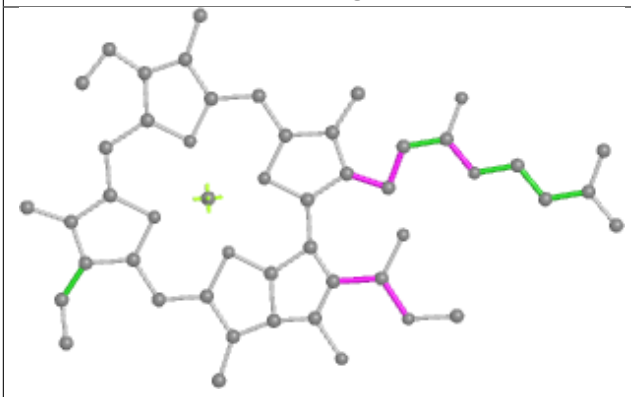
Ligand CLA c6 417



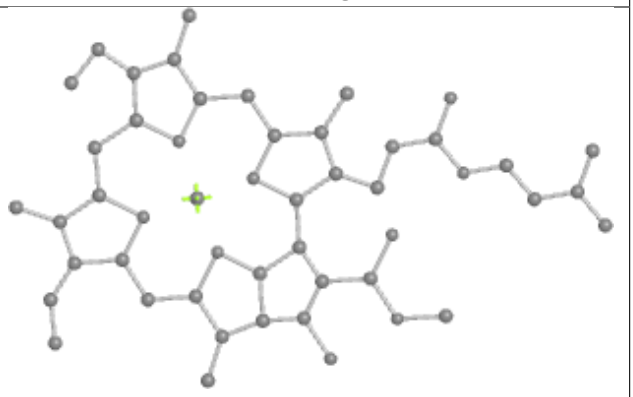
Bond lengths



Bond angles

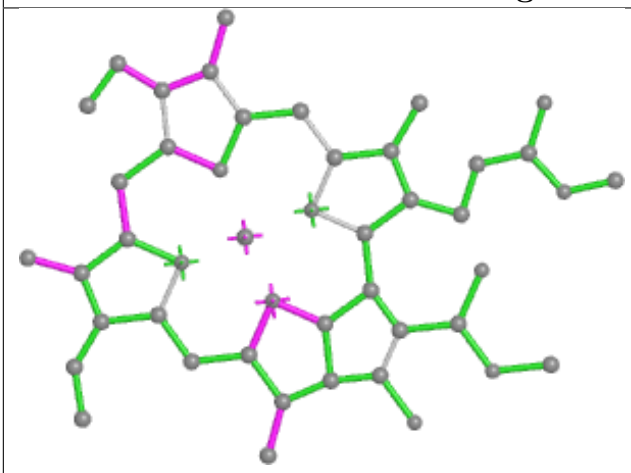


Torsions

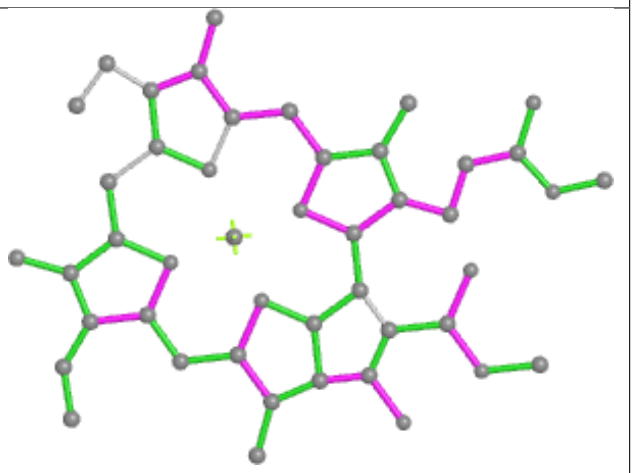


Rings

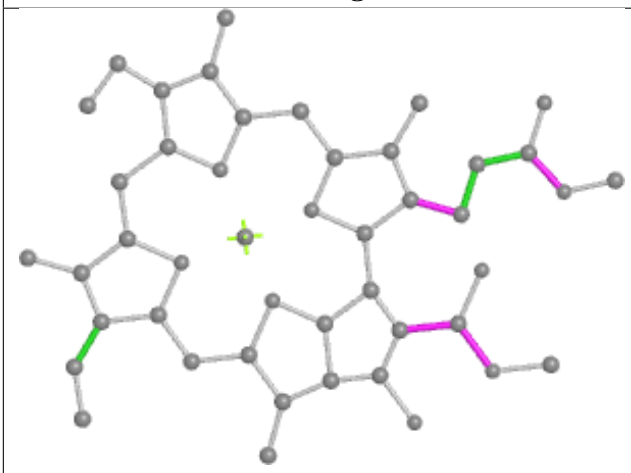
Ligand CLA cB 826



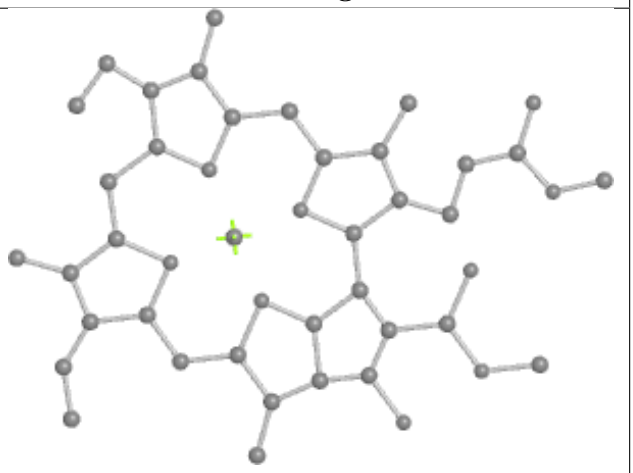
Bond lengths



Bond angles

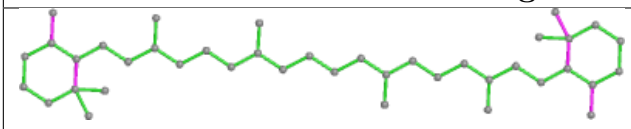


Torsions

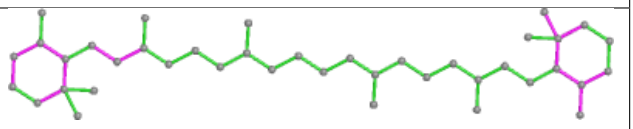


Rings

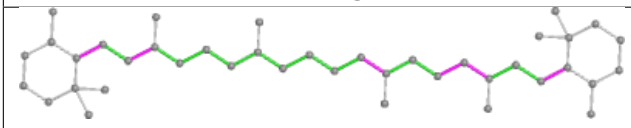
Ligand BCR c4 418



Bond lengths



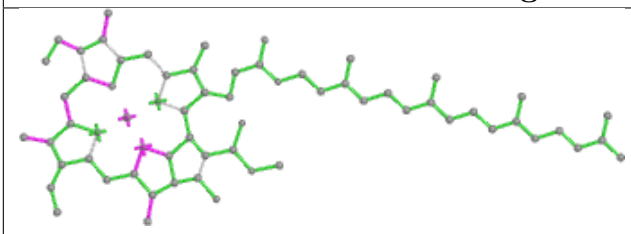
Bond angles



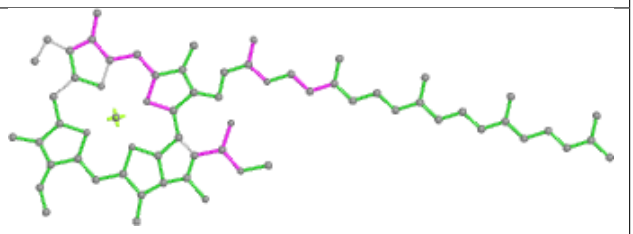
Torsions

Rings

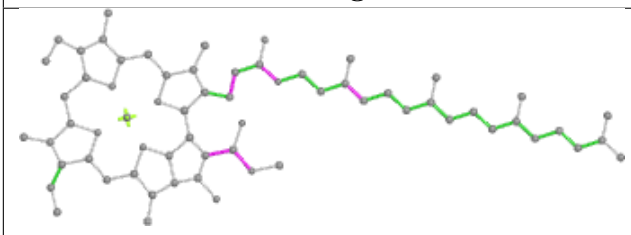
Ligand CLA c2 404



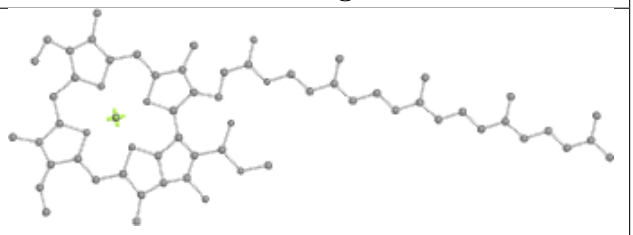
Bond lengths



Bond angles

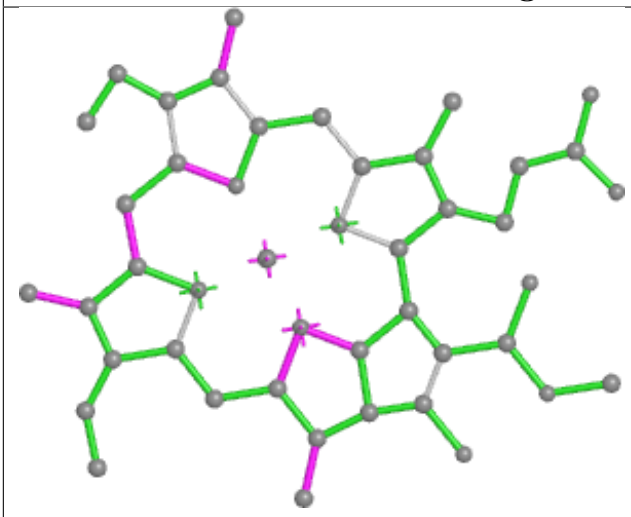


Torsions

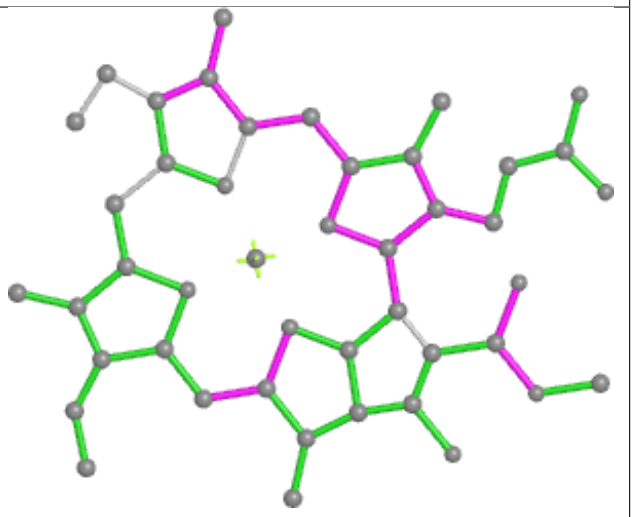


Rings

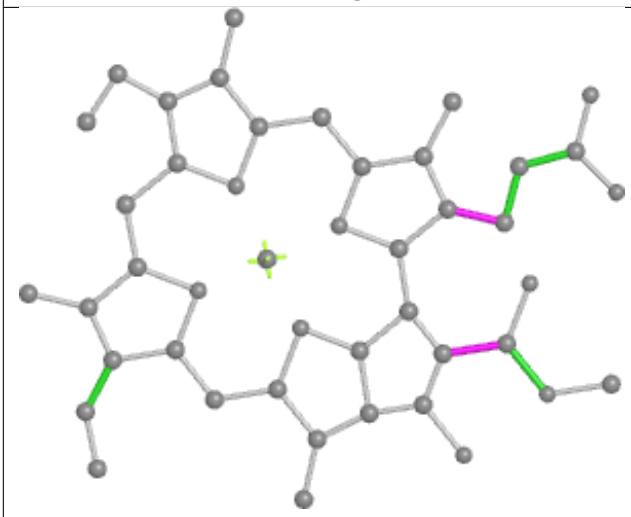
Ligand CLA b5 411



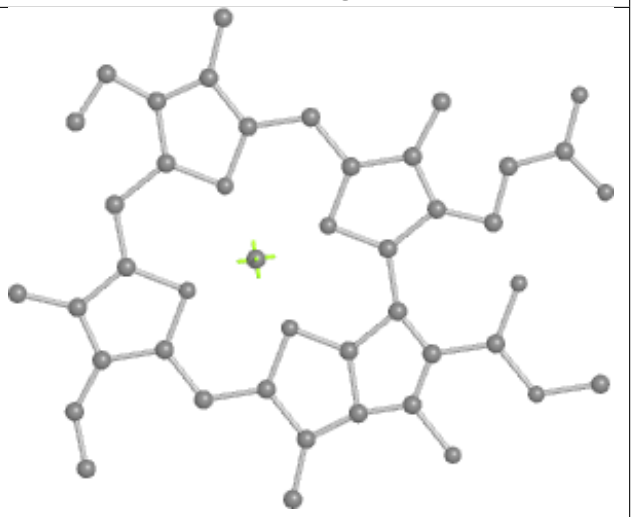
Bond lengths



Bond angles

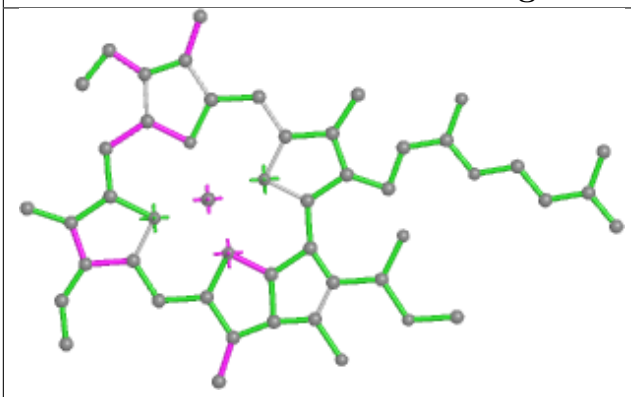


Torsions

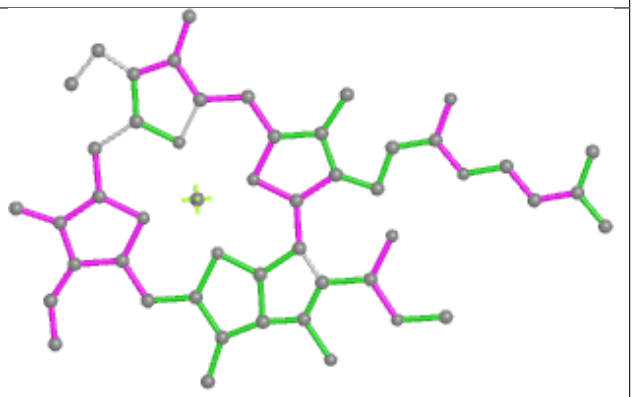


Rings

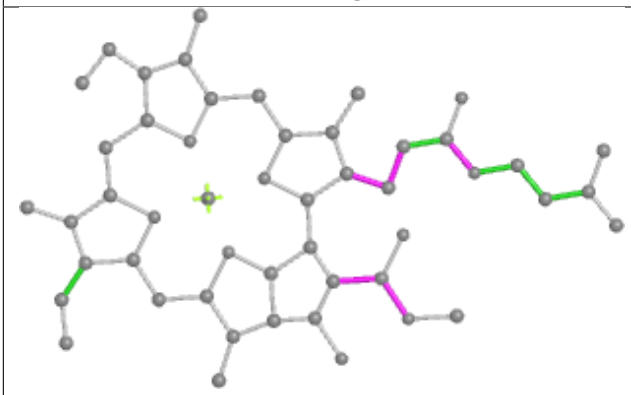
Ligand CLA b1 416



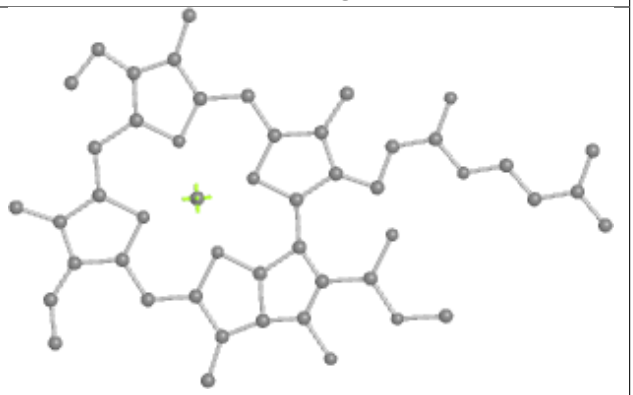
Bond lengths



Bond angles

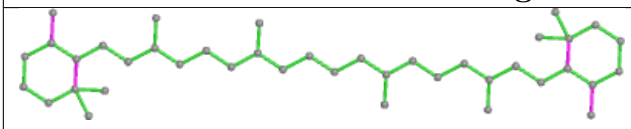


Torsions

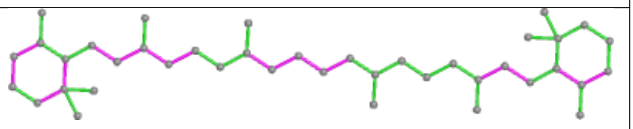


Rings

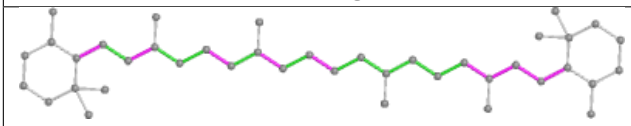
Ligand BCR cB 848



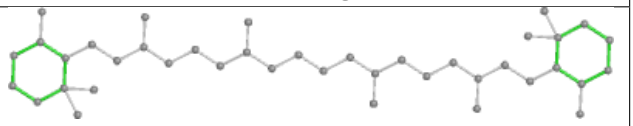
Bond lengths



Bond angles

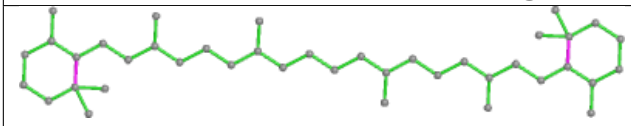


Torsions

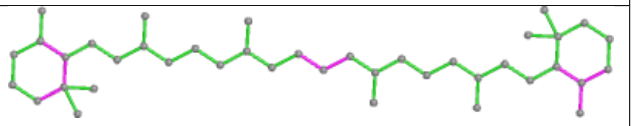


Rings

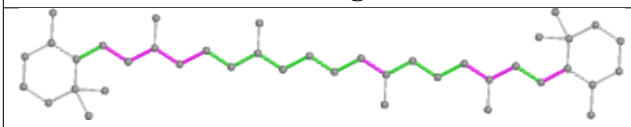
Ligand BCR cI 101



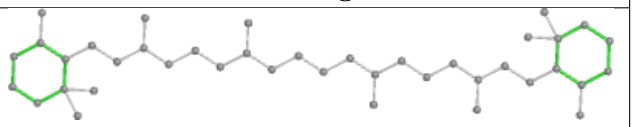
Bond lengths



Bond angles

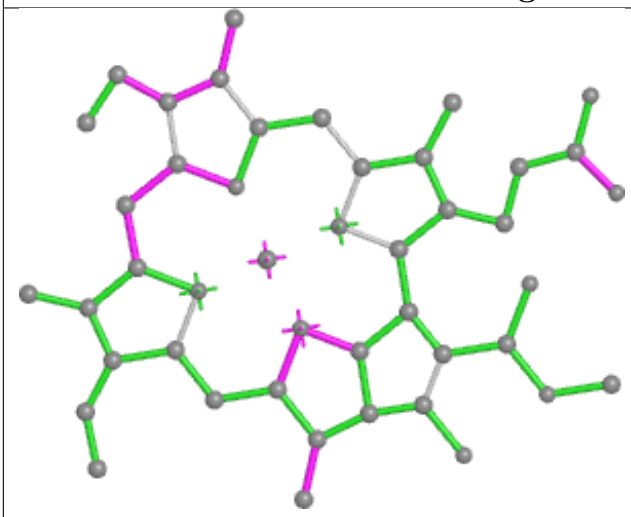


Torsions

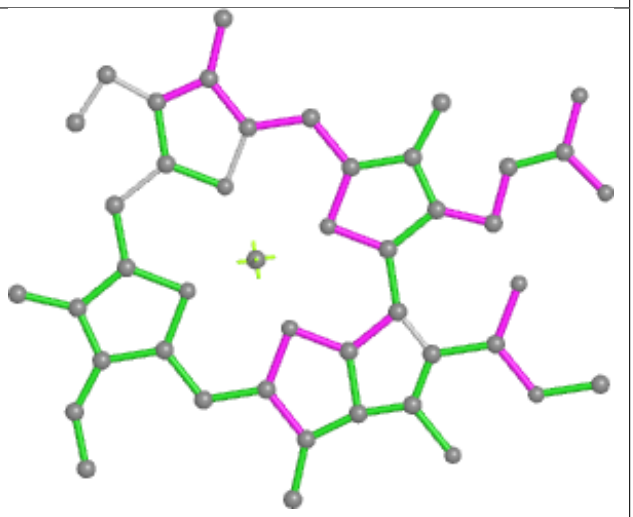


Rings

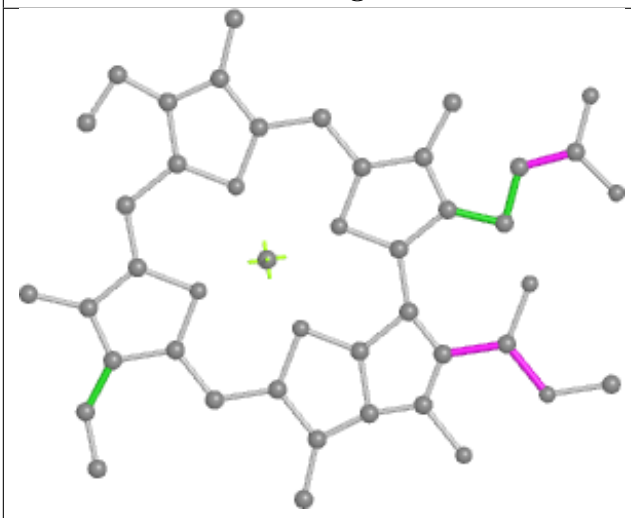
Ligand CLA b3 415



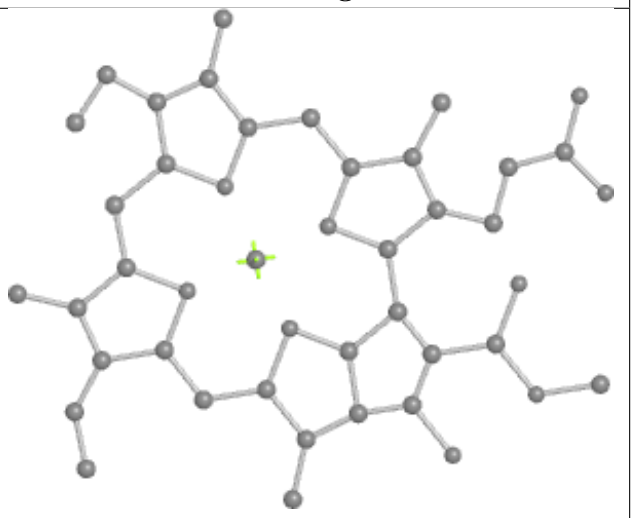
Bond lengths



Bond angles

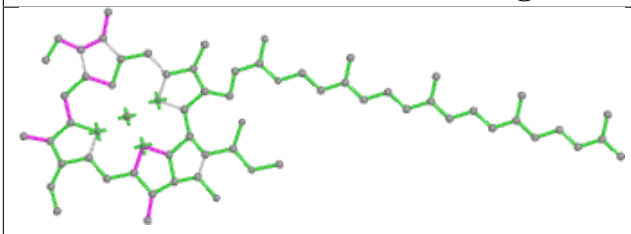


Torsions

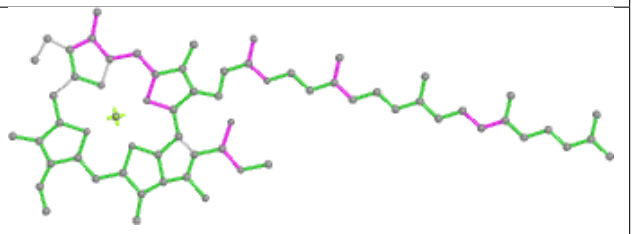


Rings

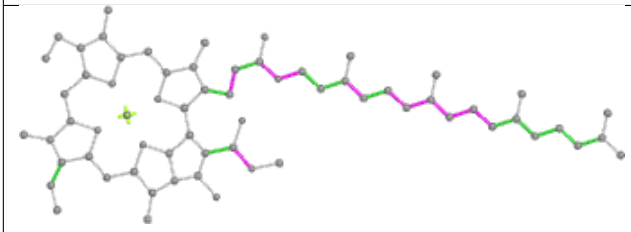
Ligand CLA cA 841



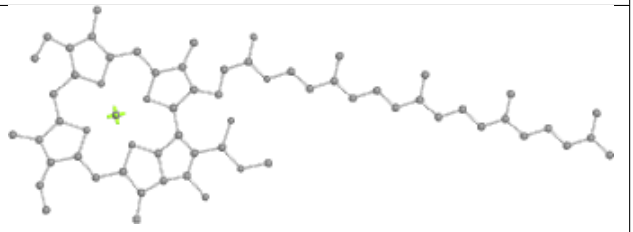
Bond lengths



Bond angles

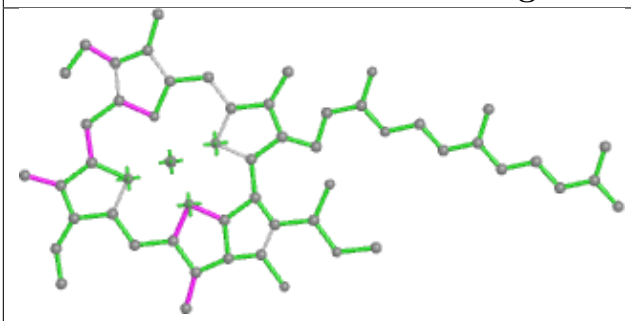


Torsions

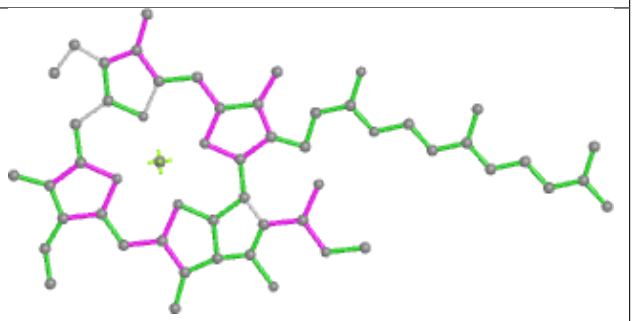


Rings

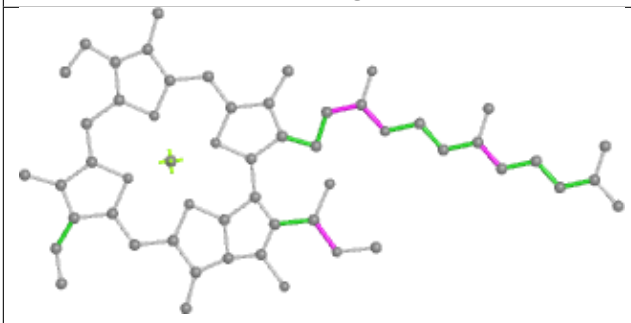
Ligand CLA b4 417



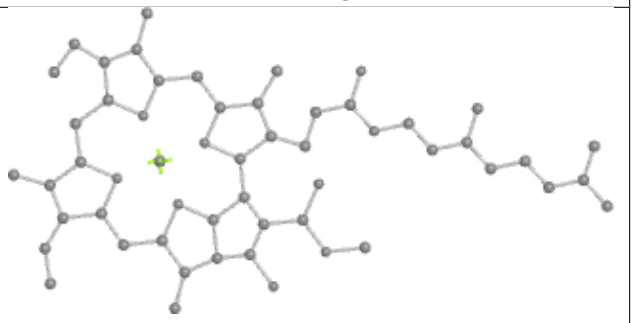
Bond lengths



Bond angles

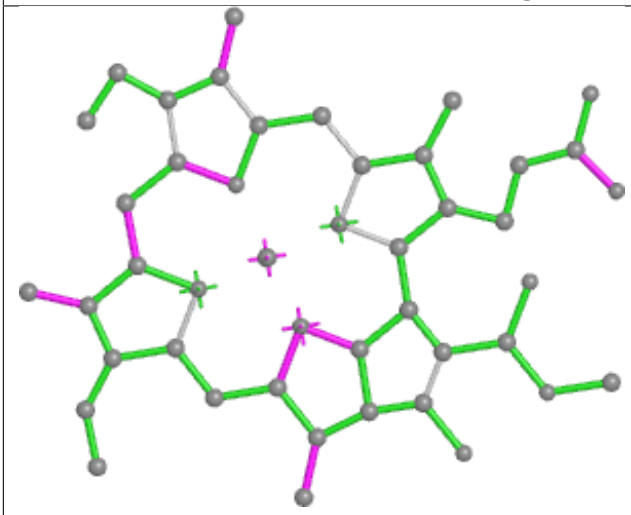


Torsions

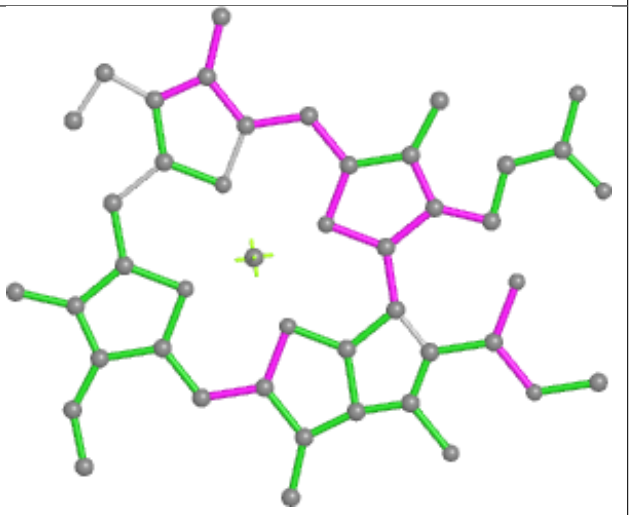


Rings

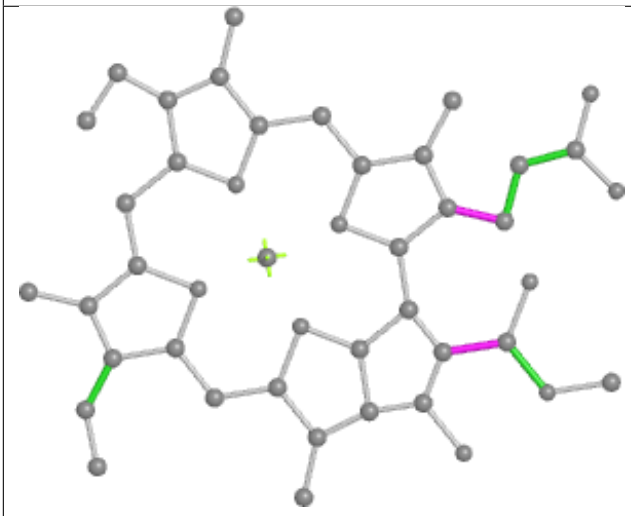
Ligand CLA b2 412



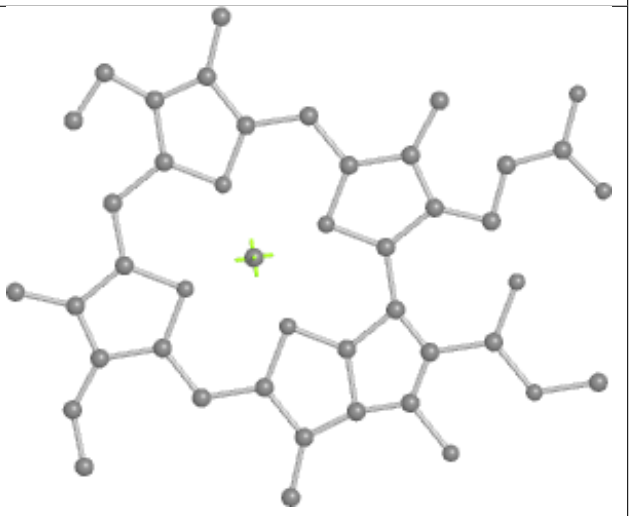
Bond lengths



Bond angles

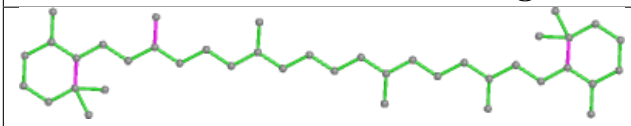


Torsions

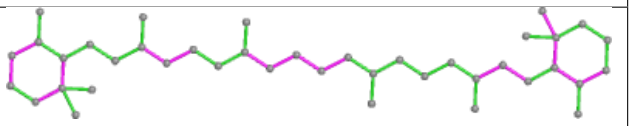


Rings

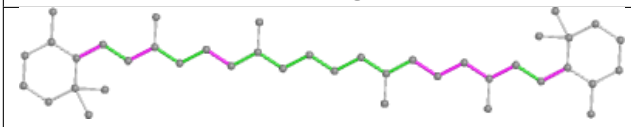
Ligand BCR b2 420



Bond lengths



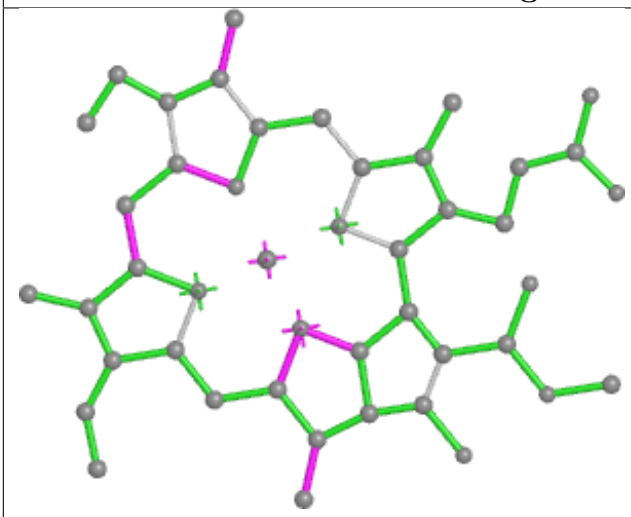
Bond angles



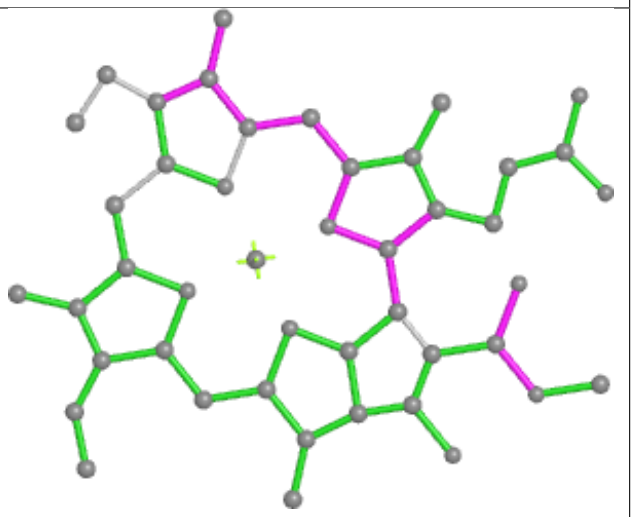
Torsions

Rings

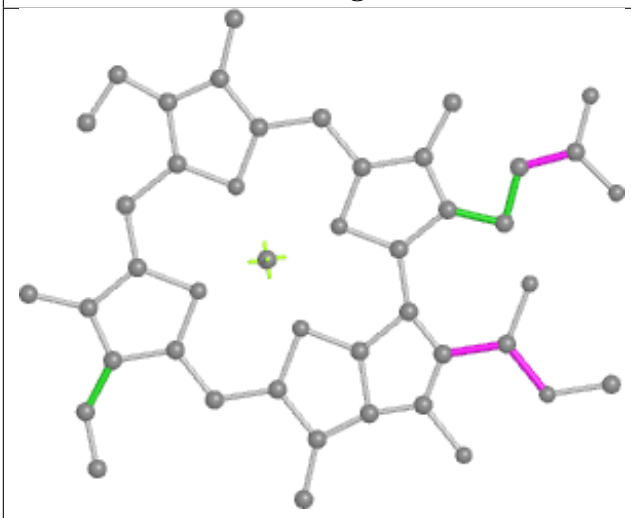
Ligand CLA c6 408



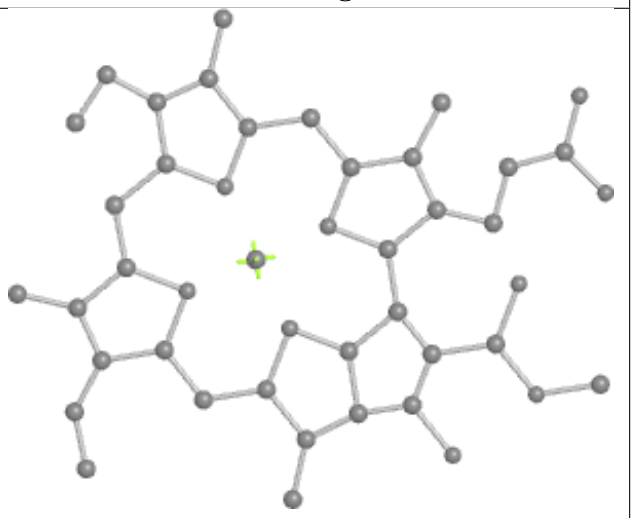
Bond lengths



Bond angles

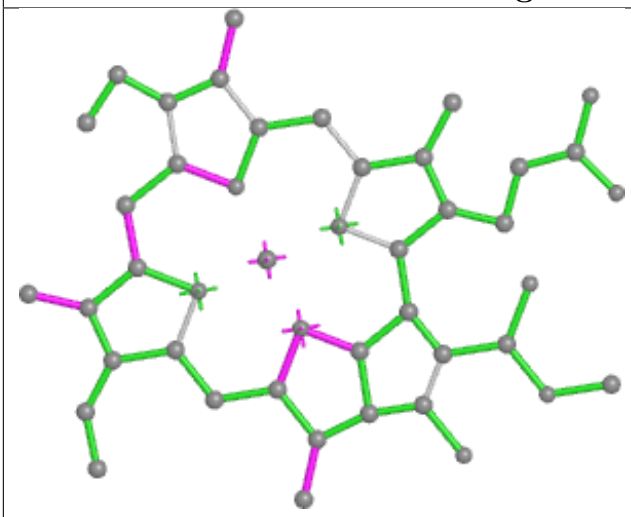


Torsions

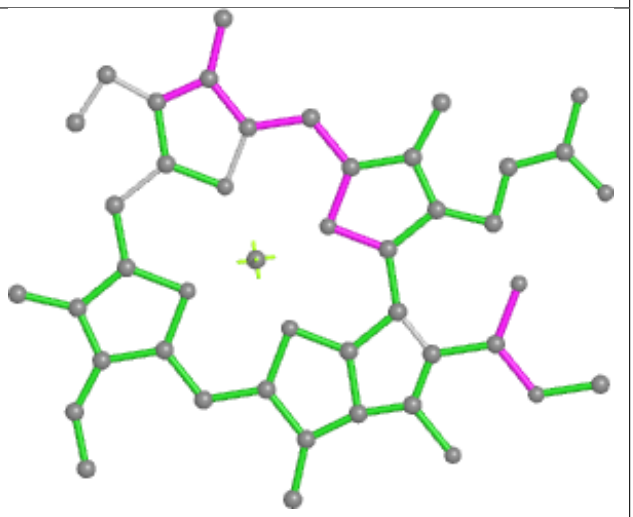


Rings

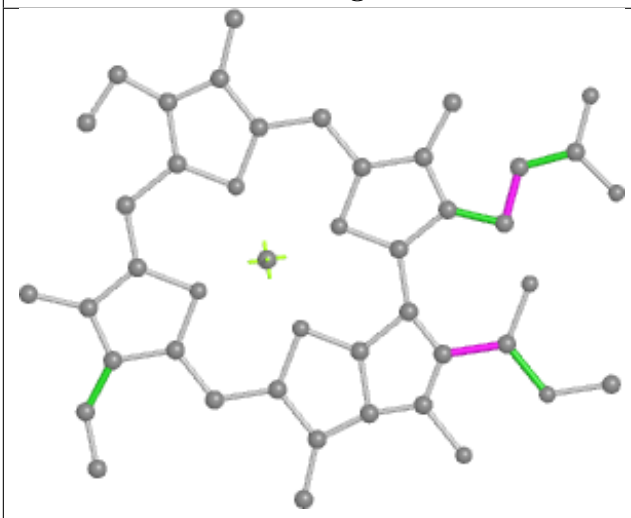
Ligand CLA cA 816



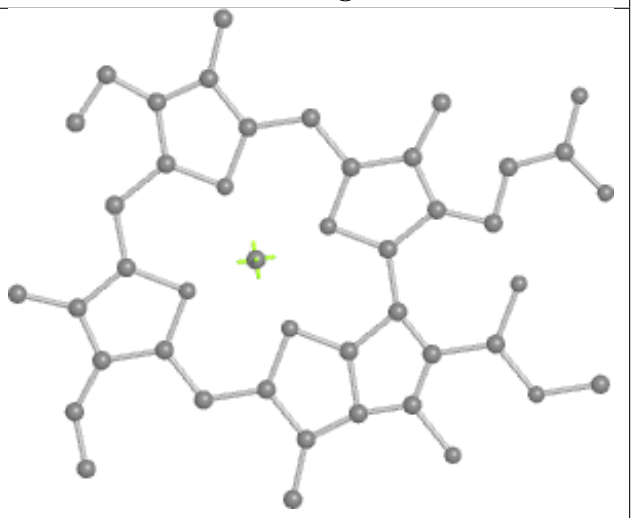
Bond lengths



Bond angles

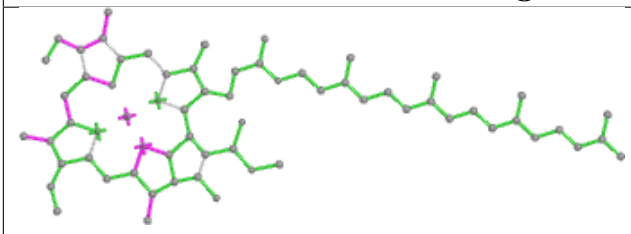


Torsions

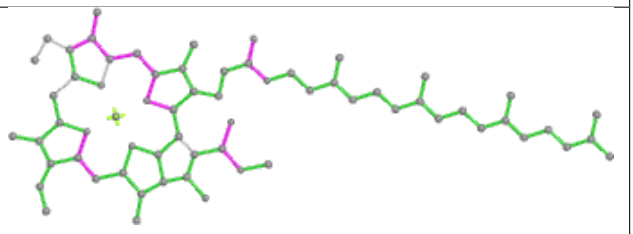


Rings

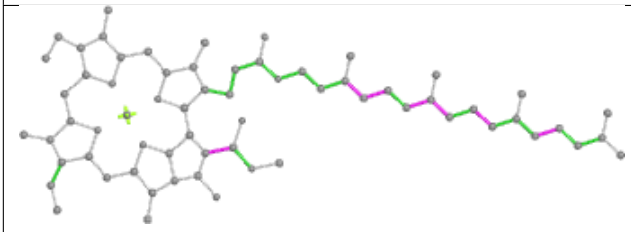
Ligand CLA cA 828



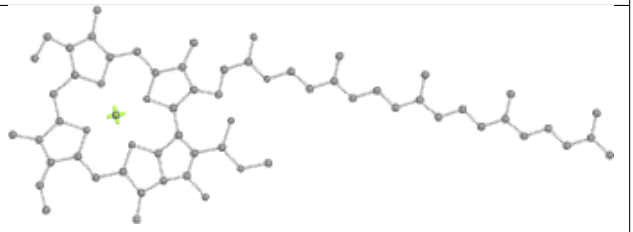
Bond lengths



Bond angles

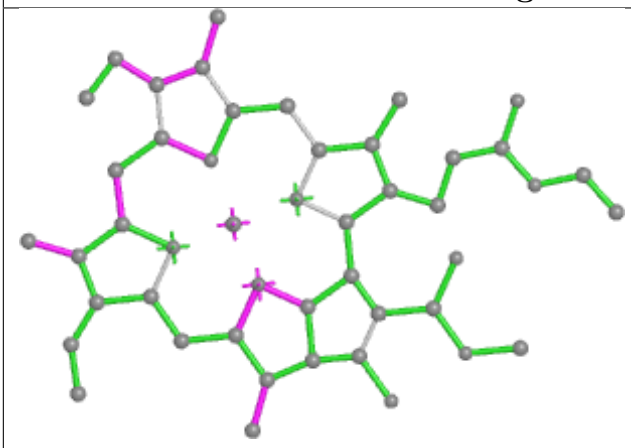


Torsions

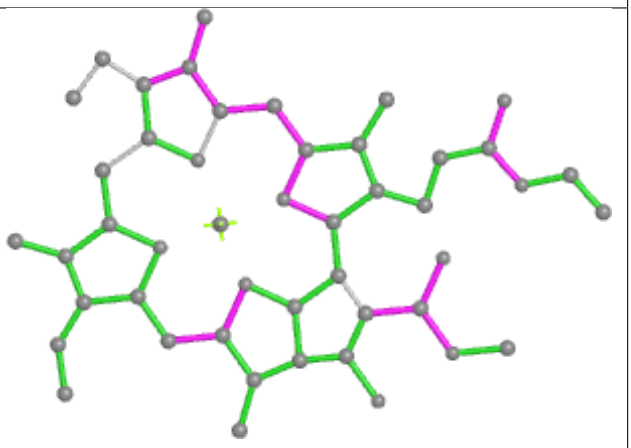


Rings

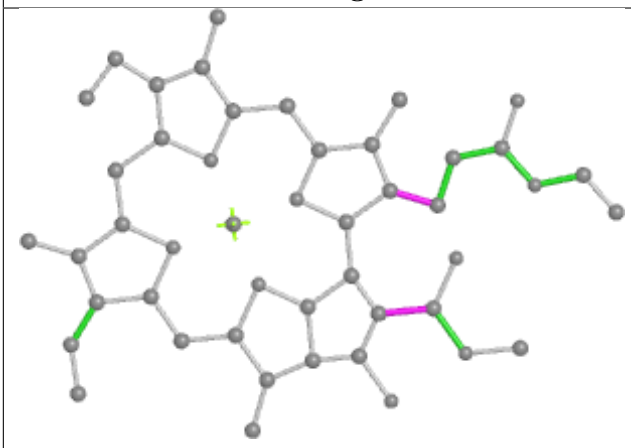
Ligand CLA cB 838



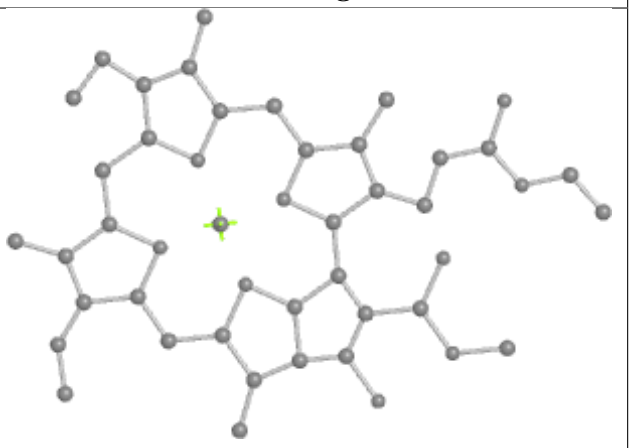
Bond lengths



Bond angles

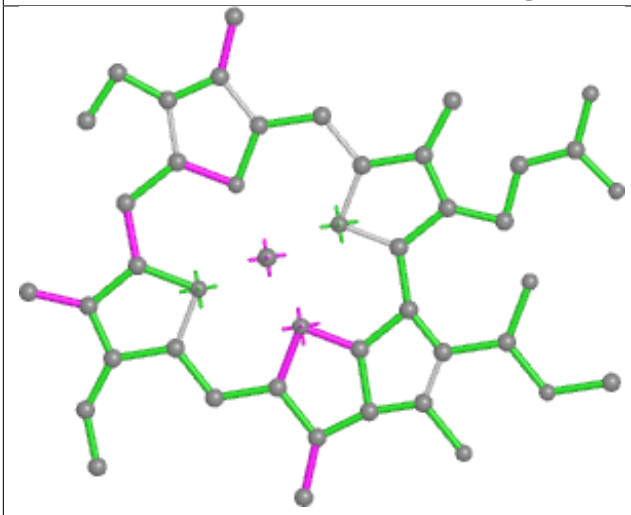


Torsions

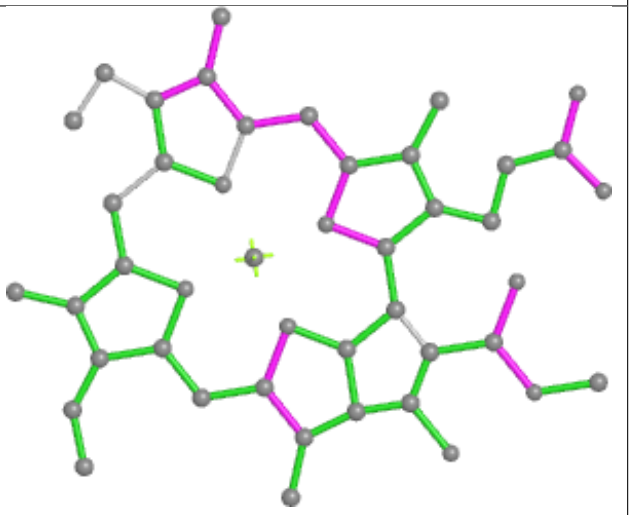


Rings

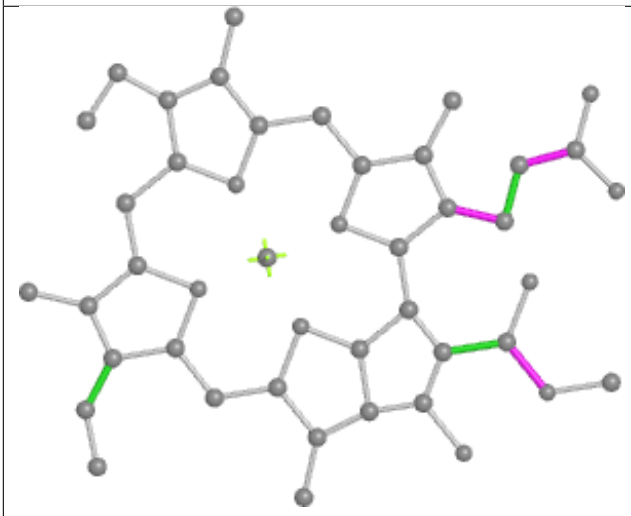
Ligand CLA c4 408



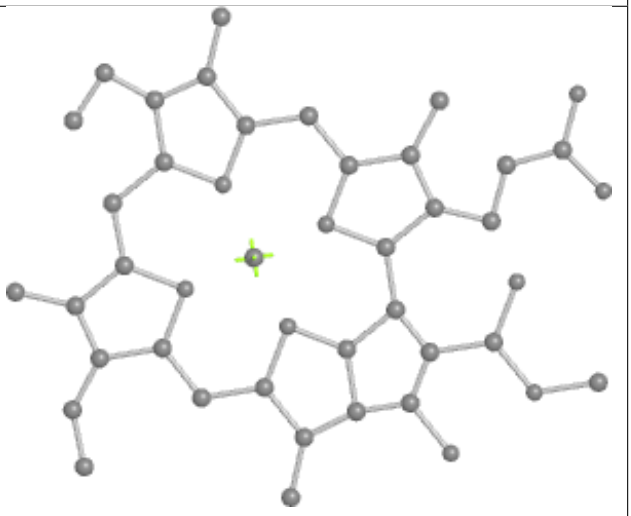
Bond lengths



Bond angles

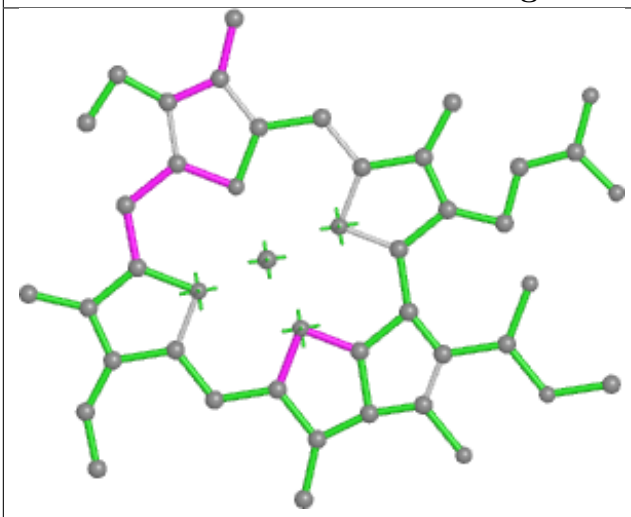


Torsions

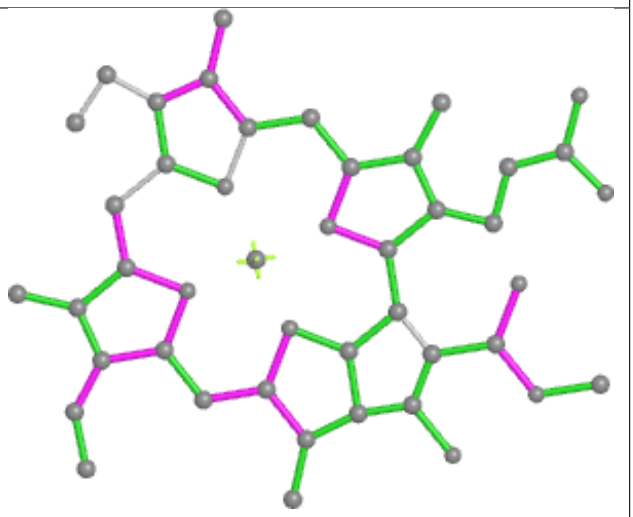


Rings

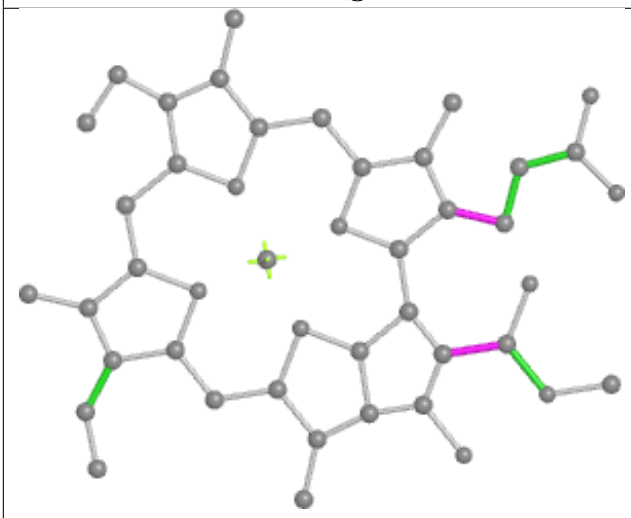
Ligand CLA c6 414



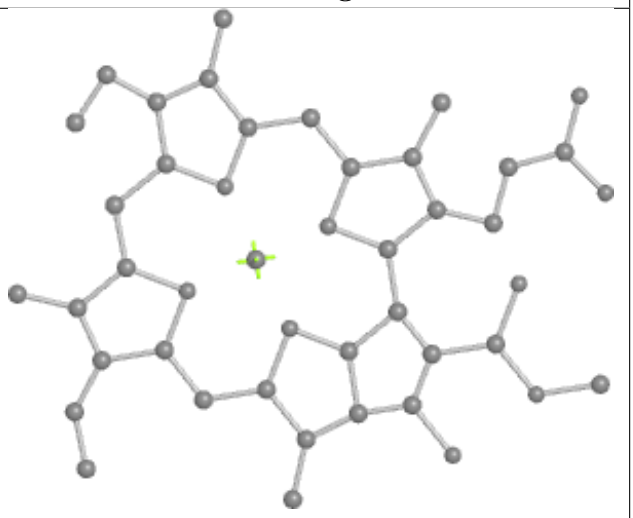
Bond lengths



Bond angles

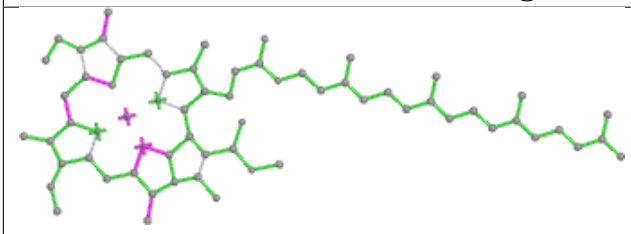


Torsions

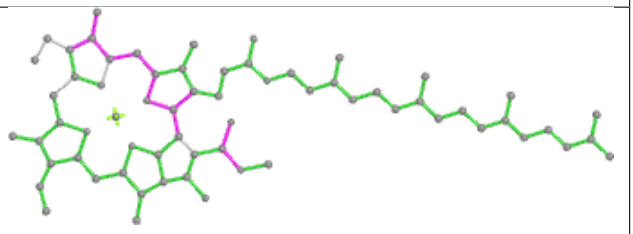


Rings

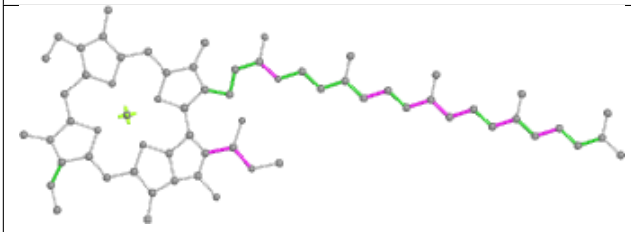
Ligand CLA b4 403



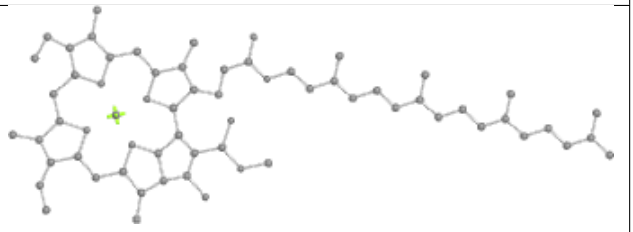
Bond lengths



Bond angles

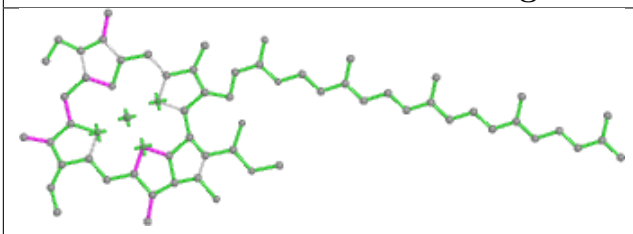


Torsions

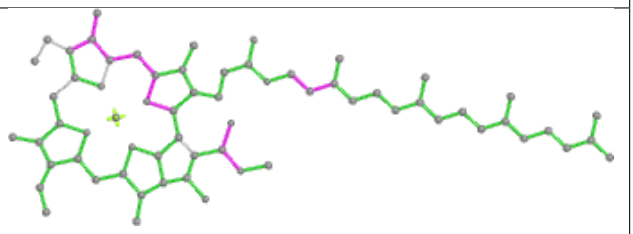


Rings

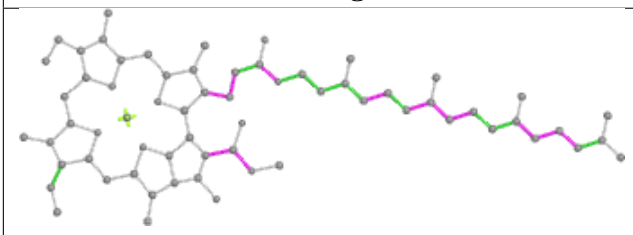
Ligand CLA a1 401



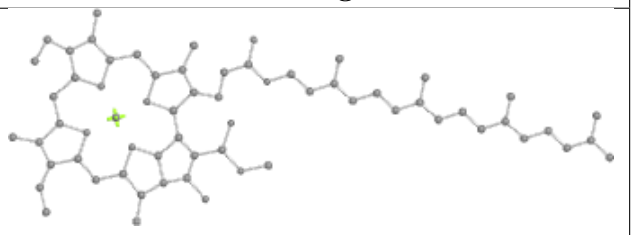
Bond lengths



Bond angles

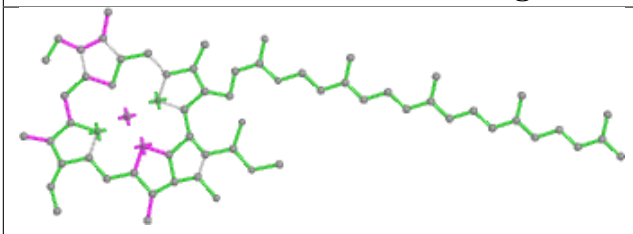


Torsions

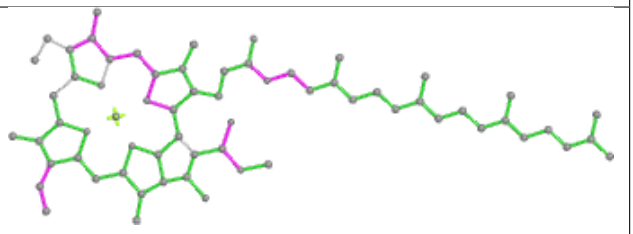


Rings

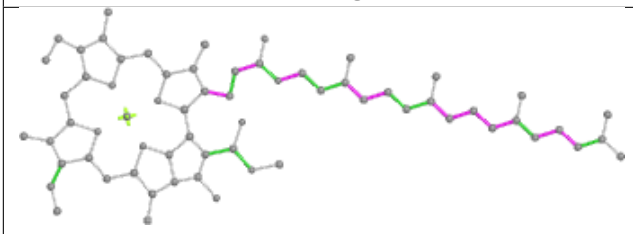
Ligand CLA bA 843



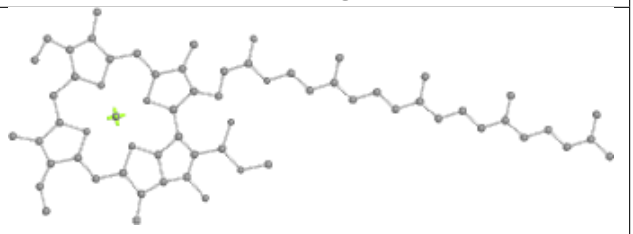
Bond lengths



Bond angles

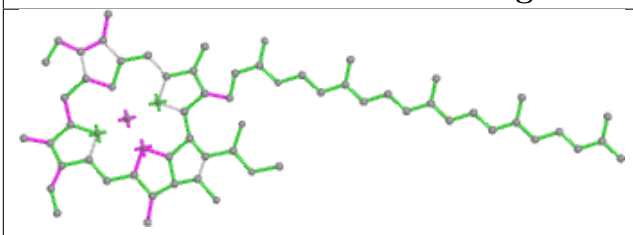


Torsions

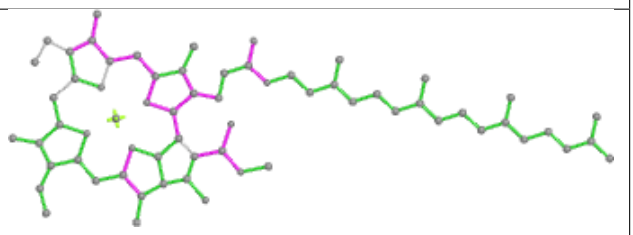


Rings

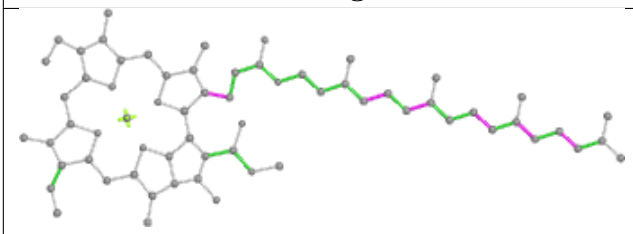
Ligand CLA cA 807



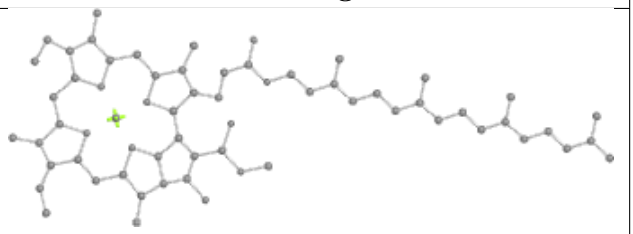
Bond lengths



Bond angles

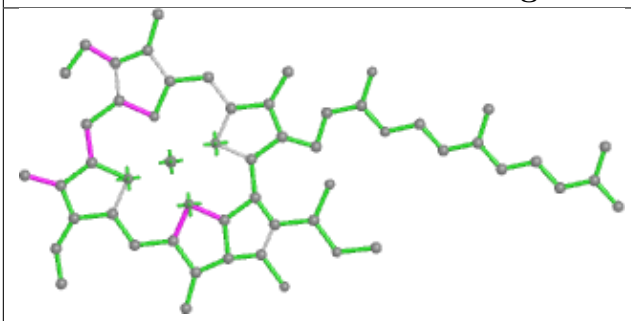


Torsions

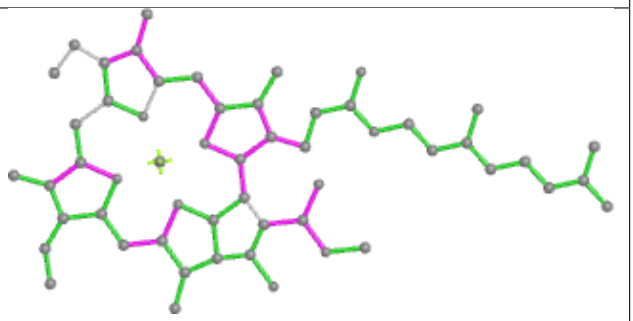


Rings

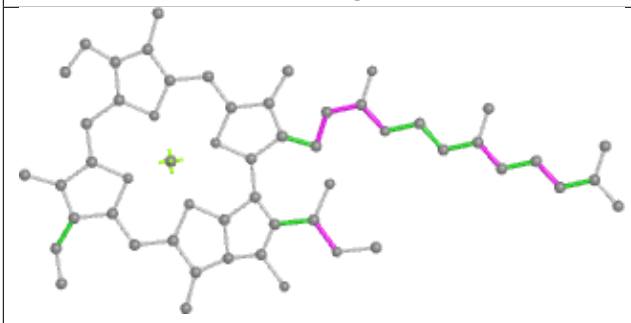
Ligand CLA c2 418



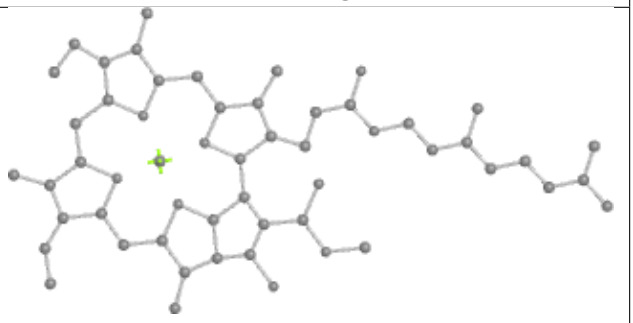
Bond lengths



Bond angles

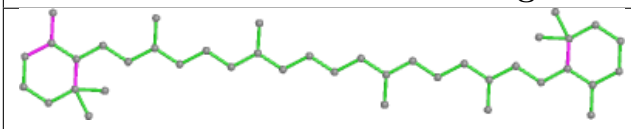


Torsions

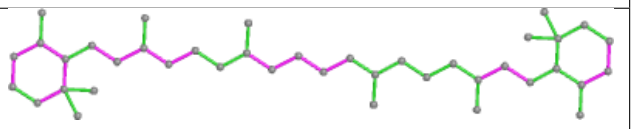


Rings

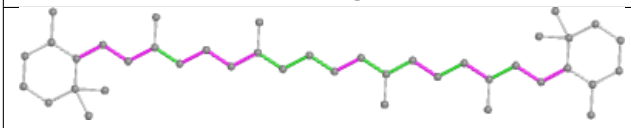
Ligand BCR a6 402



Bond lengths



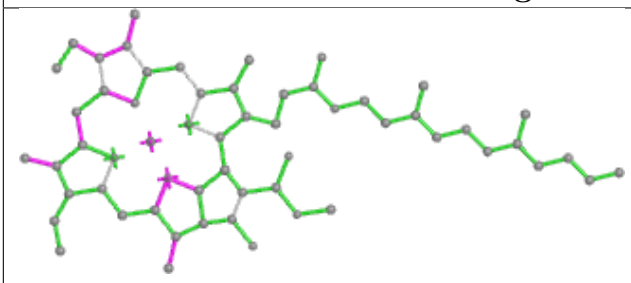
Bond angles



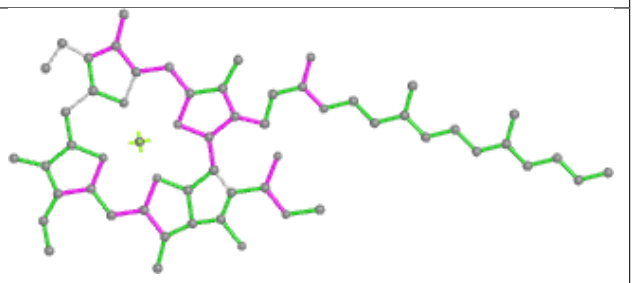
Torsions

Rings

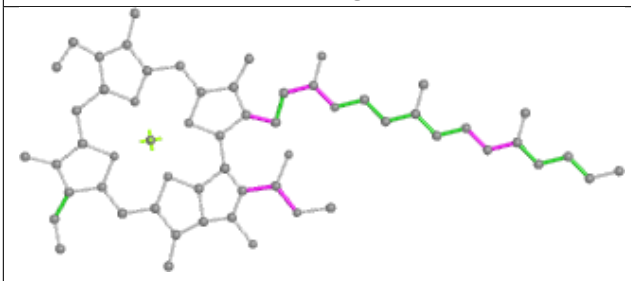
Ligand CLA bB 834



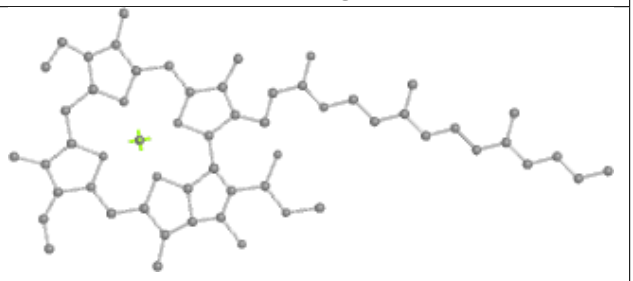
Bond lengths



Bond angles

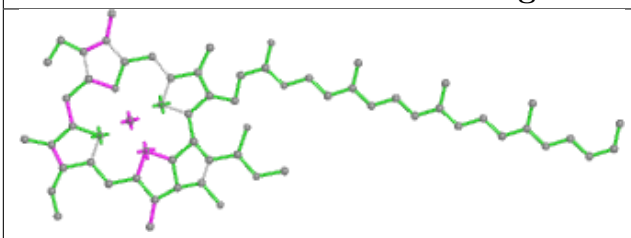


Torsions

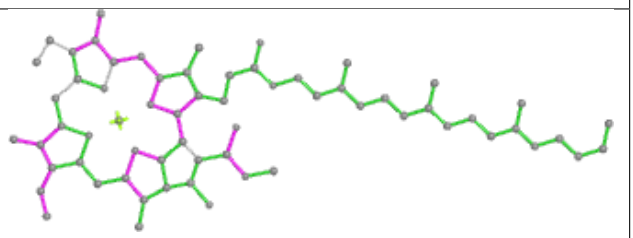


Rings

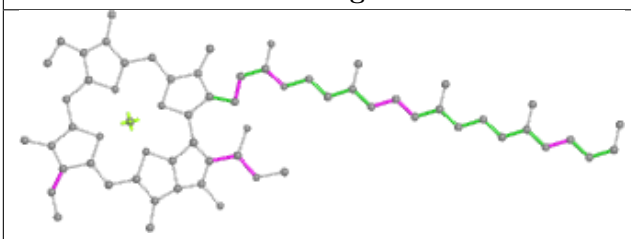
Ligand CLA b4 410



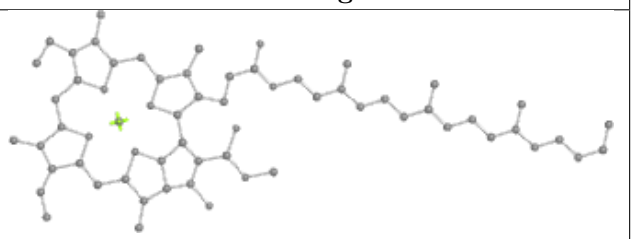
Bond lengths



Bond angles

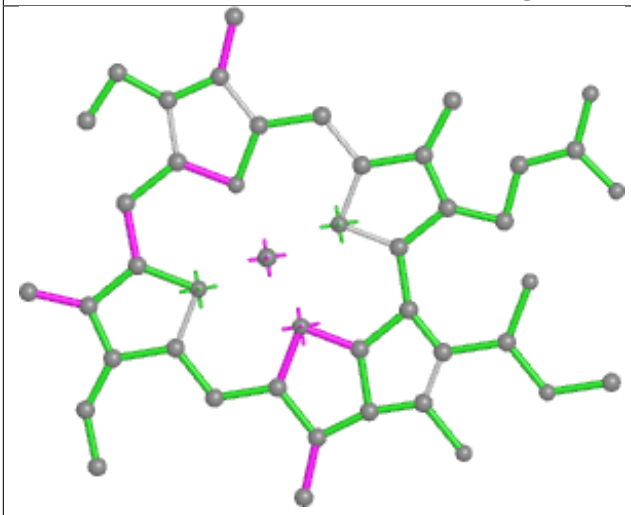


Torsions

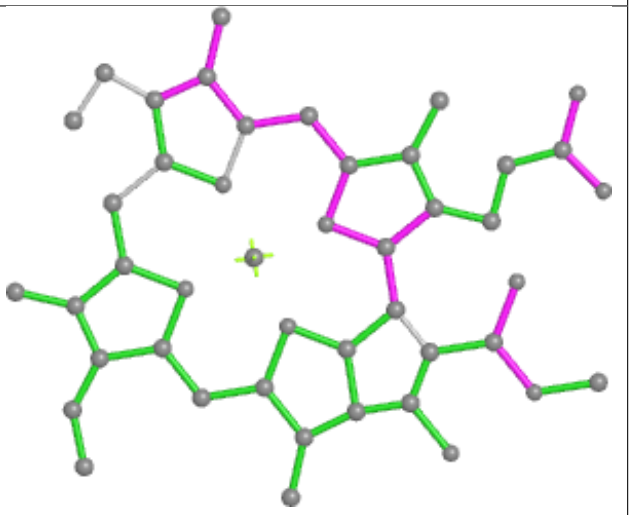


Rings

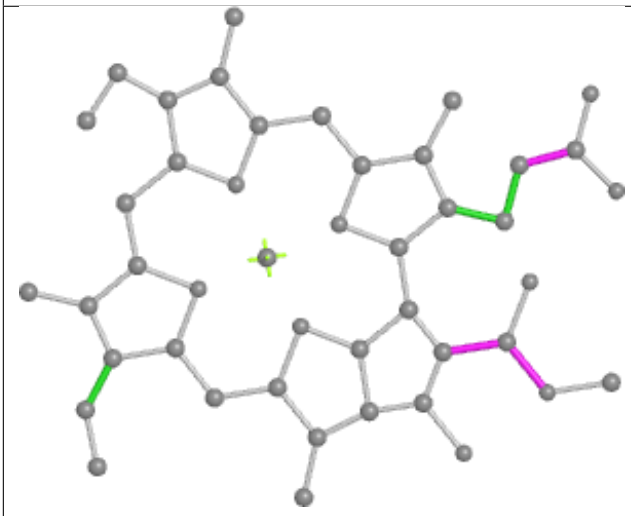
Ligand CLA b2 408



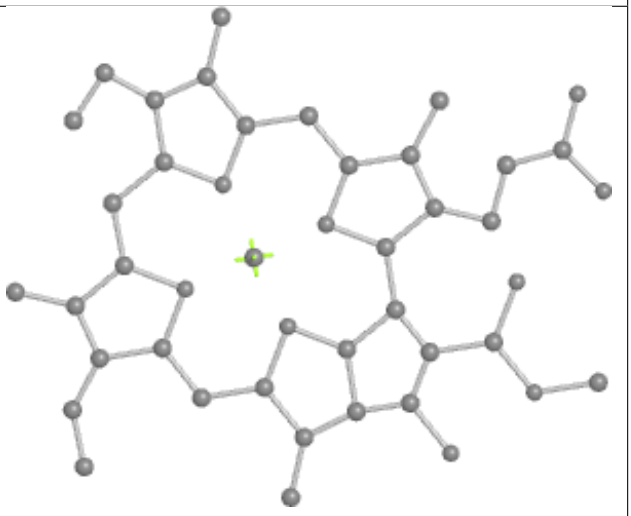
Bond lengths



Bond angles

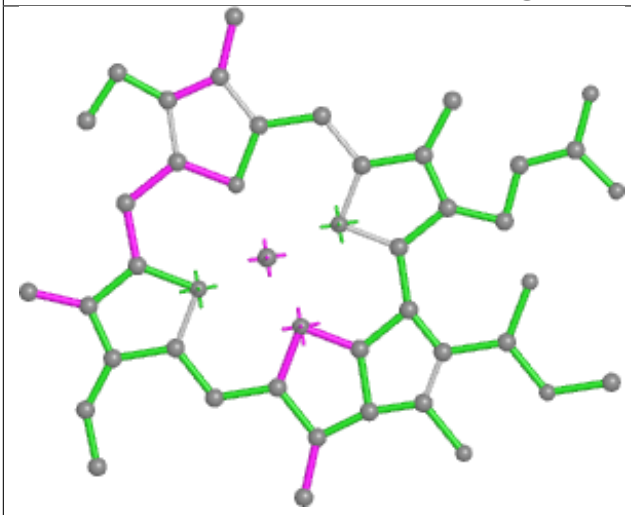


Torsions

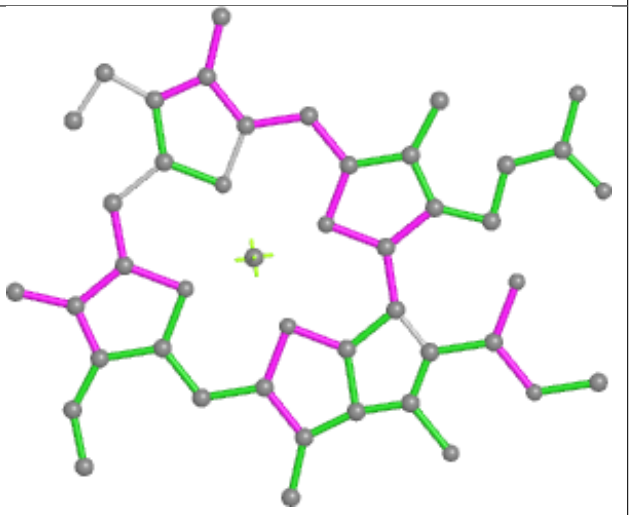


Rings

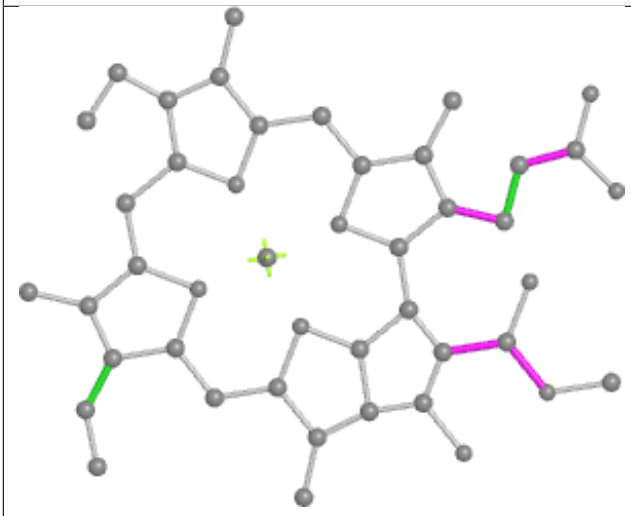
Ligand CLA b5 412



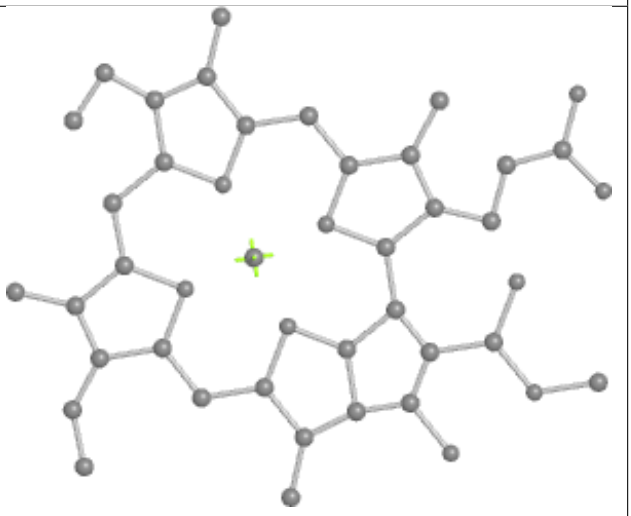
Bond lengths



Bond angles

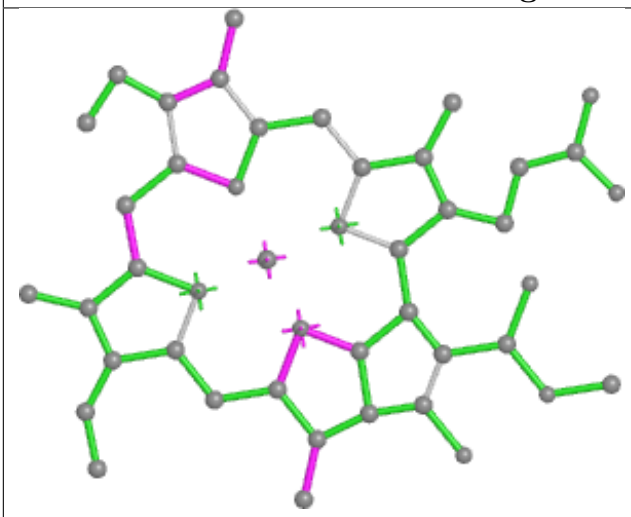


Torsions

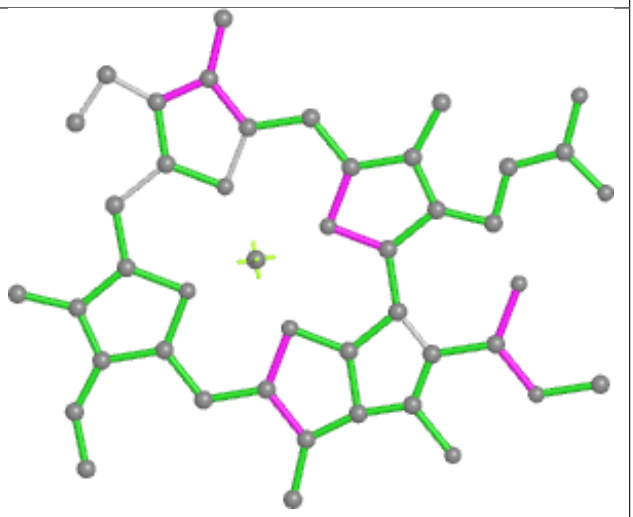


Rings

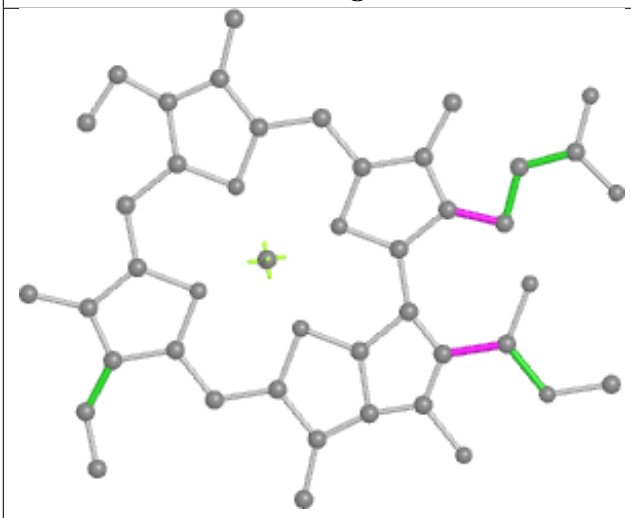
Ligand CLA a1 412



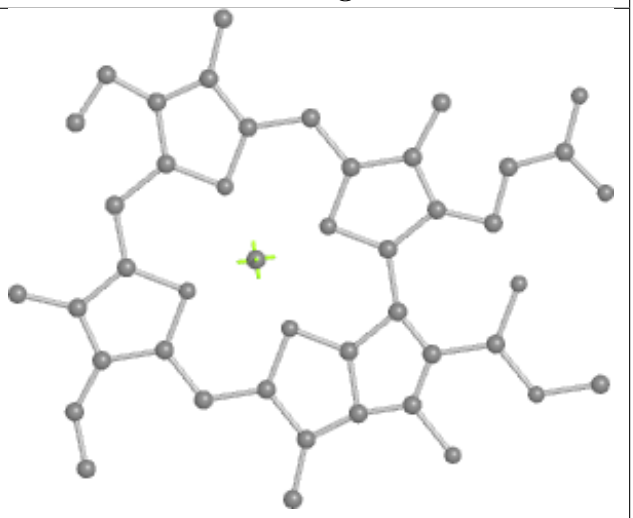
Bond lengths



Bond angles

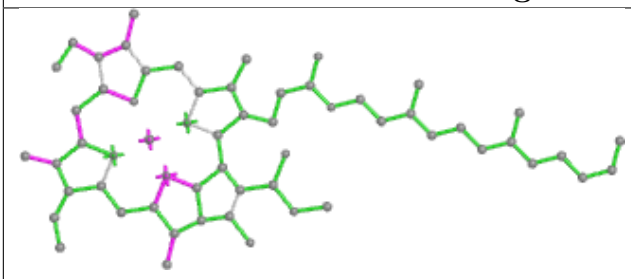


Torsions

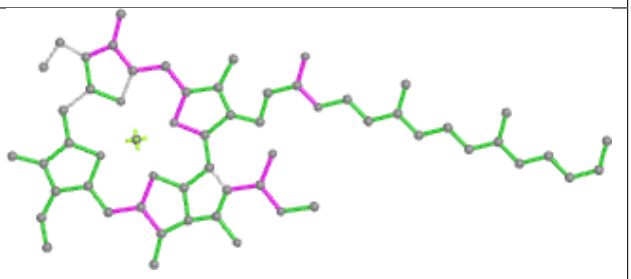


Rings

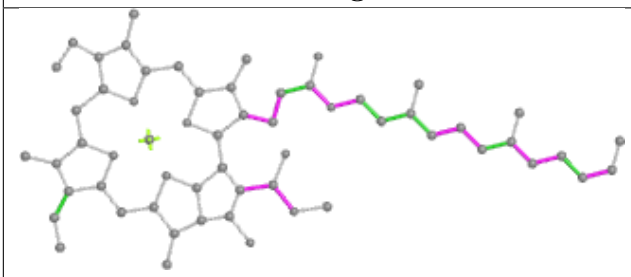
Ligand CLA bA 825



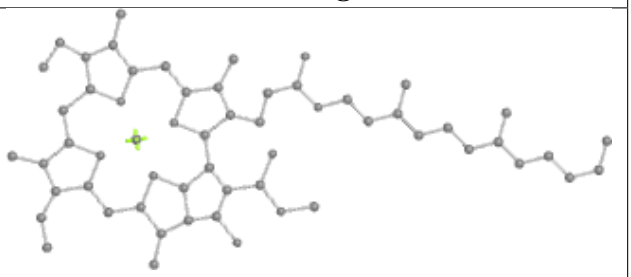
Bond lengths



Bond angles

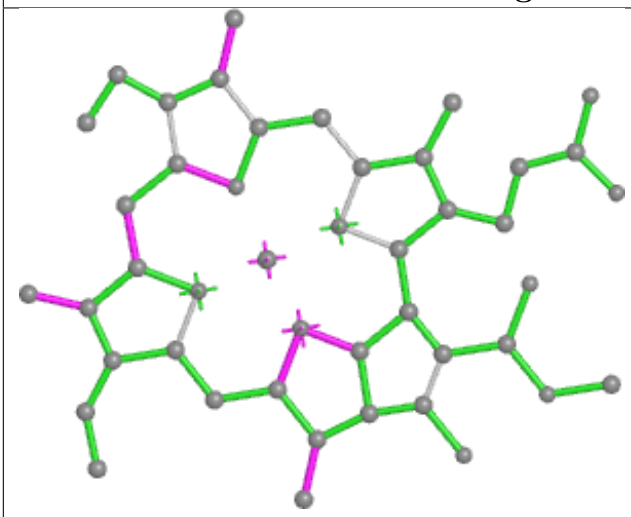


Torsions

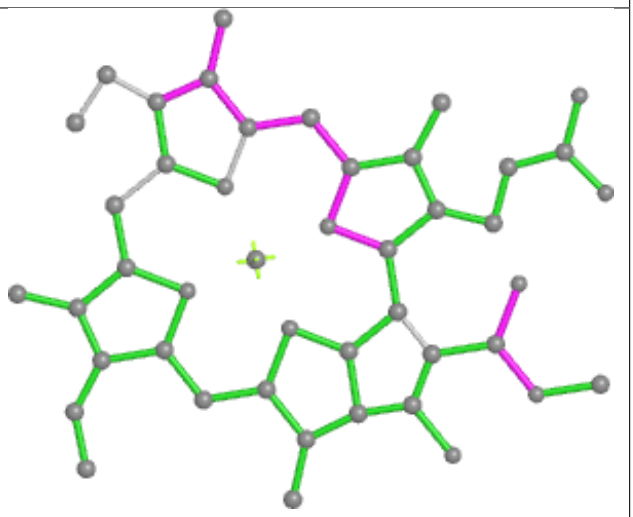


Rings

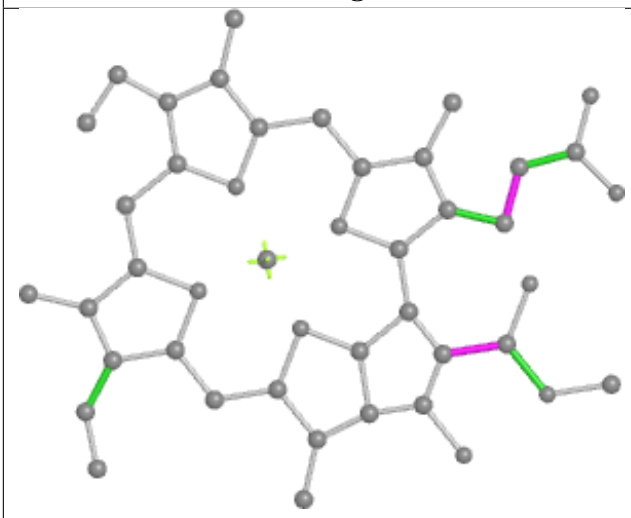
Ligand CLA aA 816



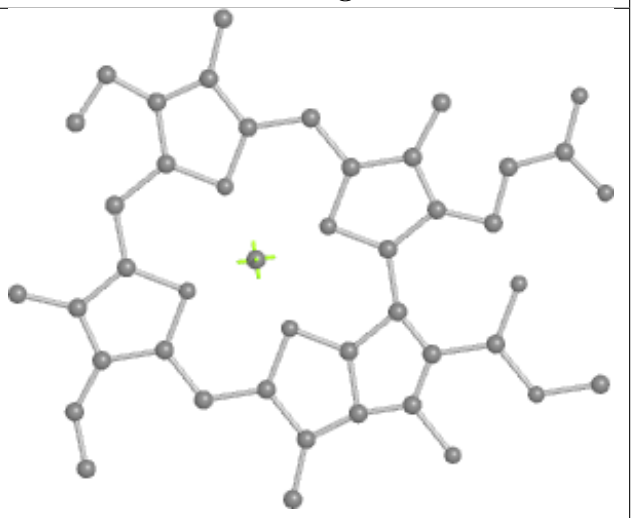
Bond lengths



Bond angles

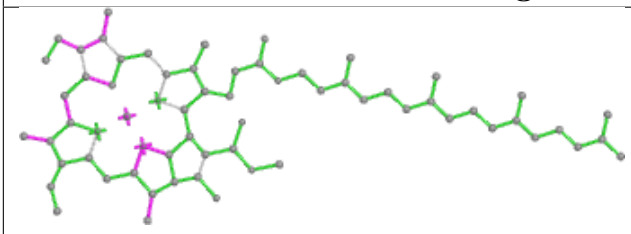


Torsions

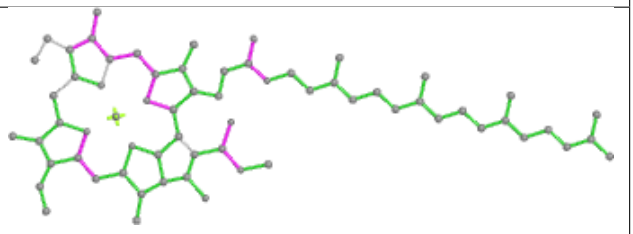


Rings

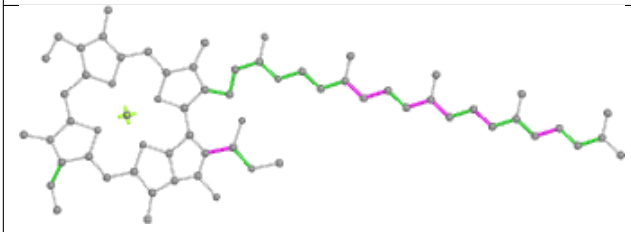
Ligand CLA aA 828



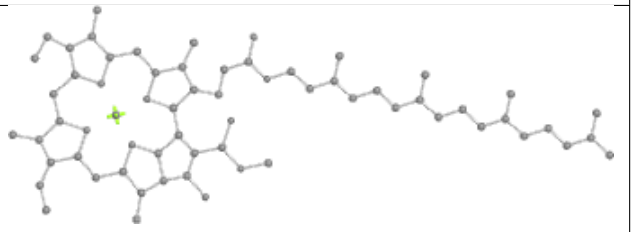
Bond lengths



Bond angles

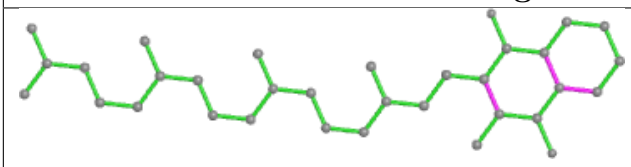


Torsions

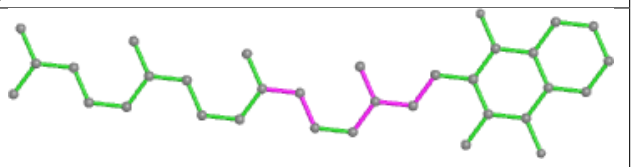


Rings

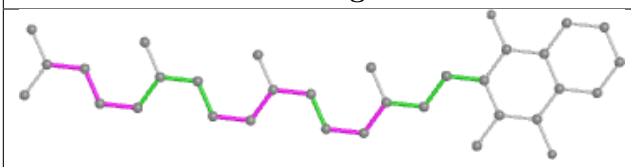
Ligand PQN cB 843



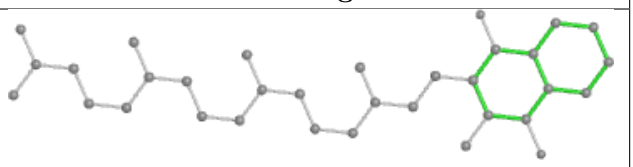
Bond lengths



Bond angles

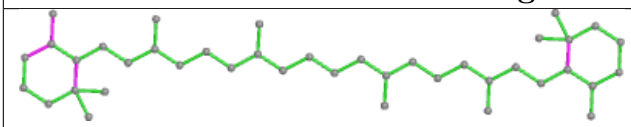


Torsions

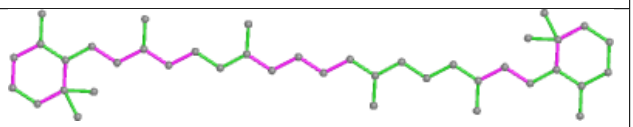


Rings

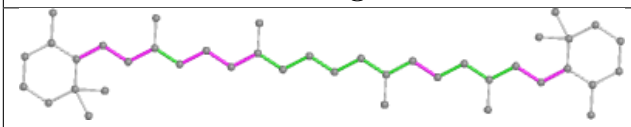
Ligand BCR a3 401



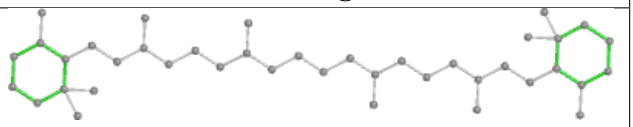
Bond lengths



Bond angles

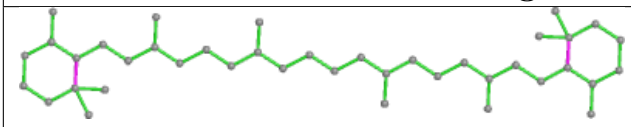


Torsions

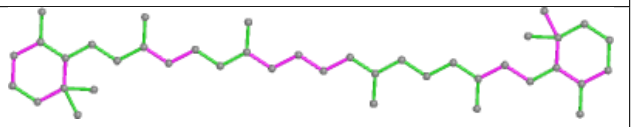


Rings

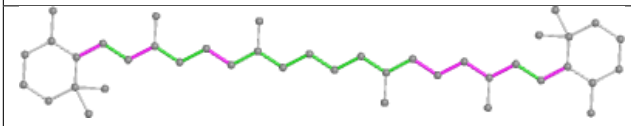
Ligand BCR c4 419



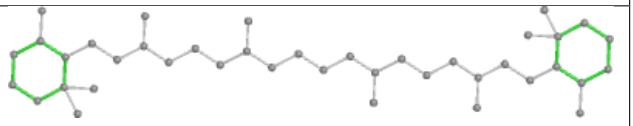
Bond lengths



Bond angles

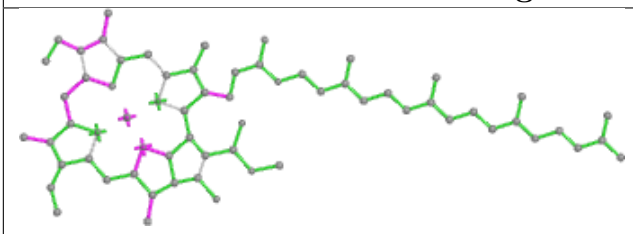


Torsions

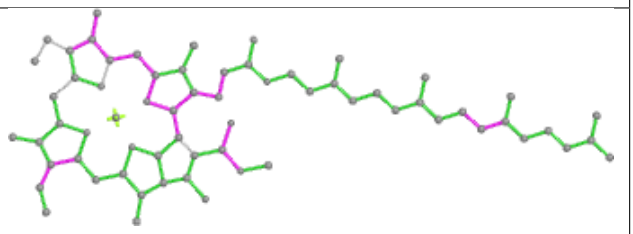


Rings

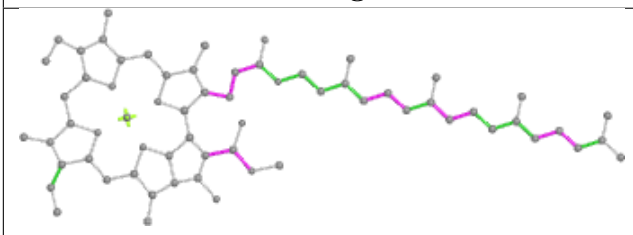
Ligand CLA aB 810



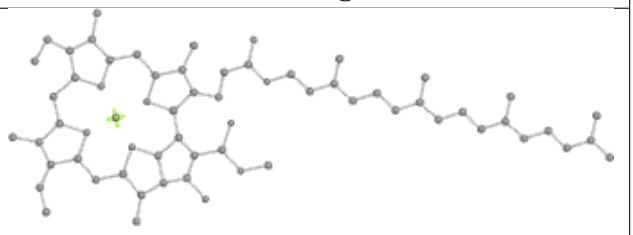
Bond lengths



Bond angles

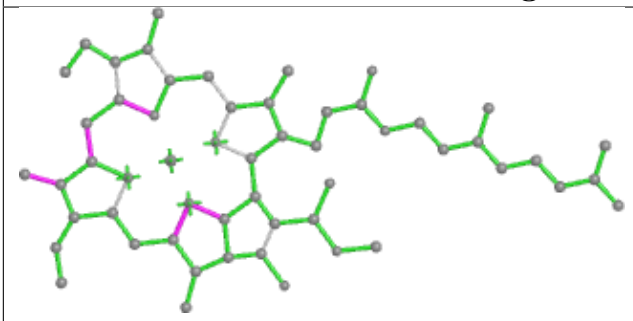


Torsions

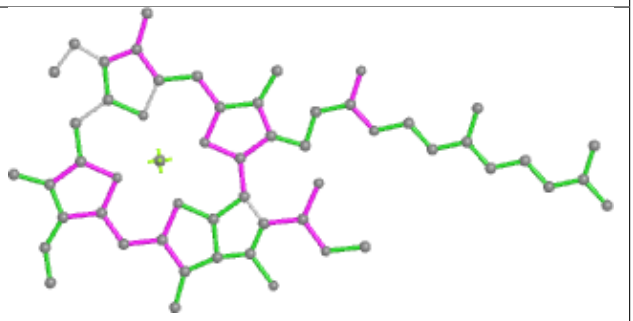


Rings

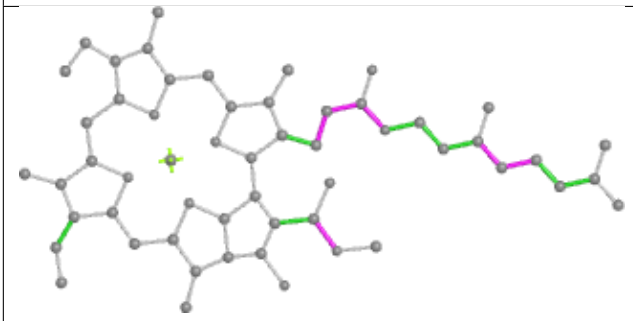
Ligand CLA c3 417



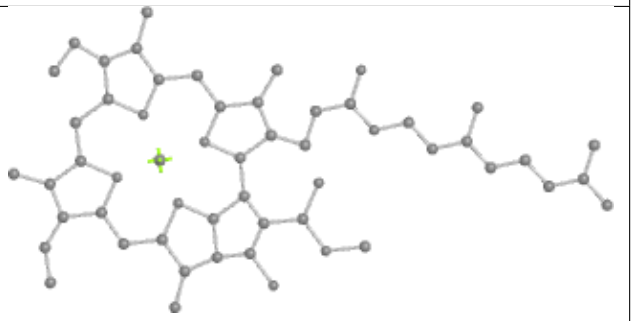
Bond lengths



Bond angles

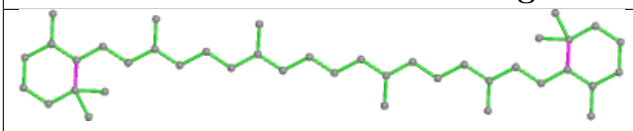


Torsions

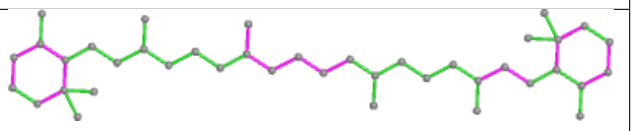


Rings

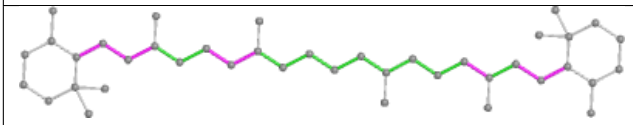
Ligand BCR a3 420



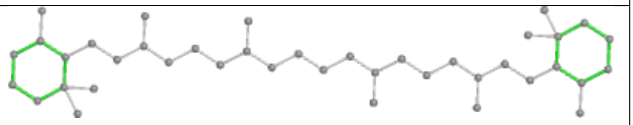
Bond lengths



Bond angles

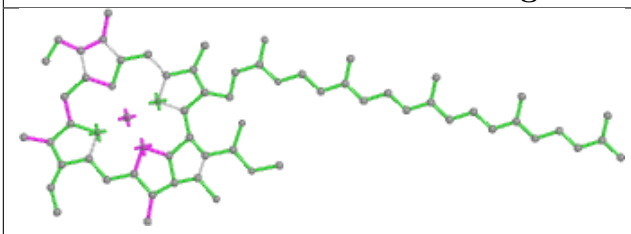


Torsions

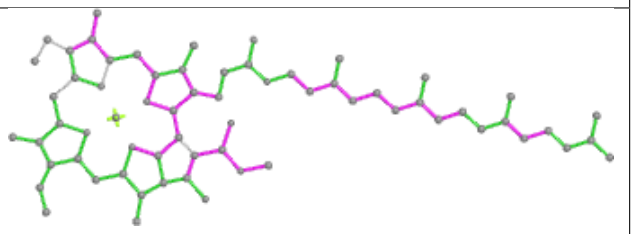


Rings

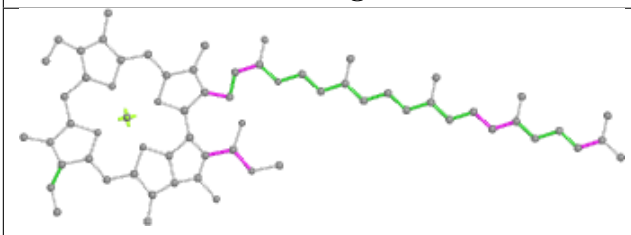
Ligand CLA c2 422



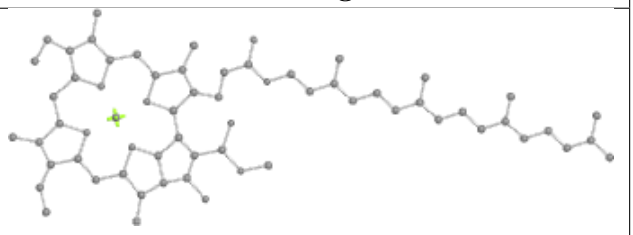
Bond lengths



Bond angles

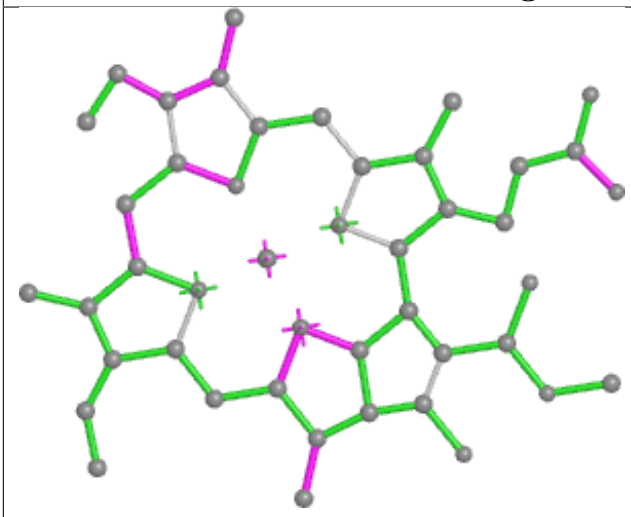


Torsions

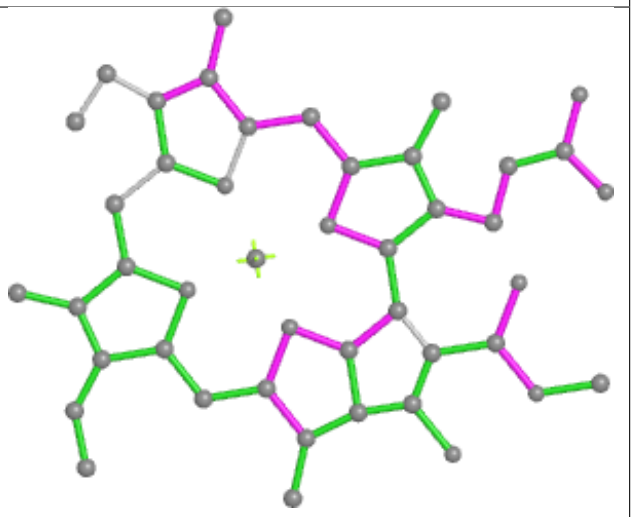


Rings

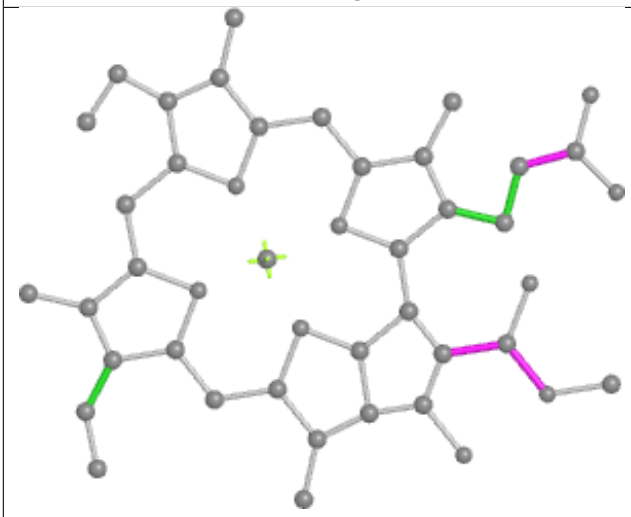
Ligand CLA a2 416



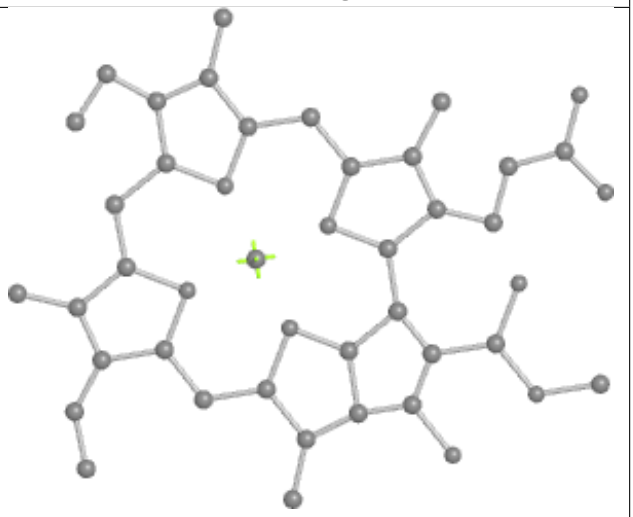
Bond lengths



Bond angles

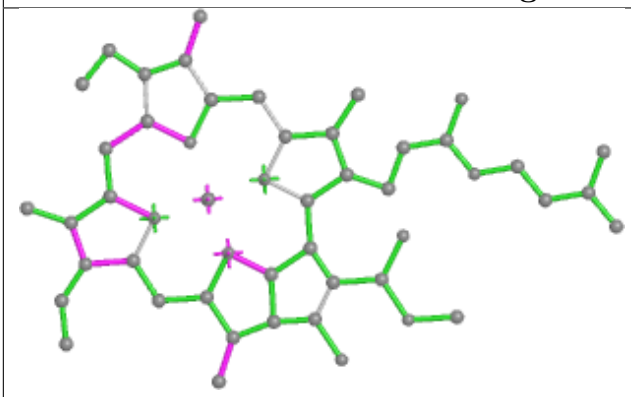


Torsions

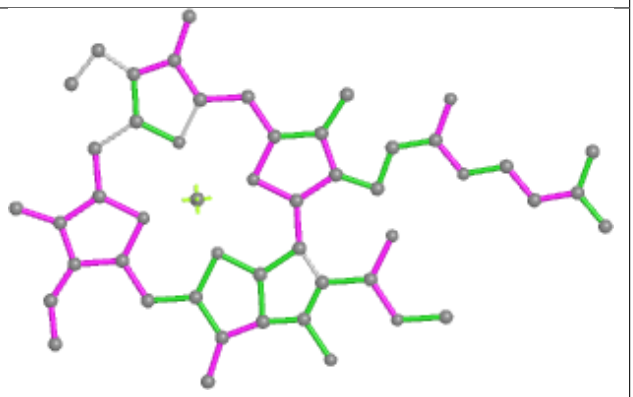


Rings

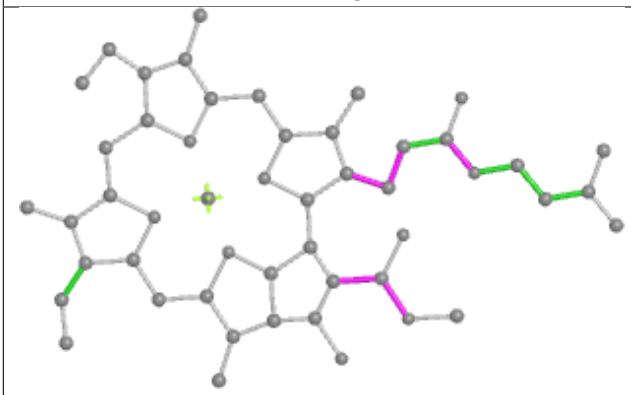
Ligand CLA a2 417



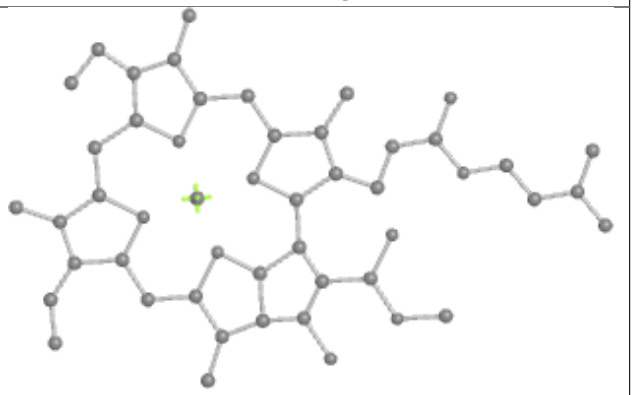
Bond lengths



Bond angles

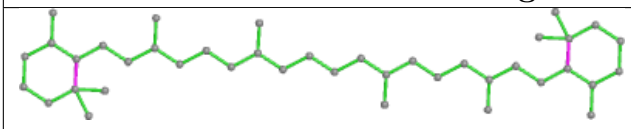


Torsions

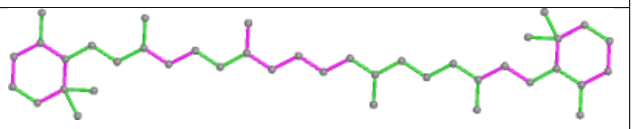


Rings

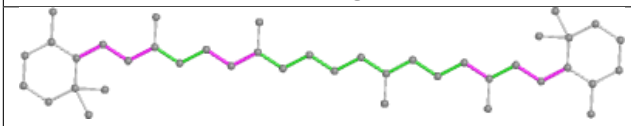
Ligand BCR c5 419



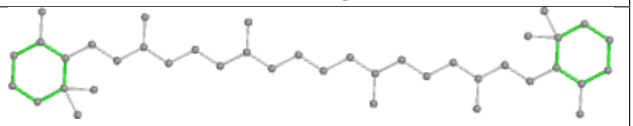
Bond lengths



Bond angles

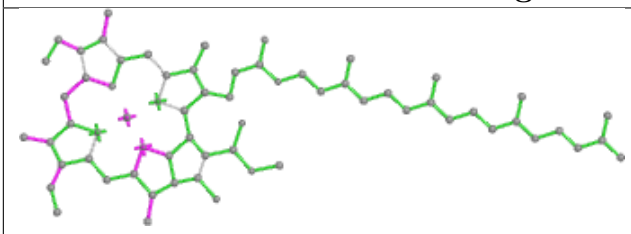


Torsions

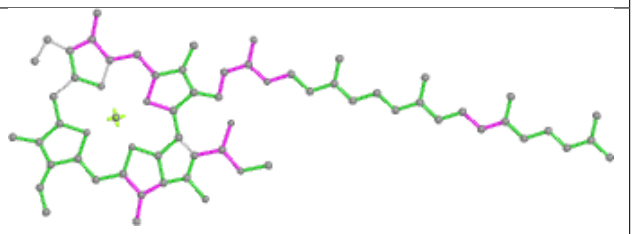


Rings

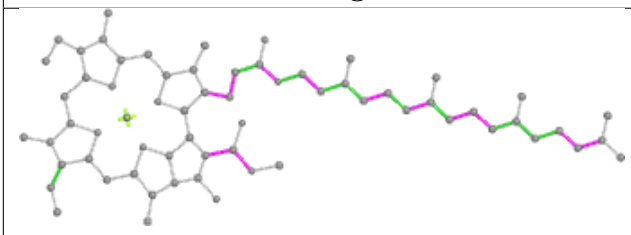
Ligand CLA aA 803



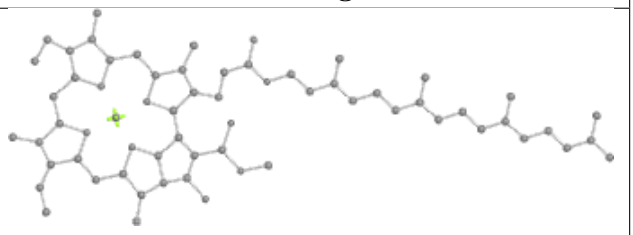
Bond lengths



Bond angles

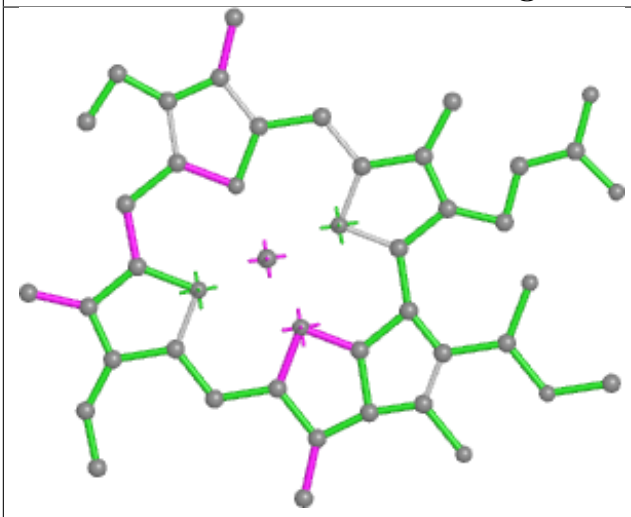


Torsions

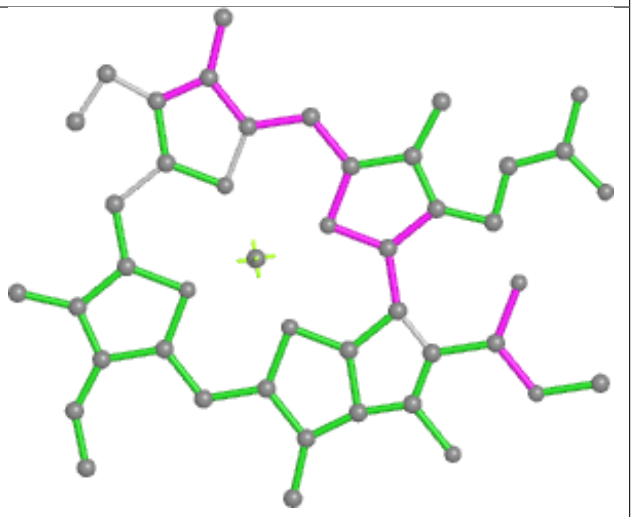


Rings

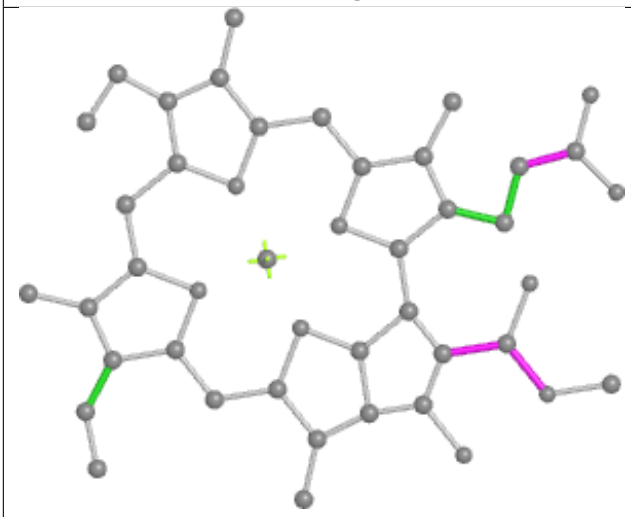
Ligand CLA b4 407



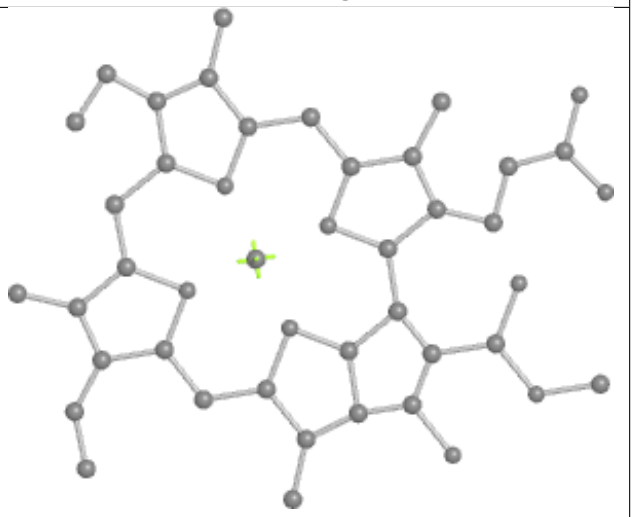
Bond lengths



Bond angles

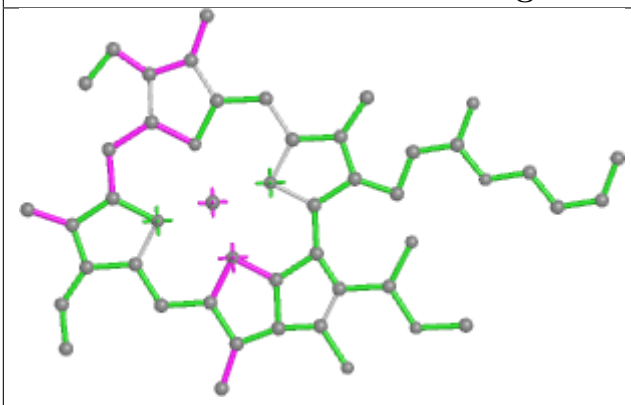


Torsions

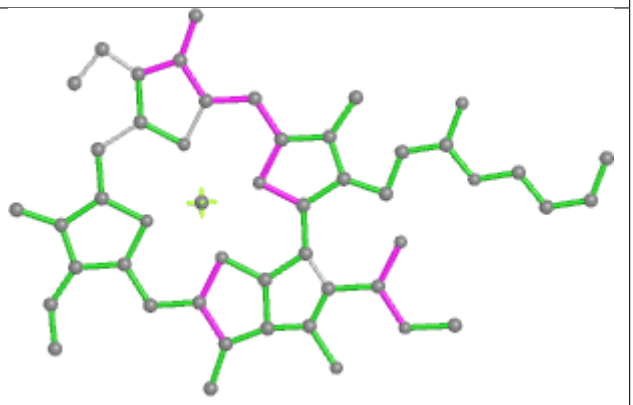


Rings

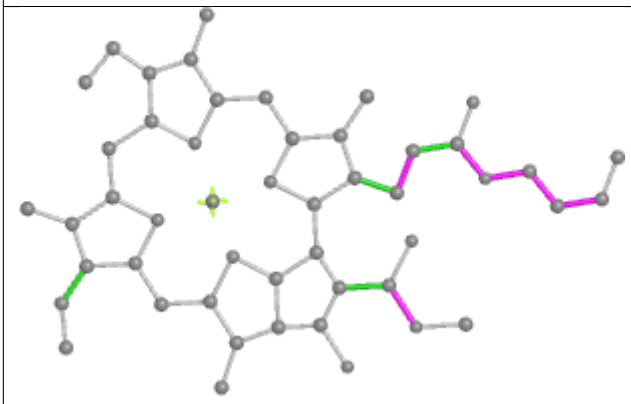
Ligand CLA cB 832



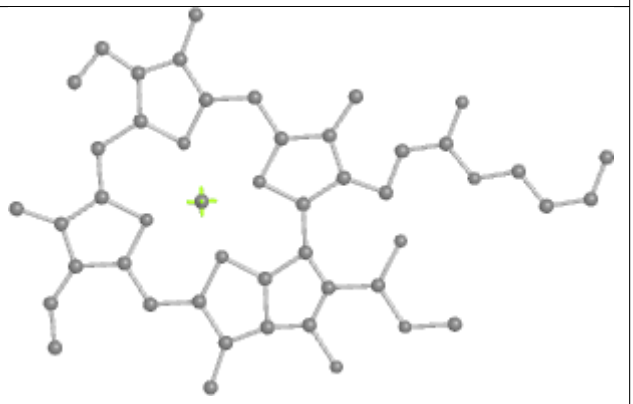
Bond lengths



Bond angles

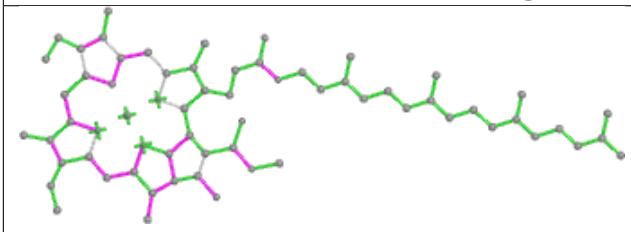


Torsions

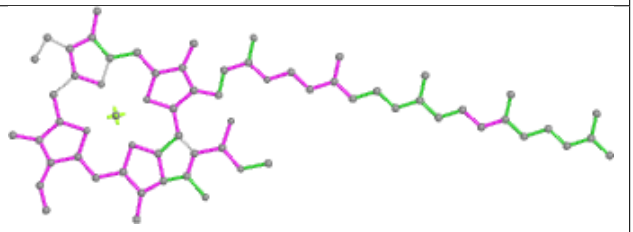


Rings

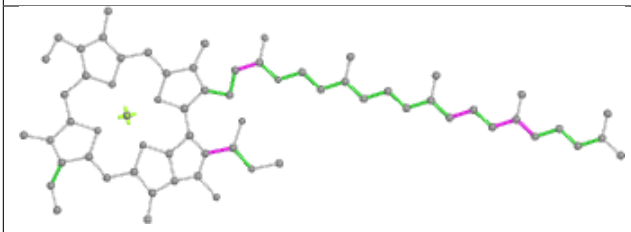
Ligand CL0 aA 801



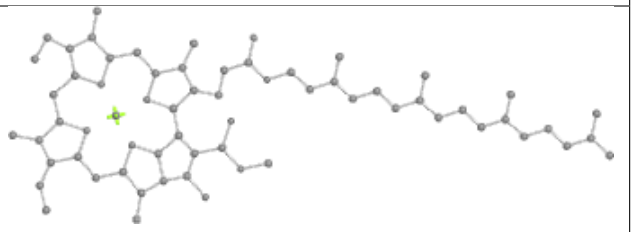
Bond lengths



Bond angles

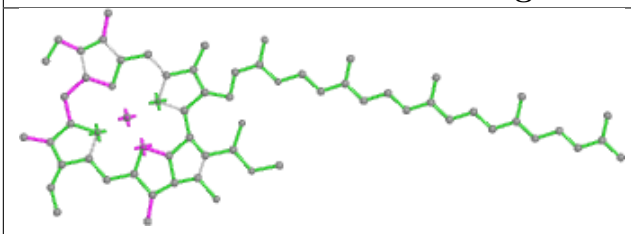


Torsions

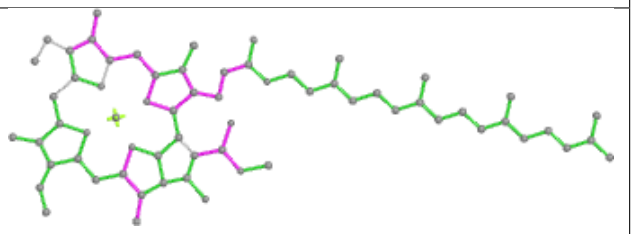


Rings

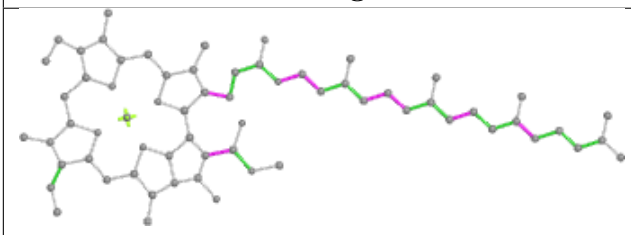
Ligand CLA aA 827



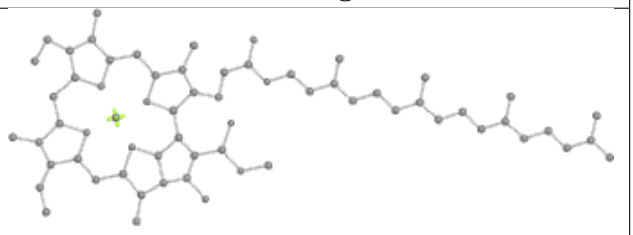
Bond lengths



Bond angles

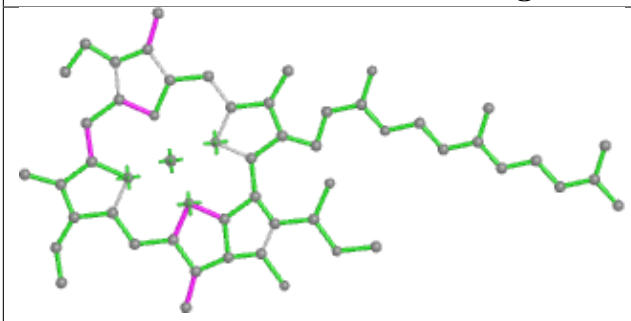


Torsions

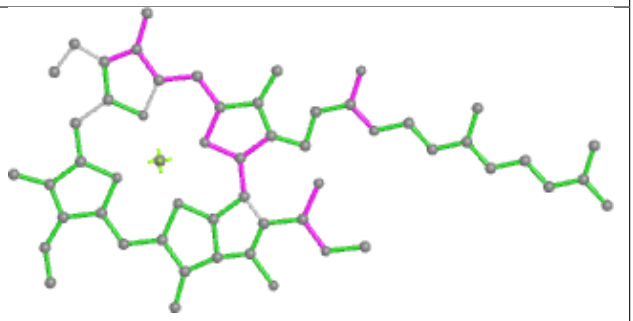


Rings

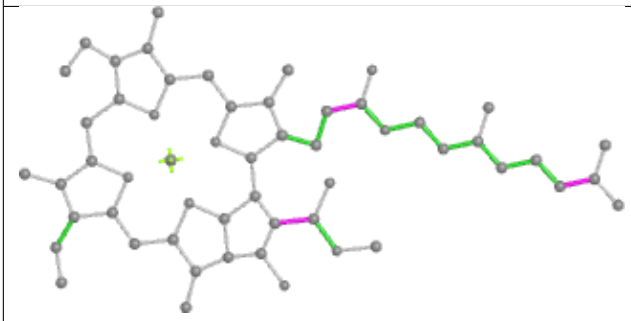
Ligand CLA aB 823



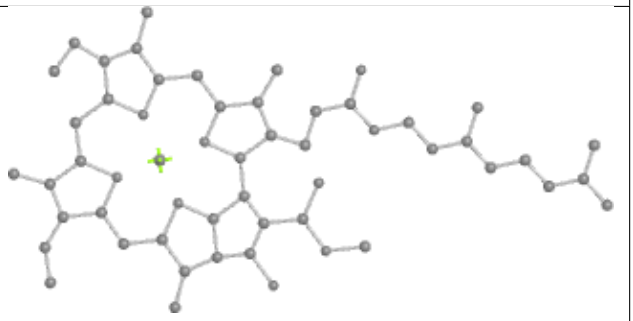
Bond lengths



Bond angles

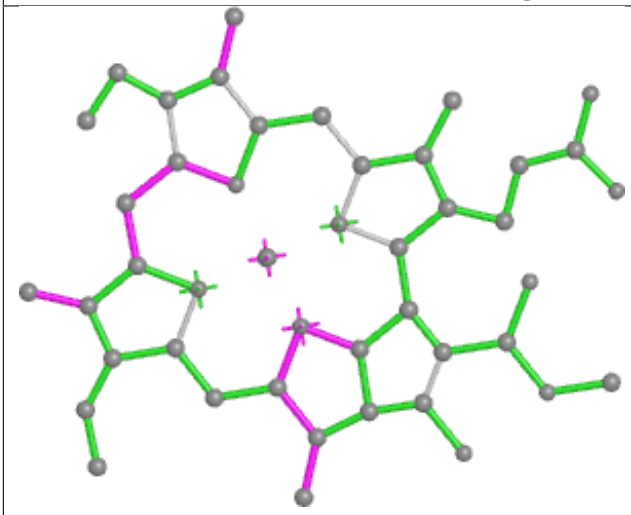


Torsions

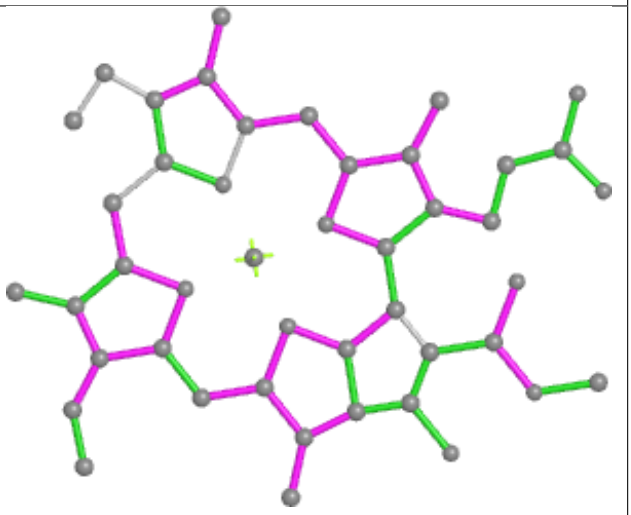


Rings

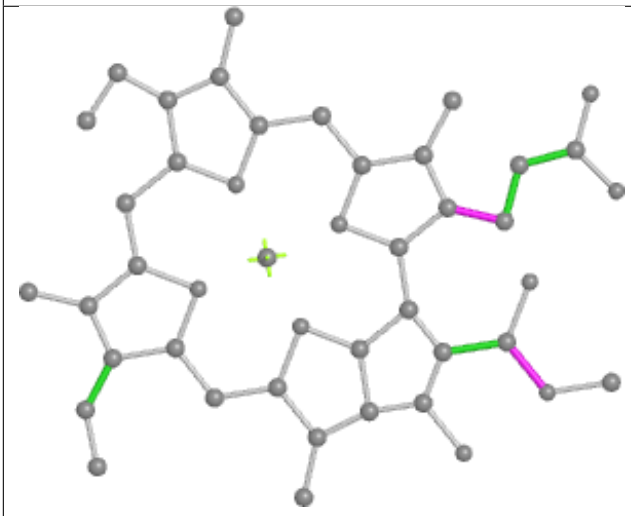
Ligand CLA b3 405



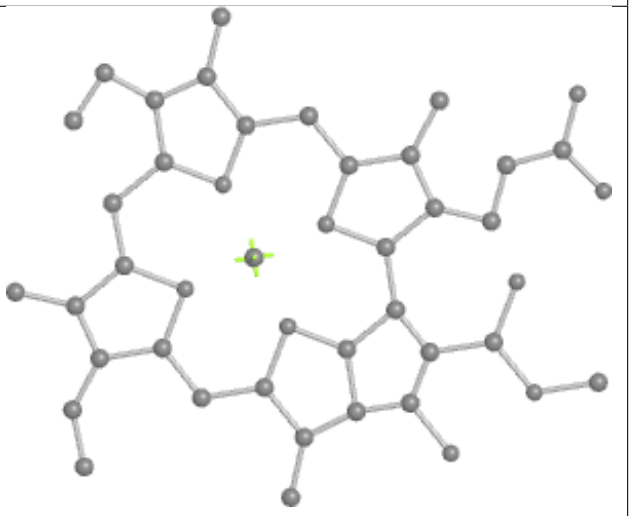
Bond lengths



Bond angles

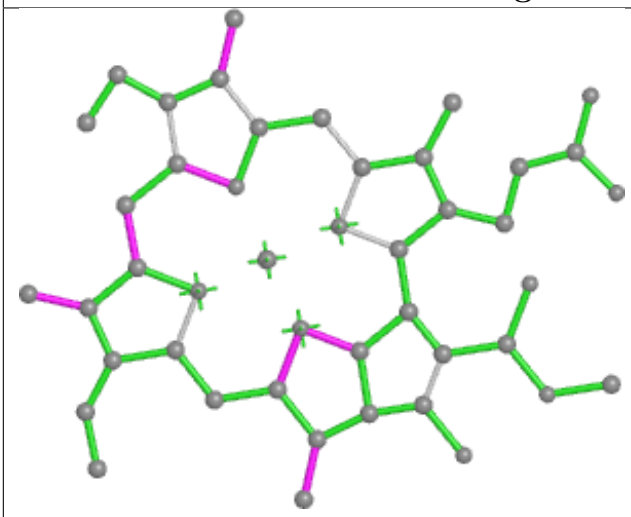


Torsions

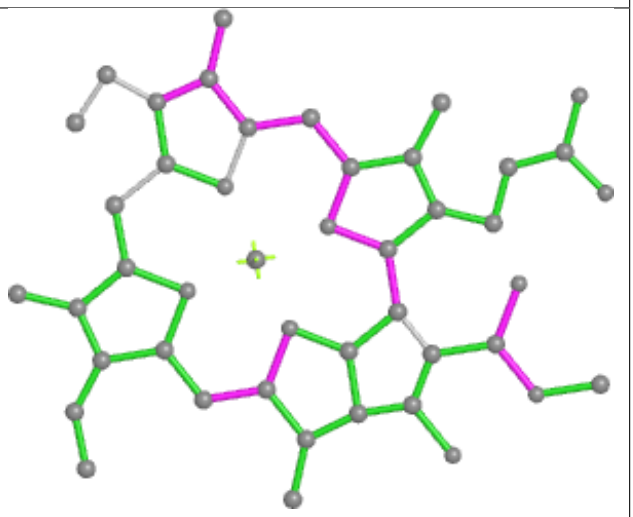


Rings

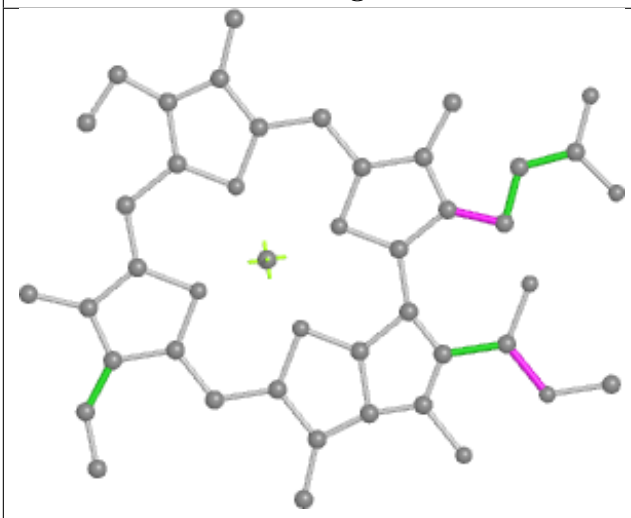
Ligand CLA bB 812



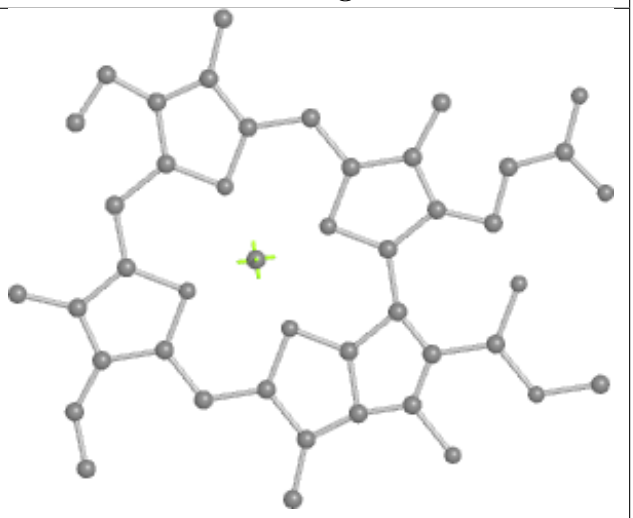
Bond lengths



Bond angles

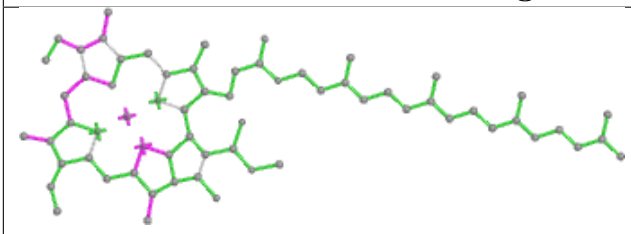


Torsions

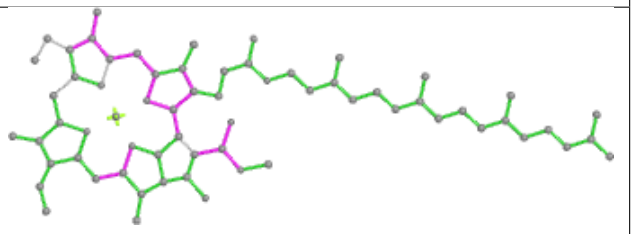


Rings

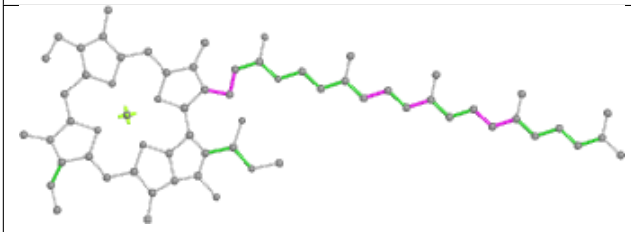
Ligand CLA bL 203



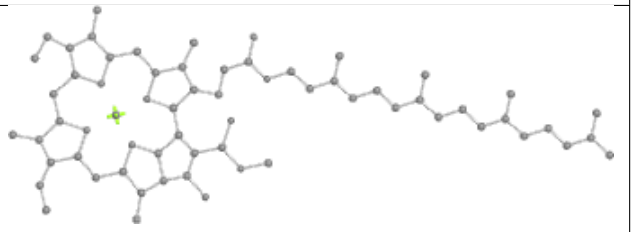
Bond lengths



Bond angles

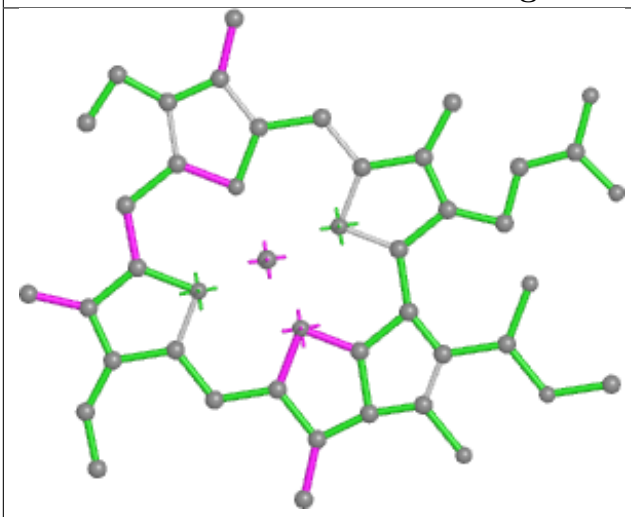


Torsions

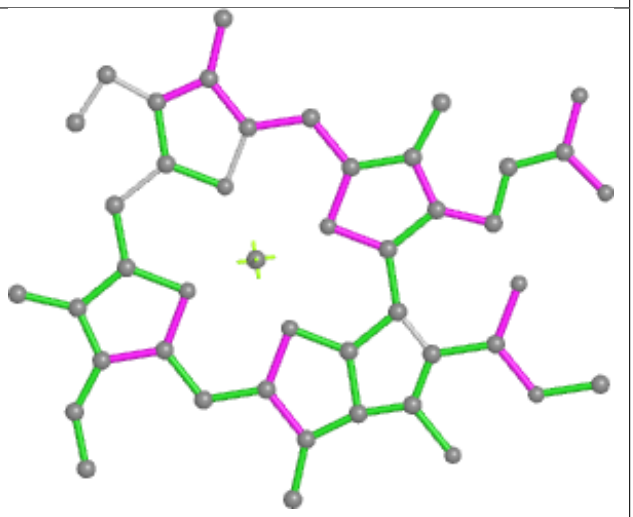


Rings

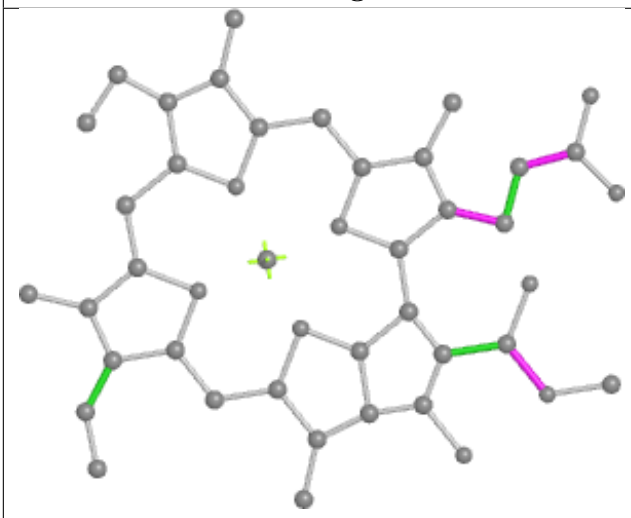
Ligand CLA a3 408



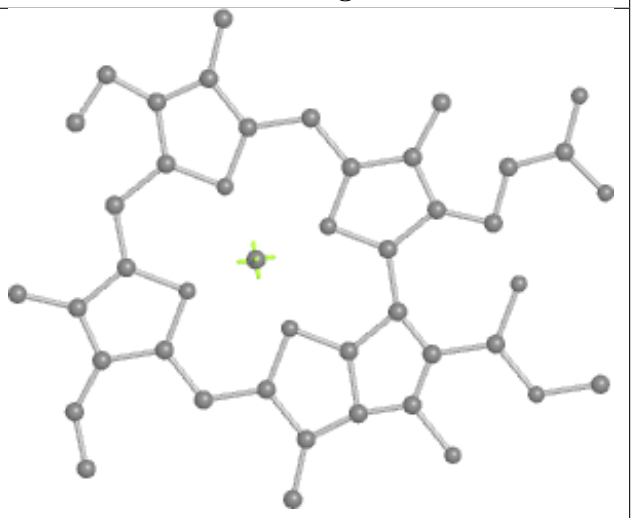
Bond lengths



Bond angles

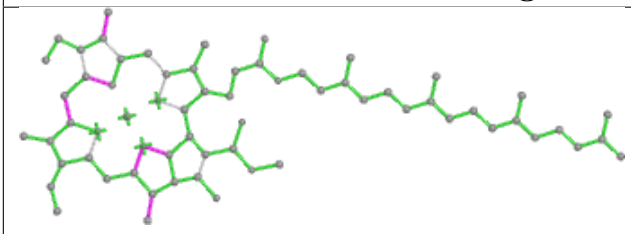


Torsions

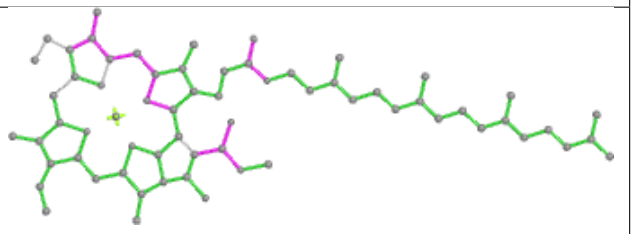


Rings

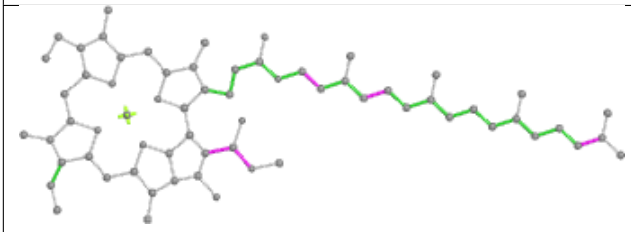
Ligand CLA b2 410



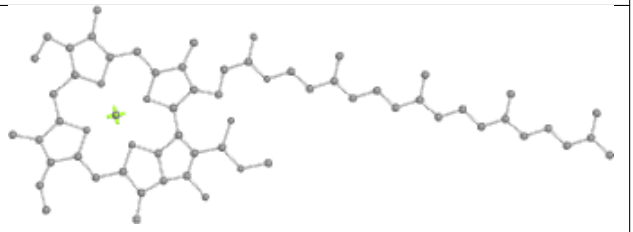
Bond lengths



Bond angles

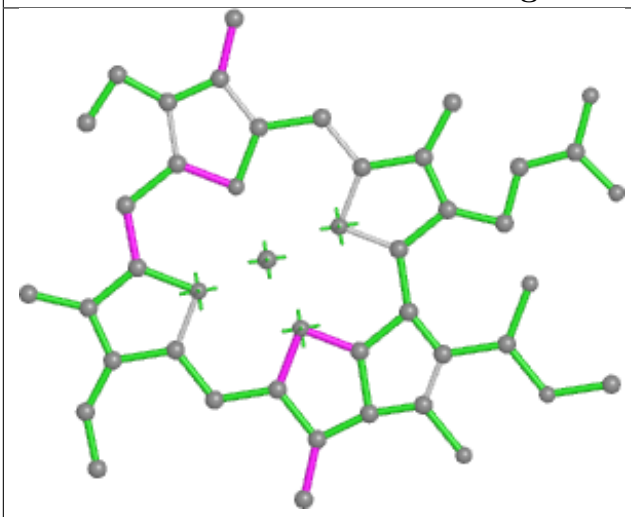


Torsions

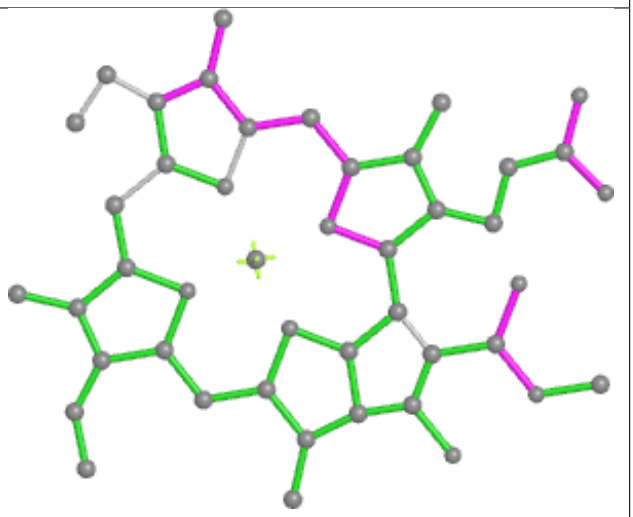


Rings

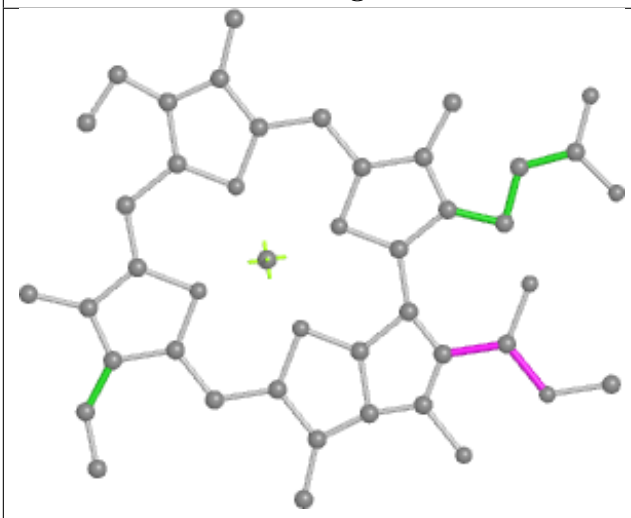
Ligand CLA c2 407



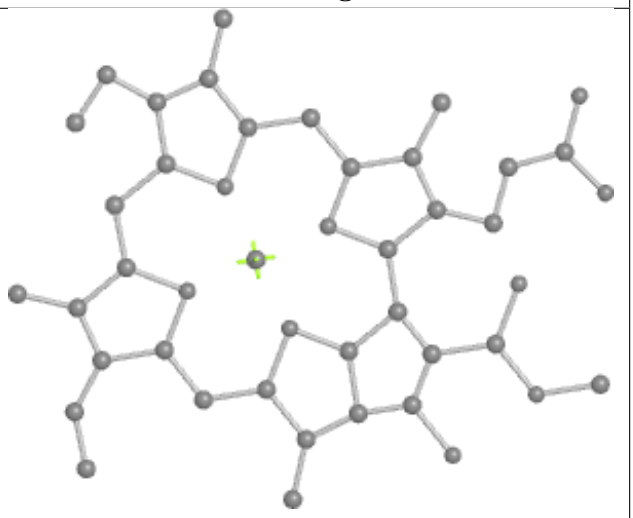
Bond lengths



Bond angles

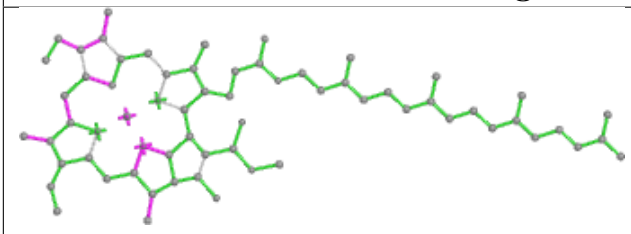


Torsions

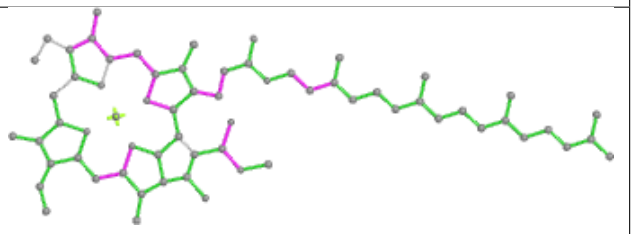


Rings

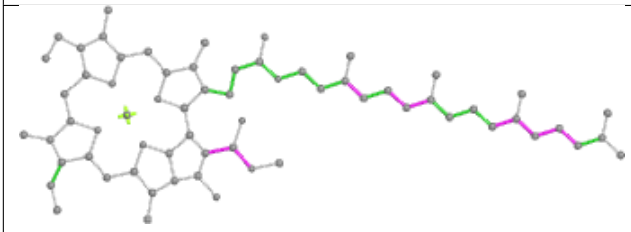
Ligand CLA bB 837



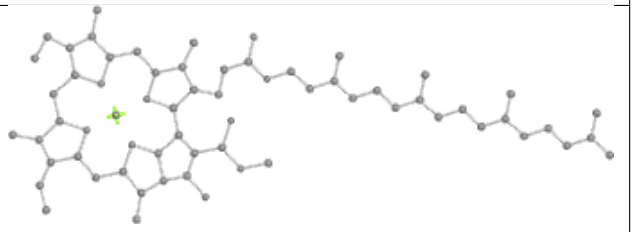
Bond lengths



Bond angles

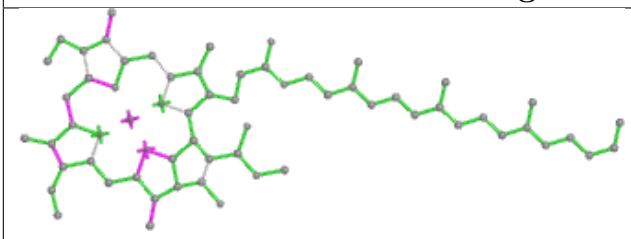


Torsions

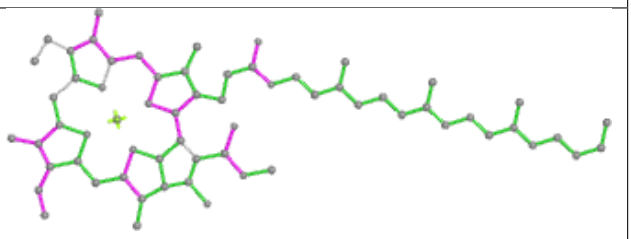


Rings

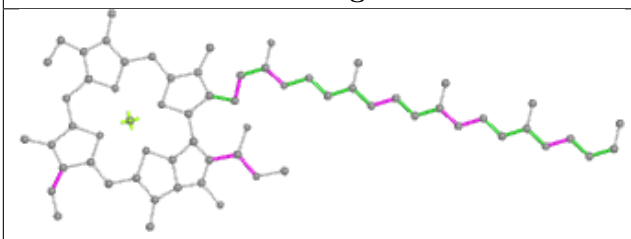
Ligand CLA b1 410



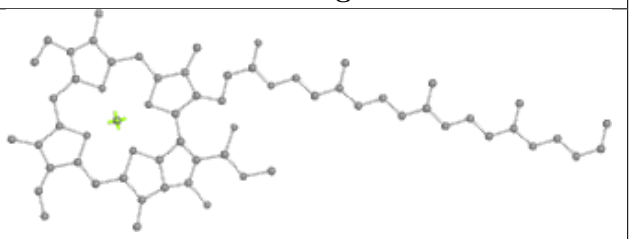
Bond lengths



Bond angles

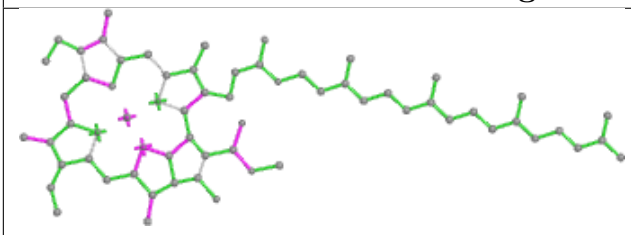


Torsions

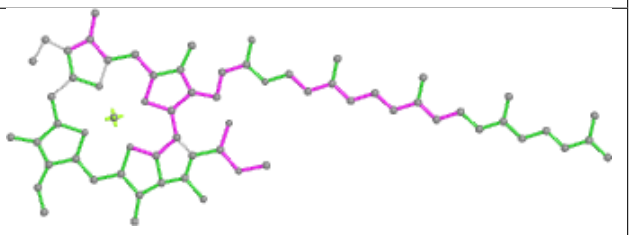


Rings

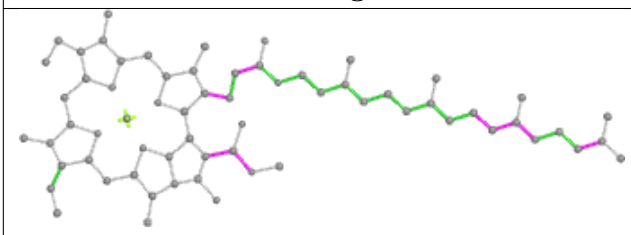
Ligand CLA b4 421



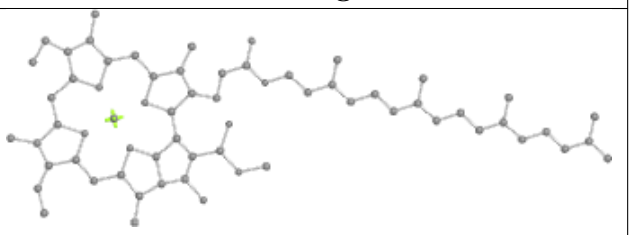
Bond lengths



Bond angles

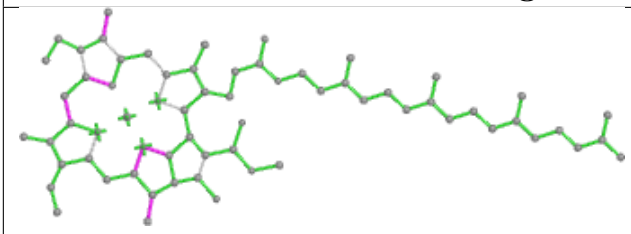


Torsions

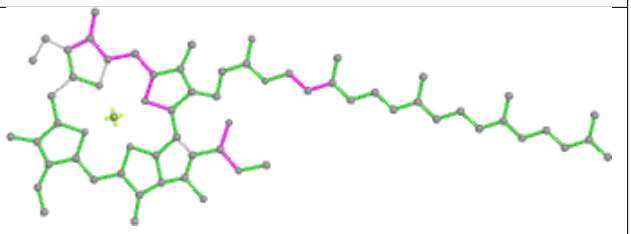


Rings

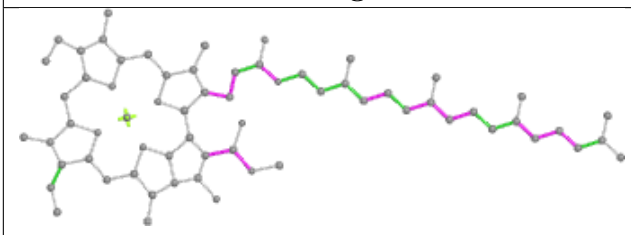
Ligand CLA b6 403



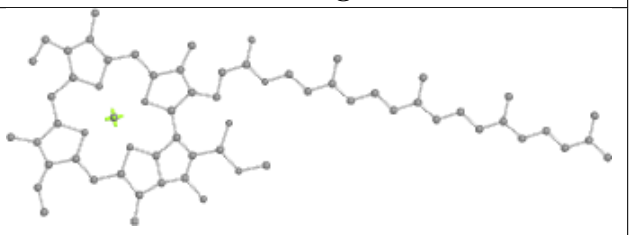
Bond lengths



Bond angles

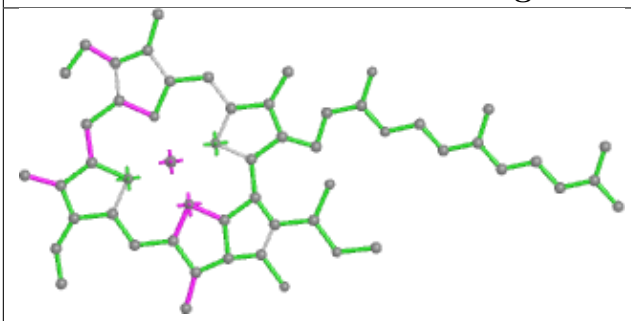


Torsions

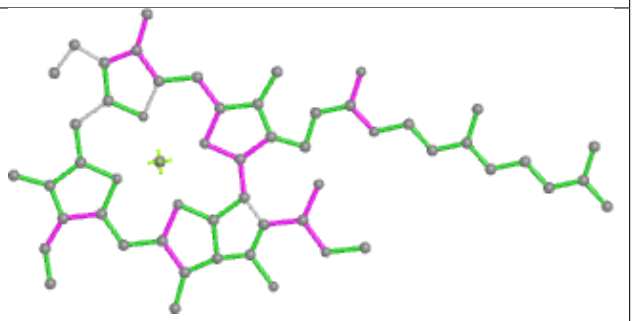


Rings

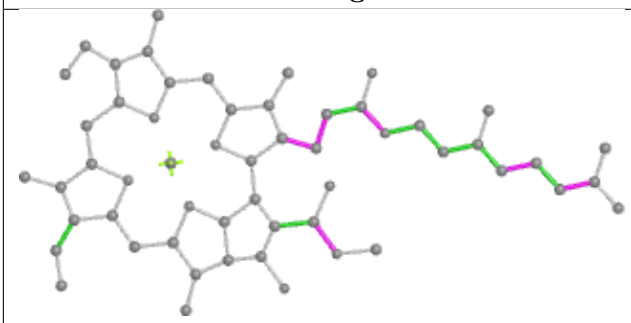
Ligand CLA bB 817



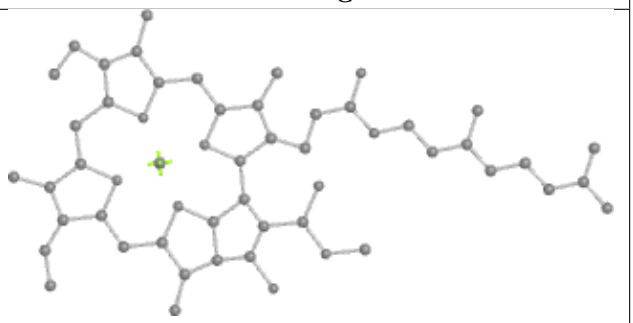
Bond lengths



Bond angles

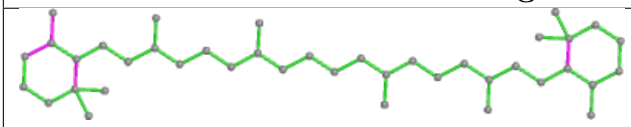


Torsions

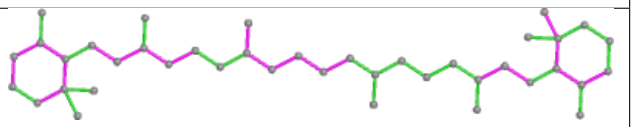


Rings

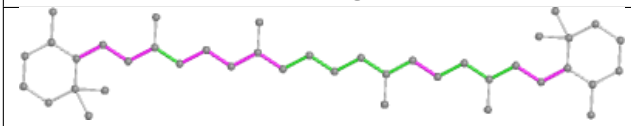
Ligand BCR a5 401



Bond lengths



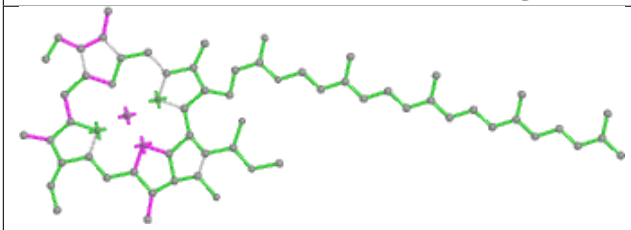
Bond angles



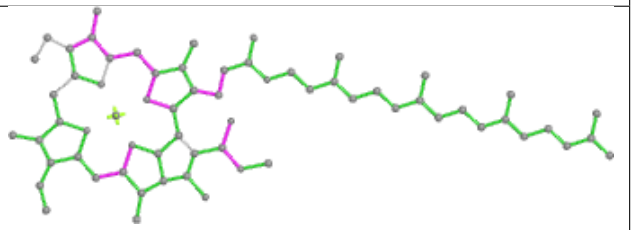
Torsions

Rings

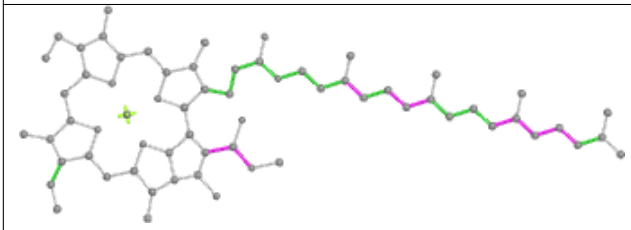
Ligand CLA cB 837



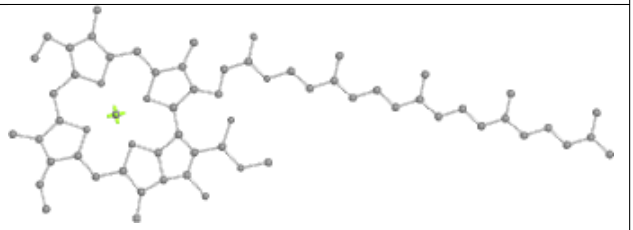
Bond lengths



Bond angles

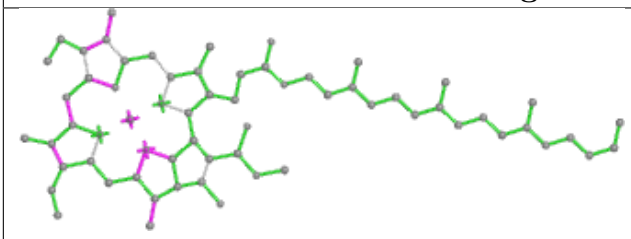


Torsions

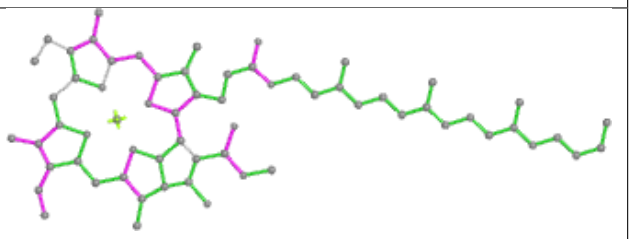


Rings

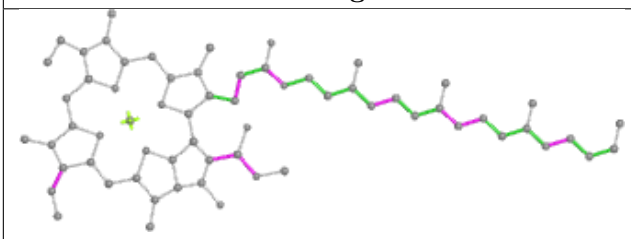
Ligand CLA c1 410



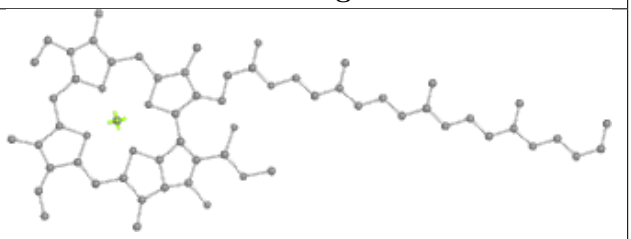
Bond lengths



Bond angles

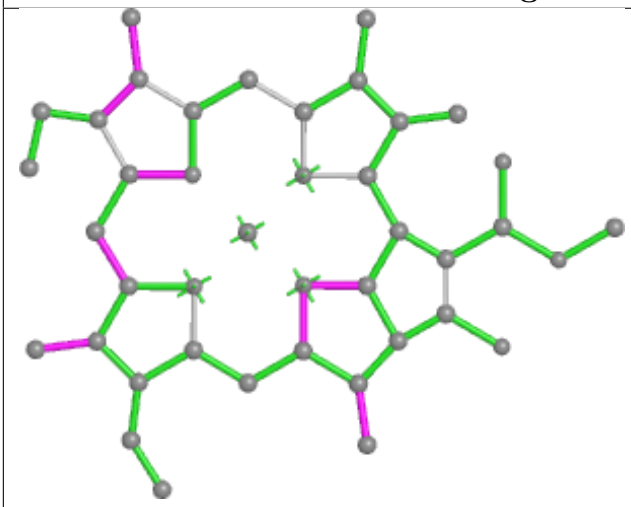


Torsions

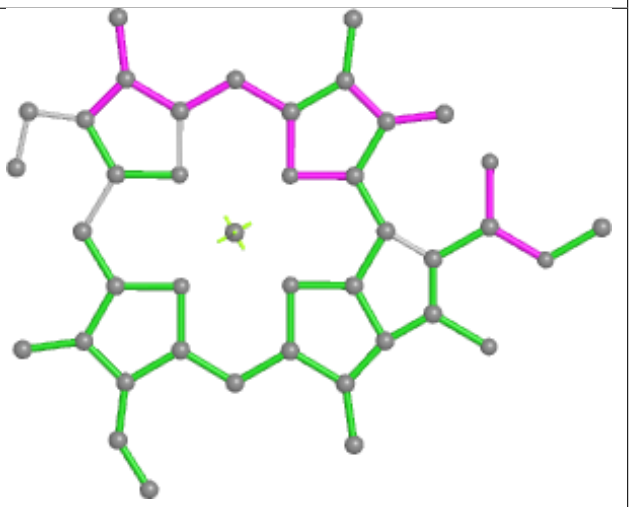


Rings

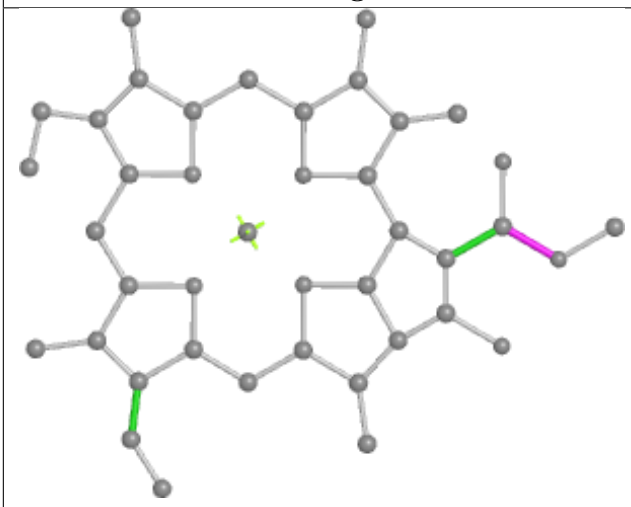
Ligand CLA c3 414



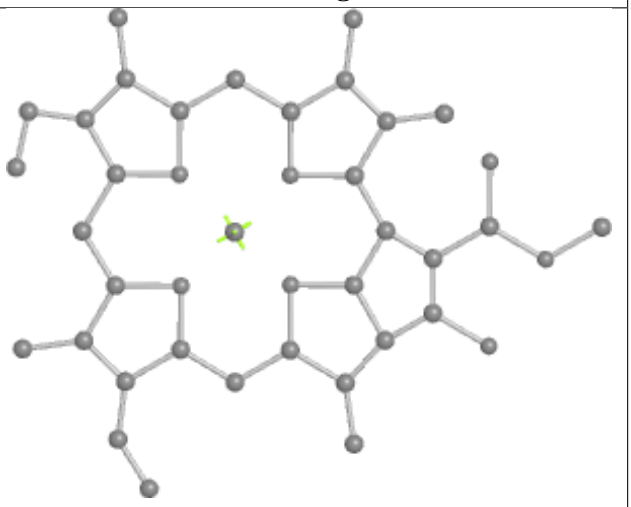
Bond lengths



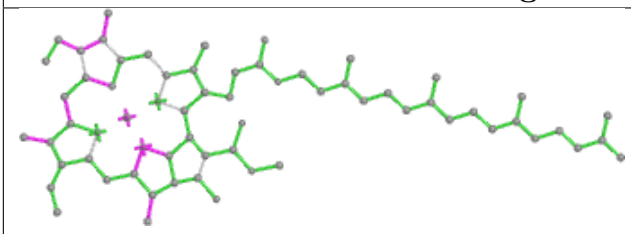
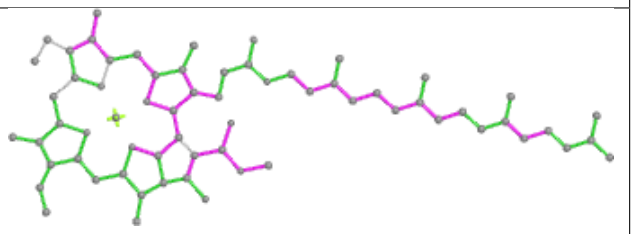
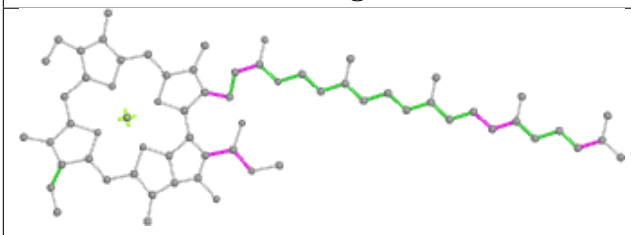
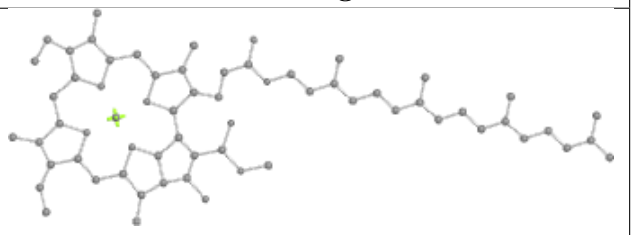
Bond angles

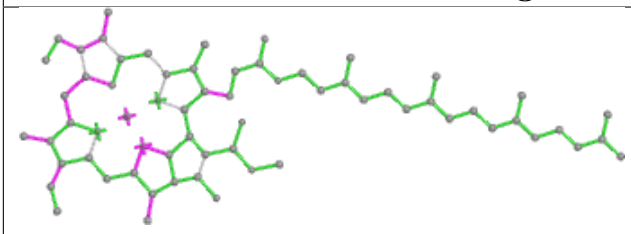
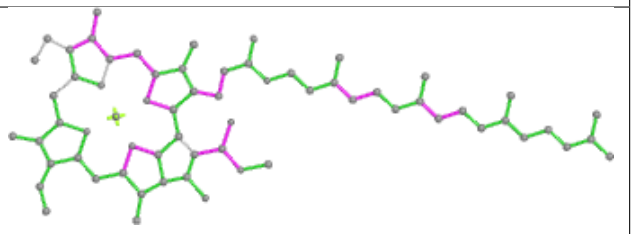
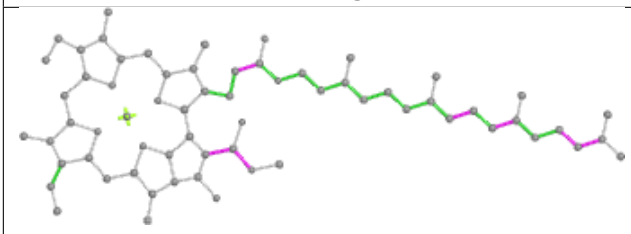
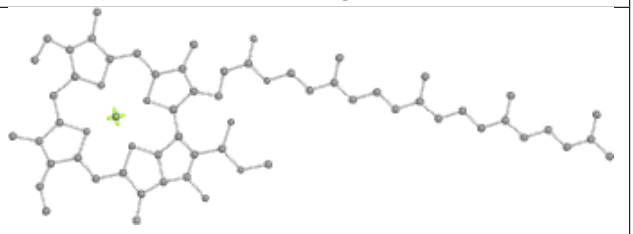


Torsions

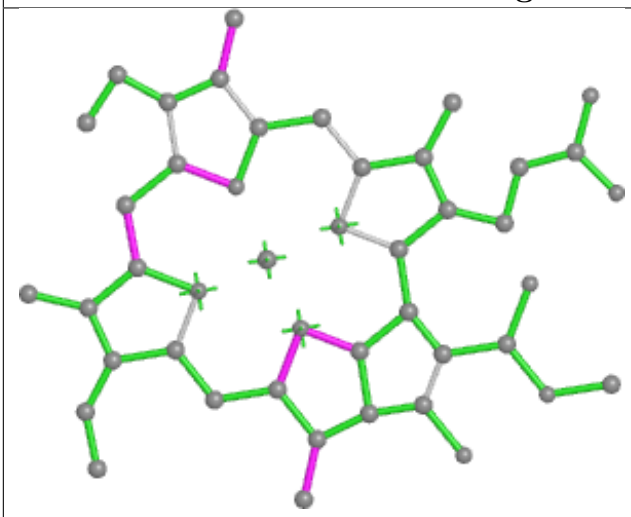


Rings

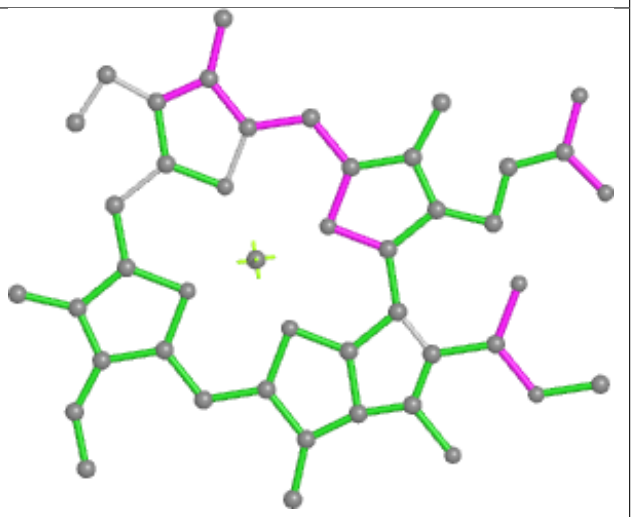
Ligand CLA a2 422	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cB 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

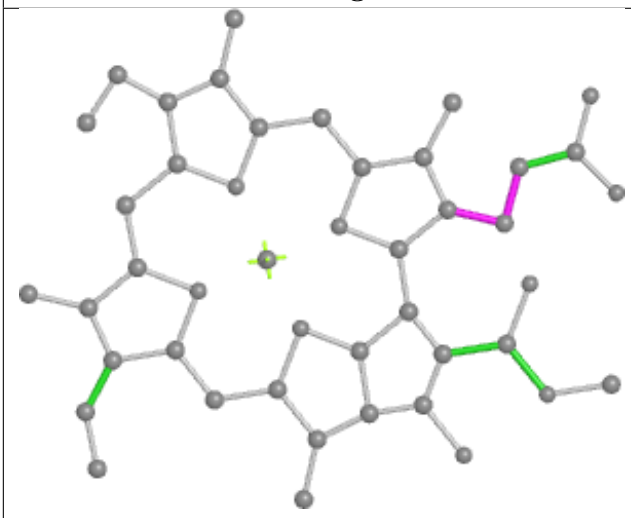
Ligand CLA aB 822



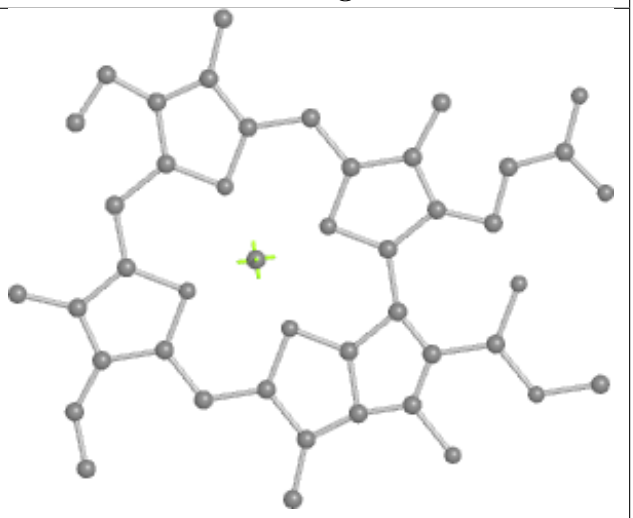
Bond lengths



Bond angles

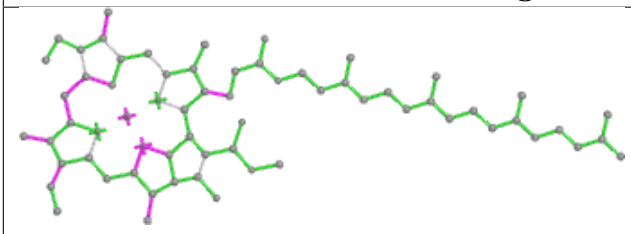


Torsions

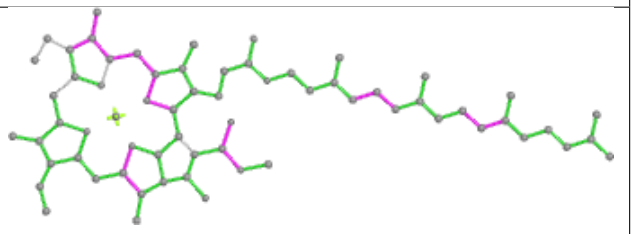


Rings

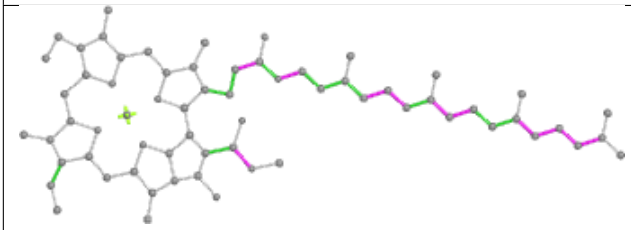
Ligand CLA cB 807



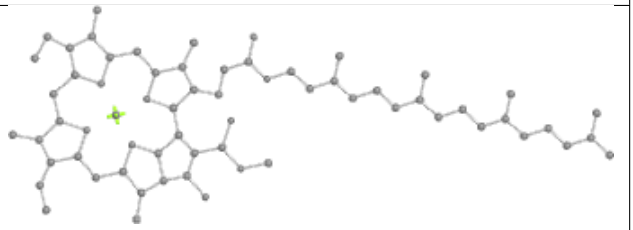
Bond lengths



Bond angles

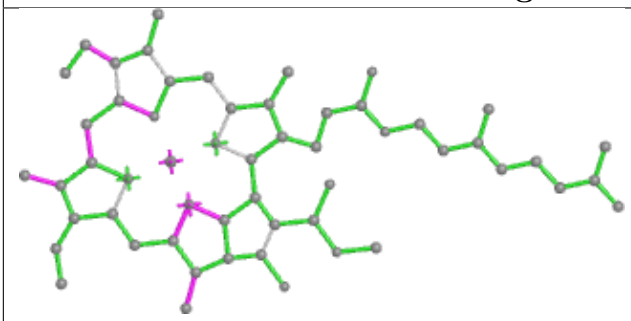


Torsions

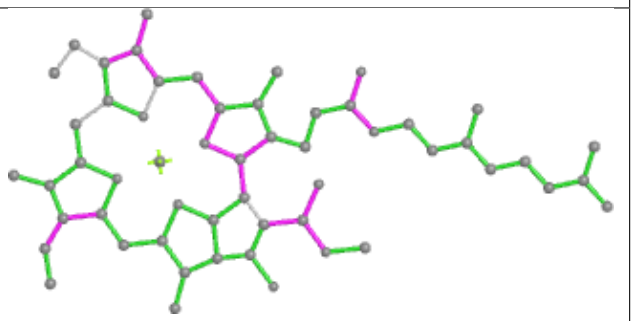


Rings

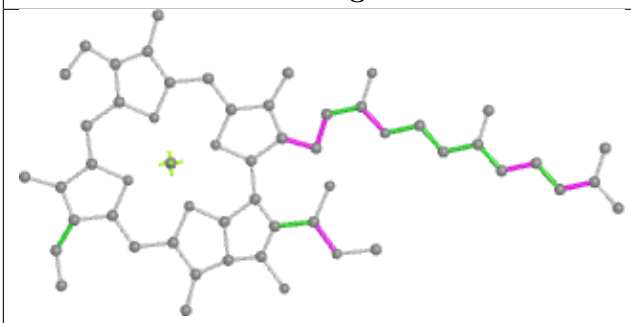
Ligand CLA aB 817



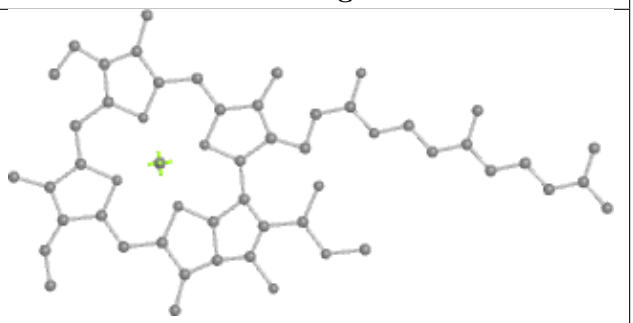
Bond lengths



Bond angles

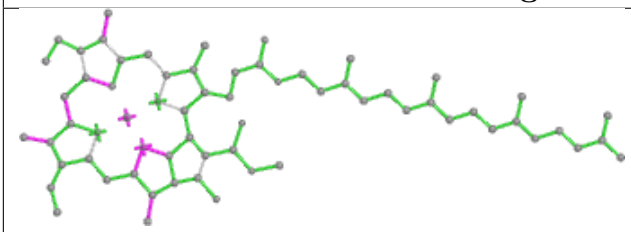


Torsions

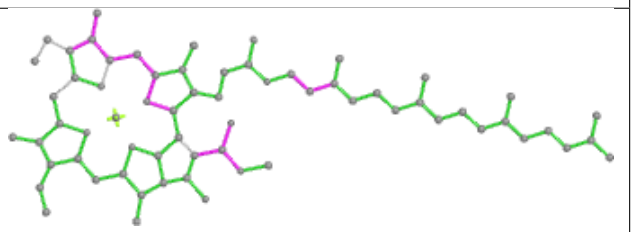


Rings

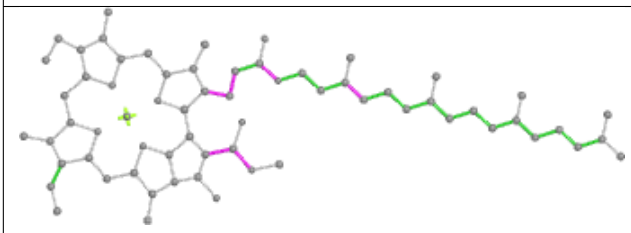
Ligand CLA c4 404



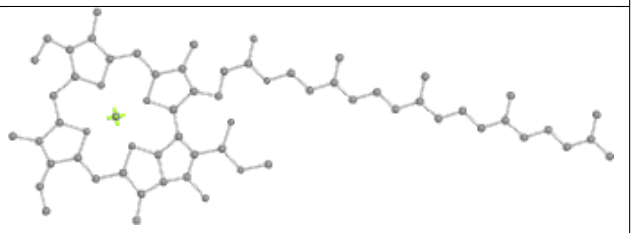
Bond lengths



Bond angles



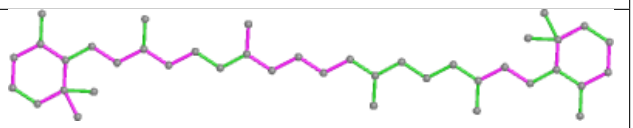
Torsions



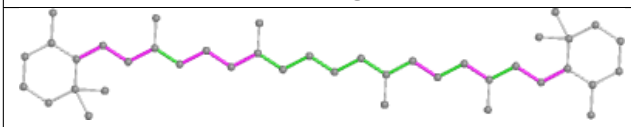
Rings

Ligand BCR b2 401

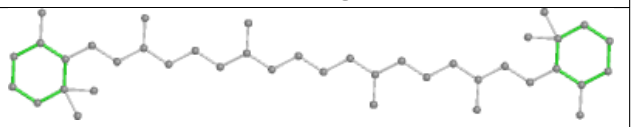
Bond lengths



Bond angles

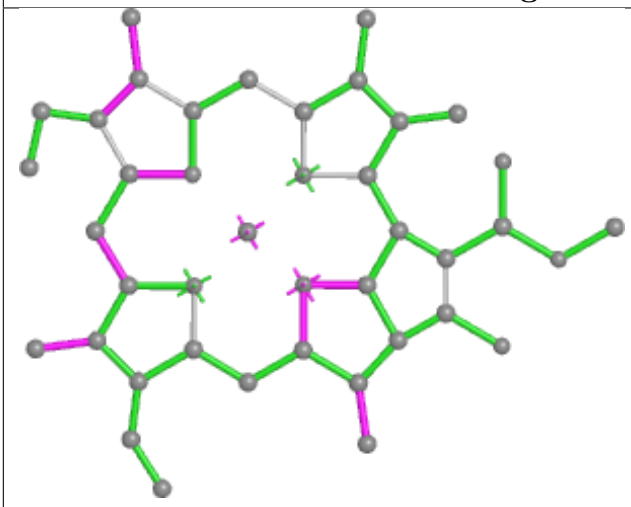


Torsions

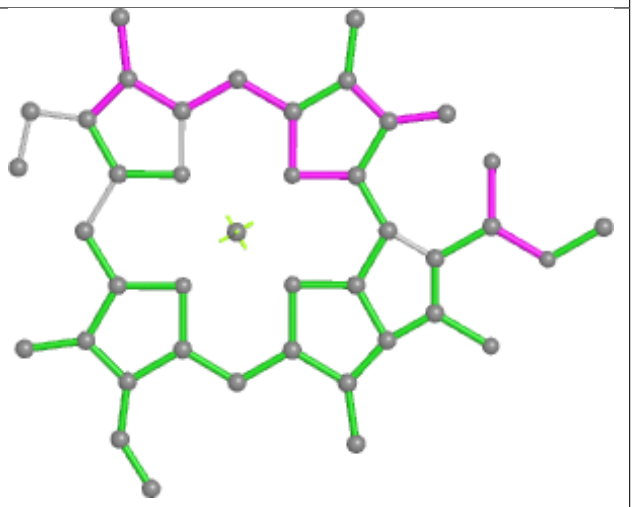


Rings

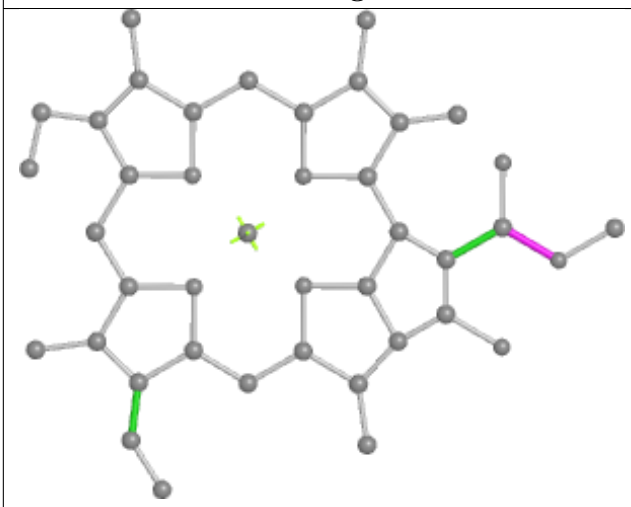
Ligand CLA c4 414



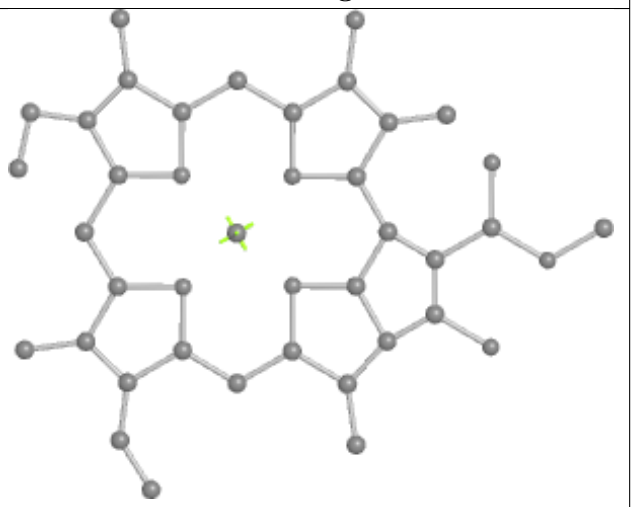
Bond lengths



Bond angles

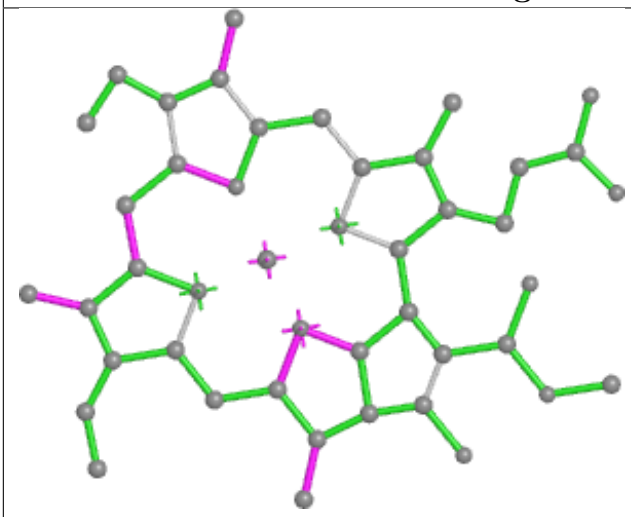


Torsions

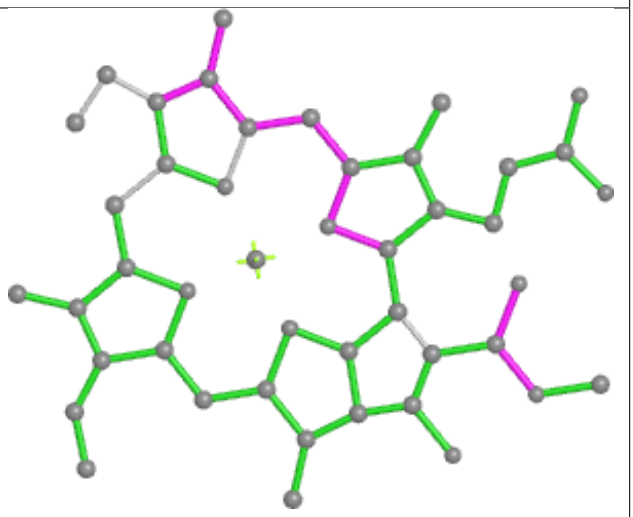


Rings

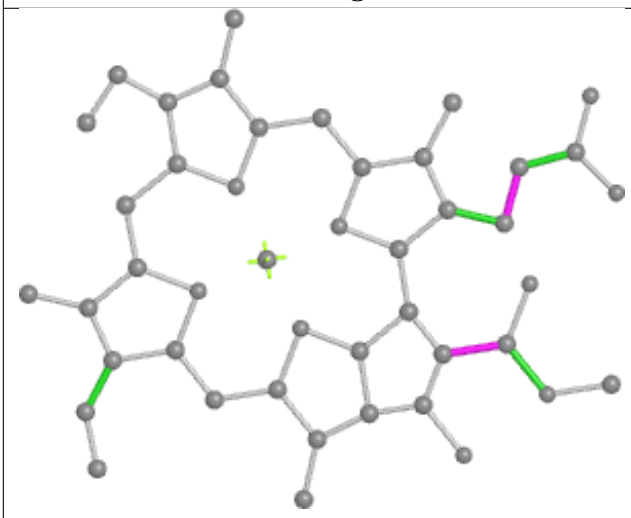
Ligand CLA bA 816



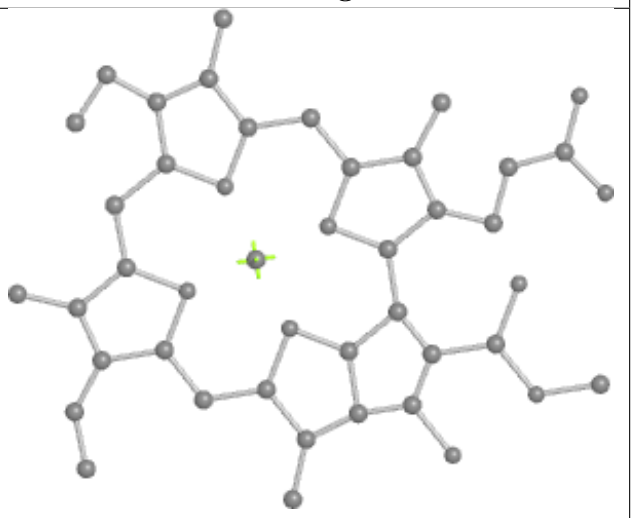
Bond lengths



Bond angles

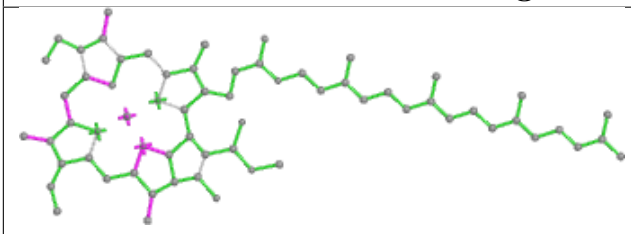


Torsions

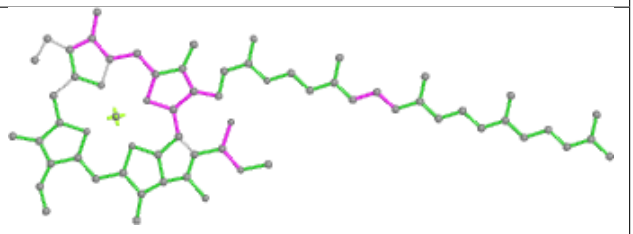


Rings

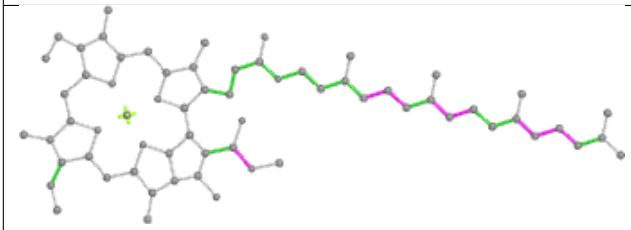
Ligand CLA cA 826



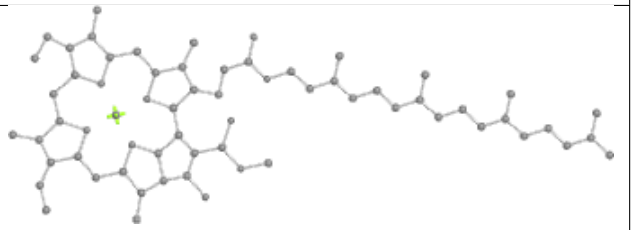
Bond lengths



Bond angles

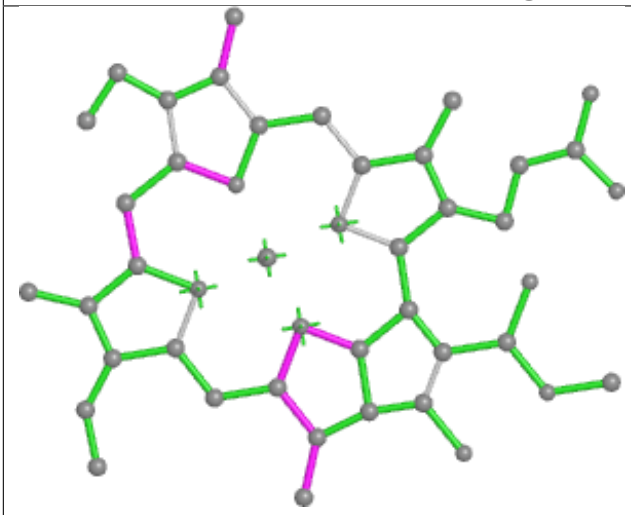


Torsions

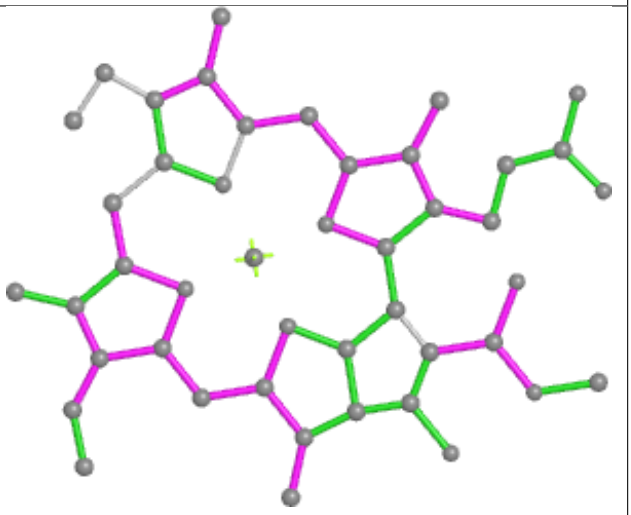


Rings

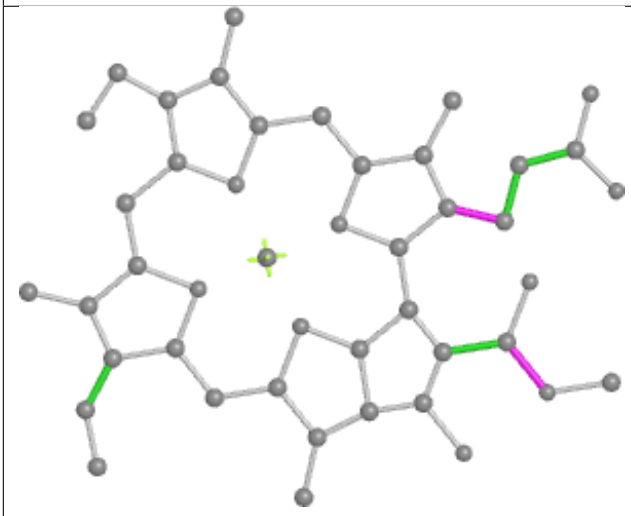
Ligand CLA c6 406



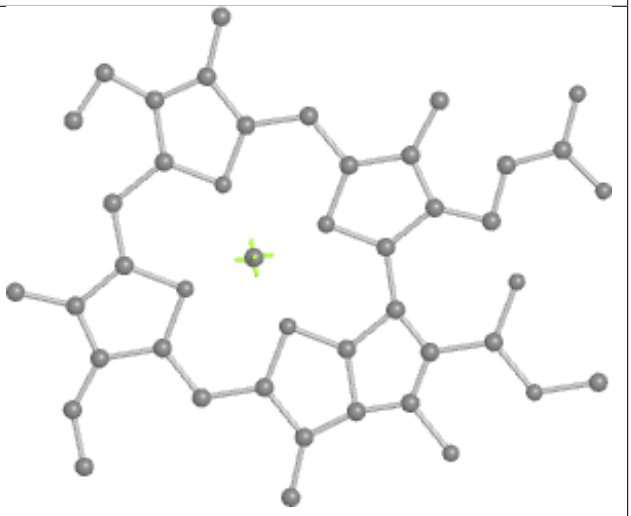
Bond lengths



Bond angles

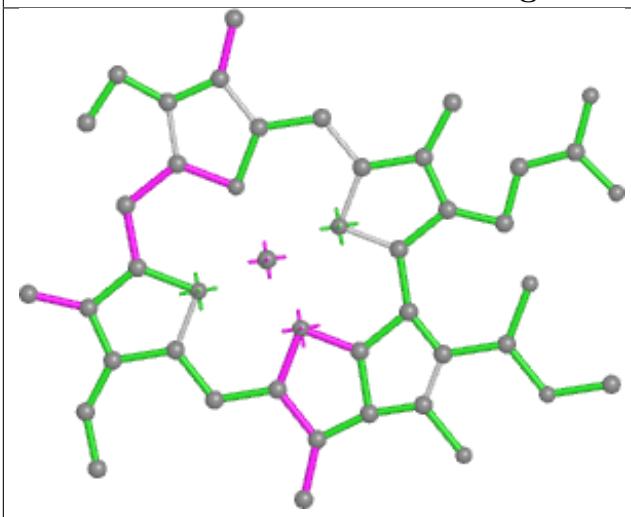


Torsions

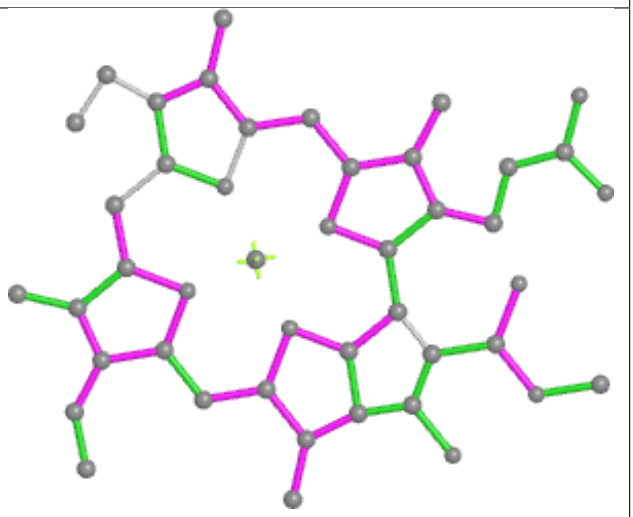


Rings

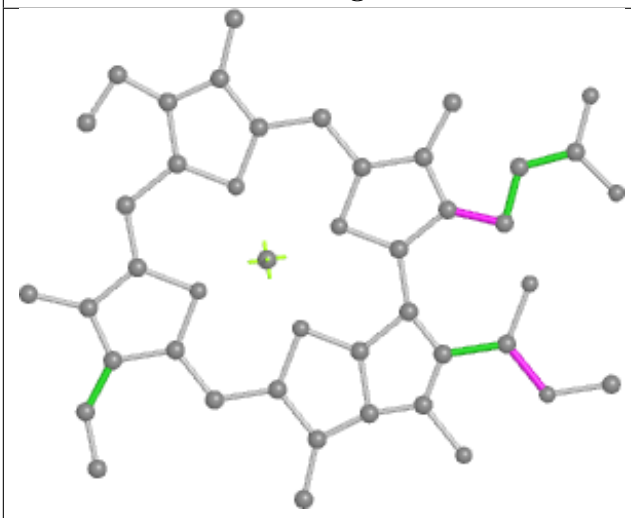
Ligand CLA a3 405



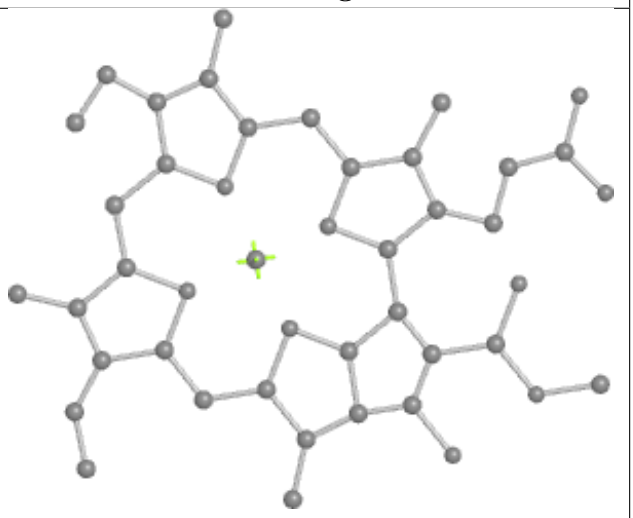
Bond lengths



Bond angles

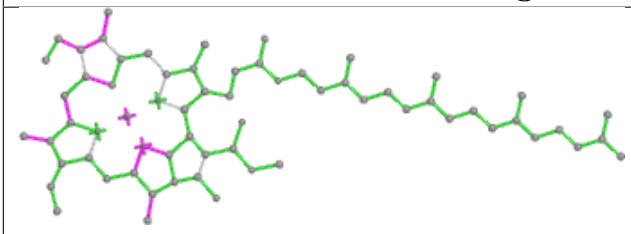


Torsions

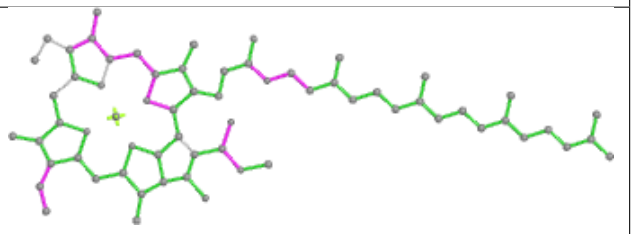


Rings

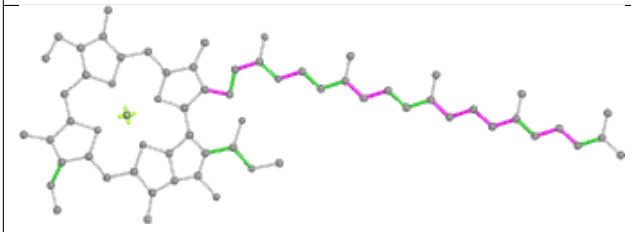
Ligand CLA cA 842



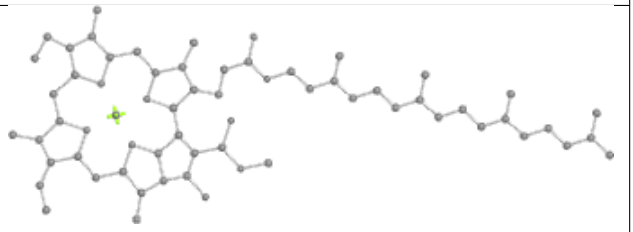
Bond lengths



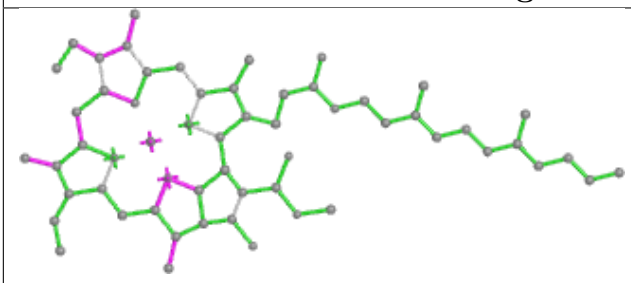
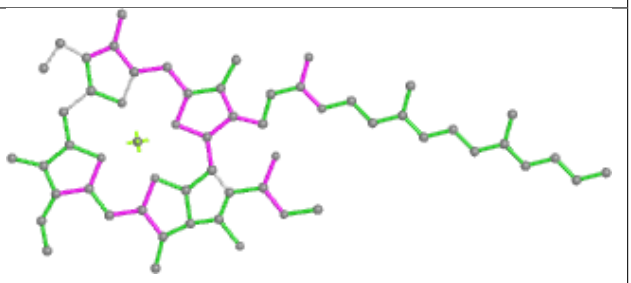
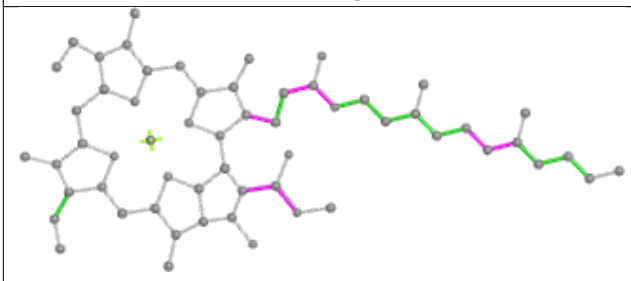
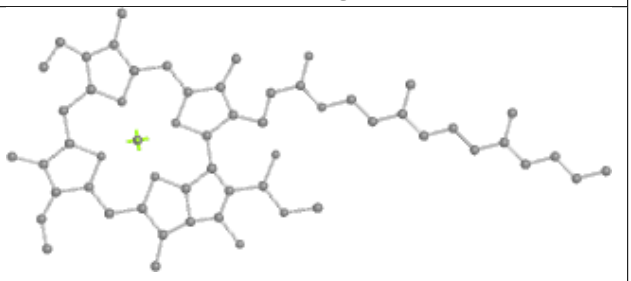
Bond angles

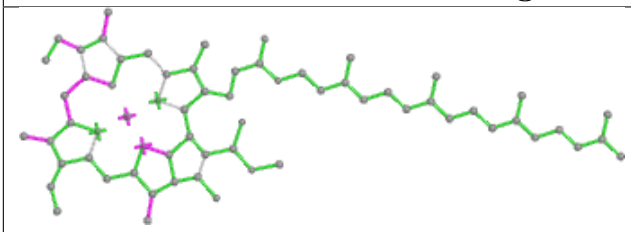
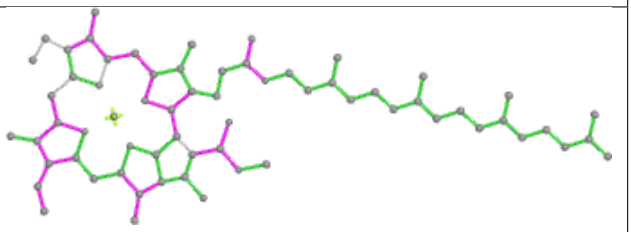
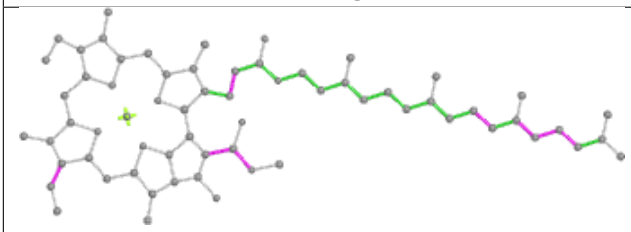
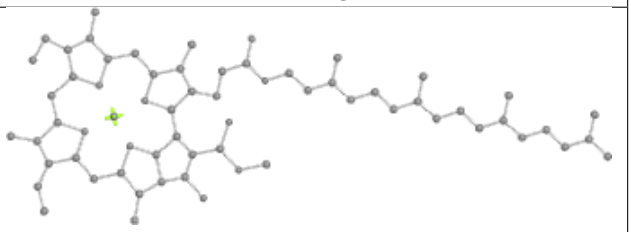


Torsions

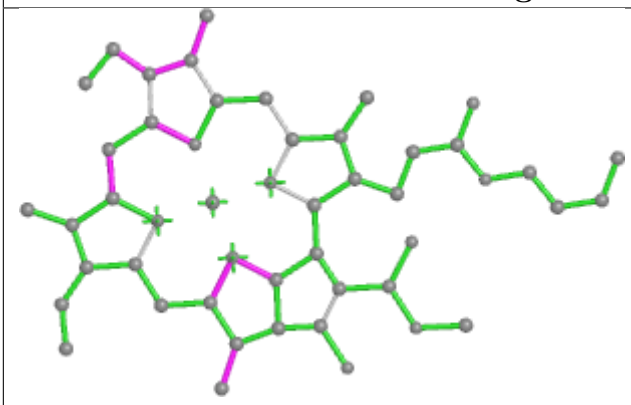


Rings

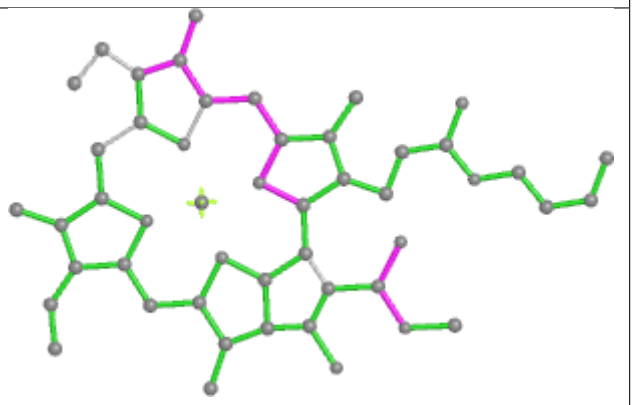
Ligand CLA cB 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cB 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

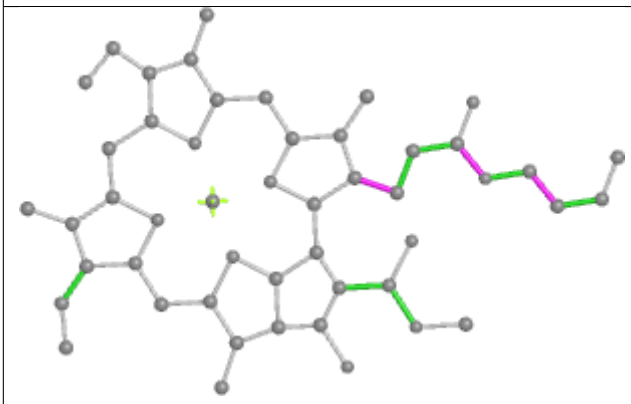
Ligand CLA aA 817



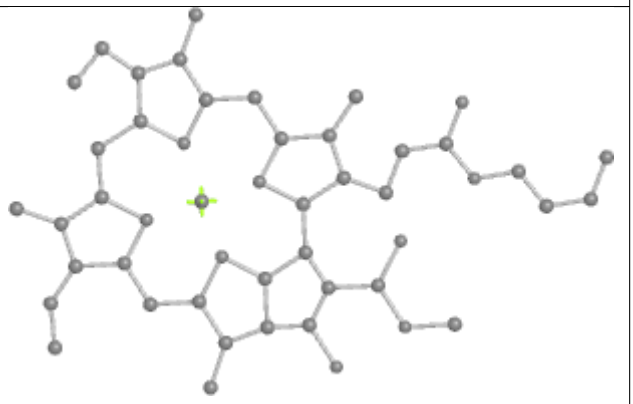
Bond lengths



Bond angles

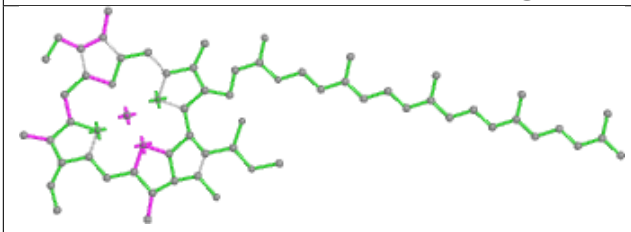


Torsions

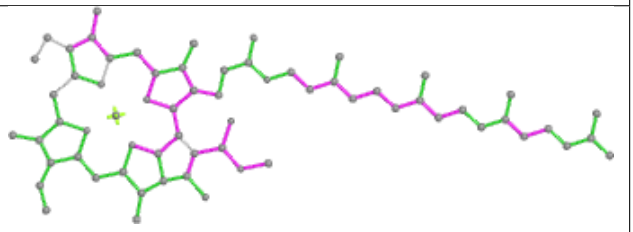


Rings

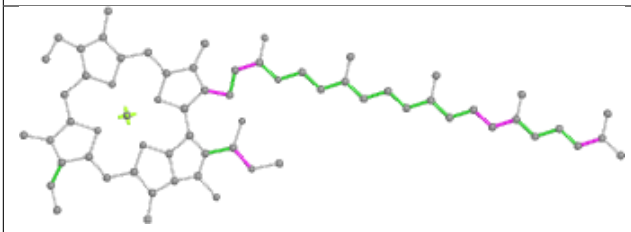
Ligand CLA b2 422



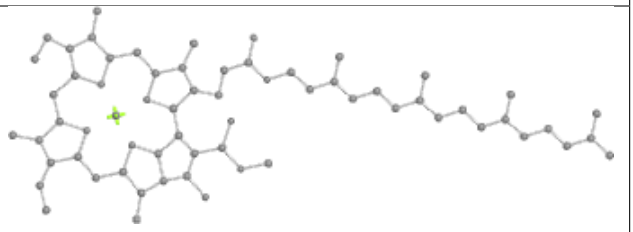
Bond lengths



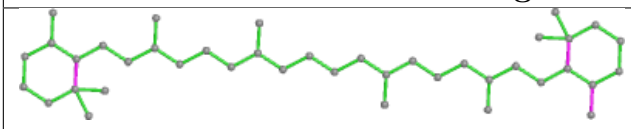
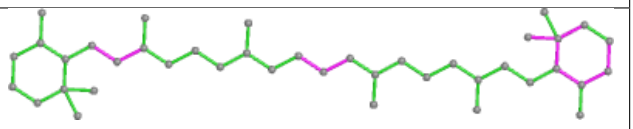
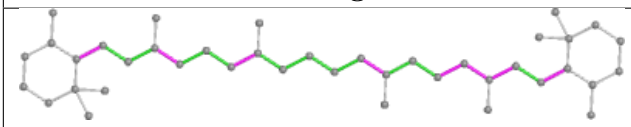
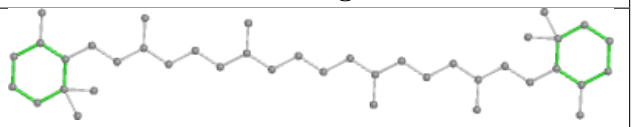
Bond angles

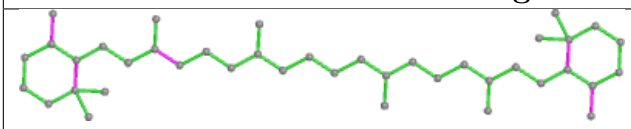
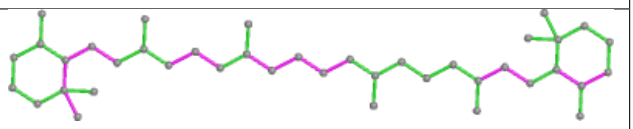
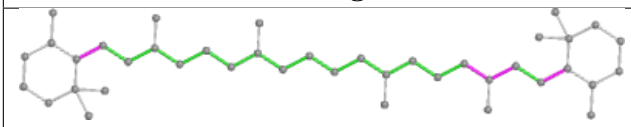
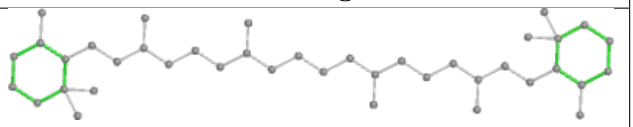


Torsions

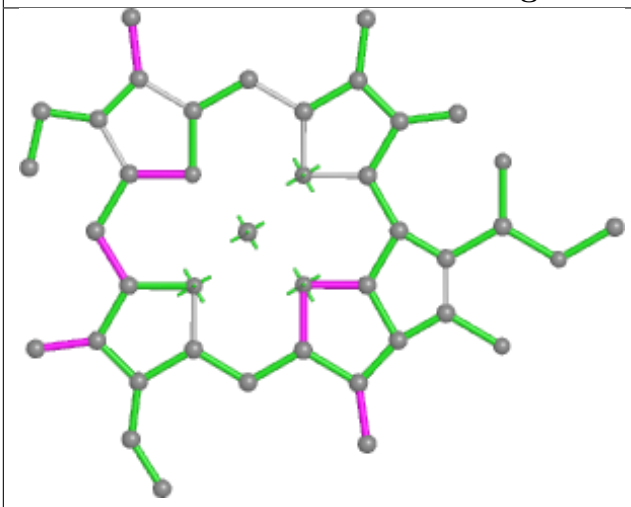


Rings

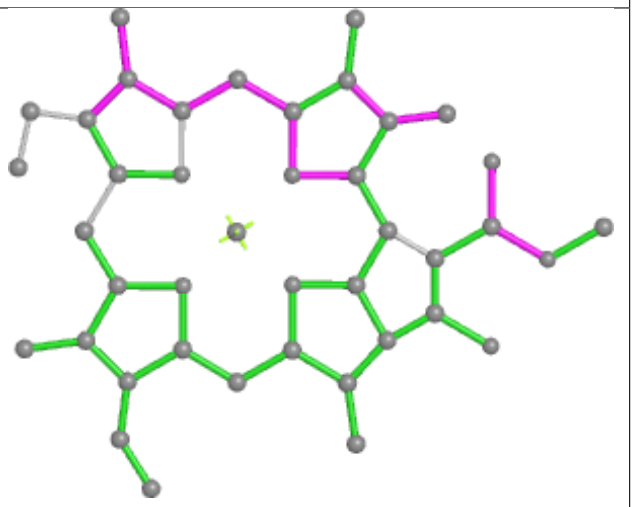
Ligand BCR aB 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR aA 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

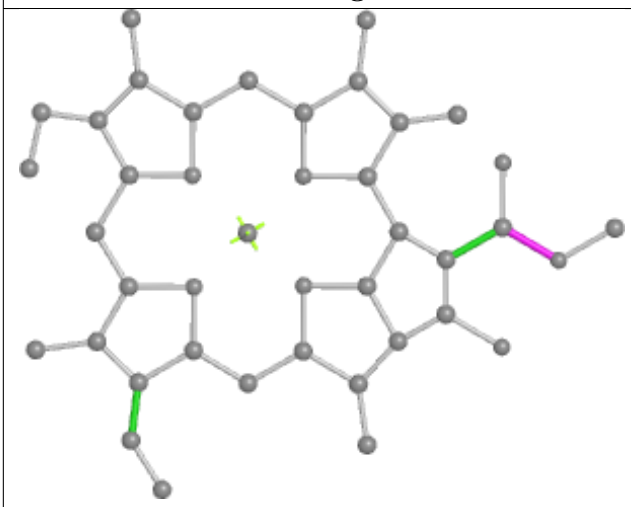
Ligand CLA c6 415



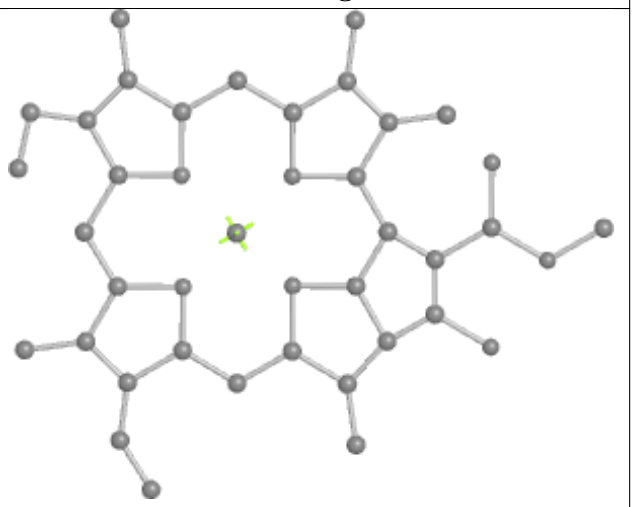
Bond lengths



Bond angles

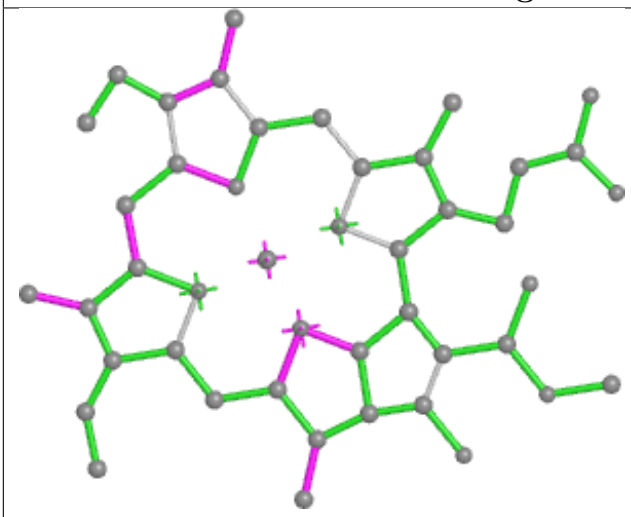


Torsions

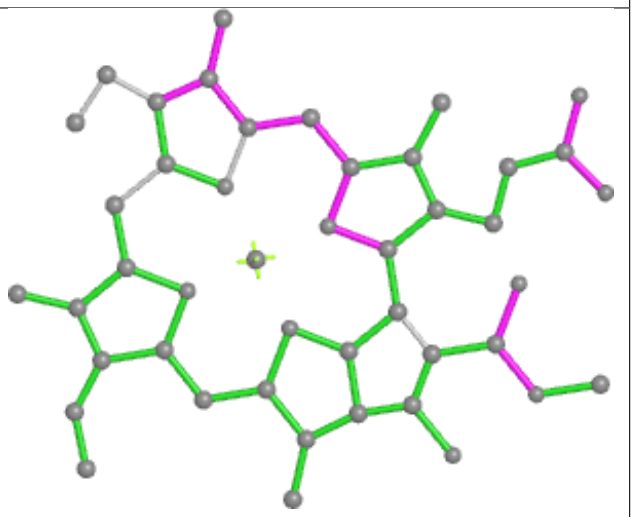


Rings

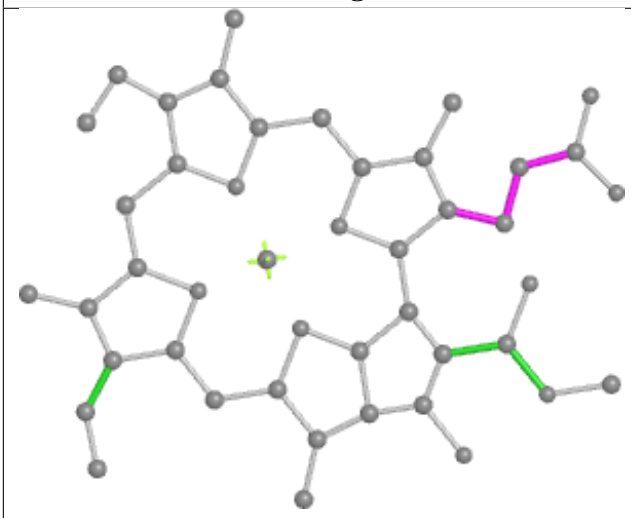
Ligand CLA cB 813



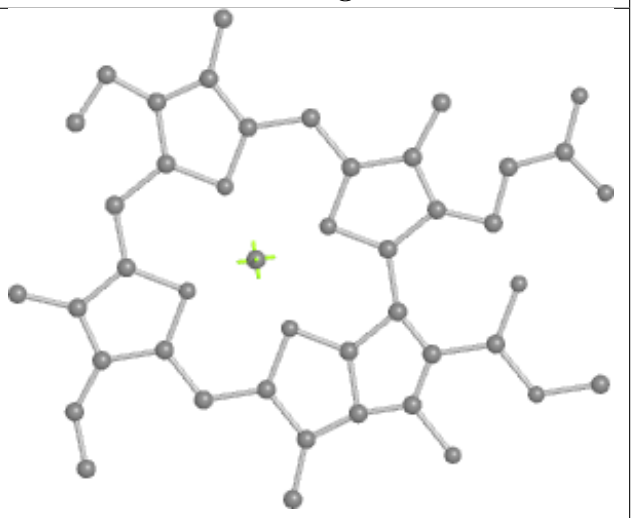
Bond lengths



Bond angles

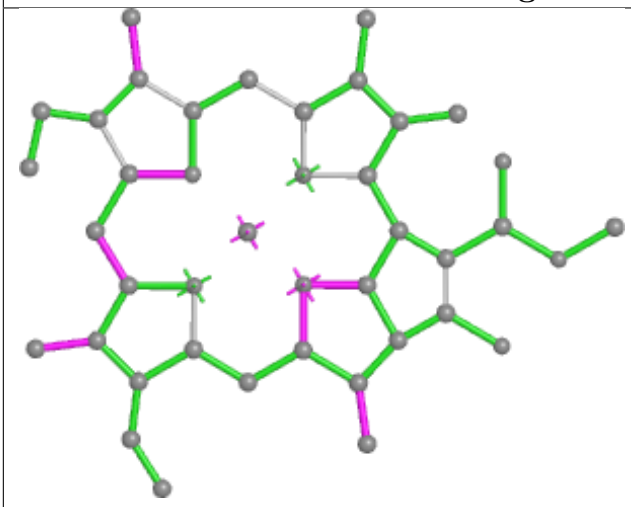


Torsions

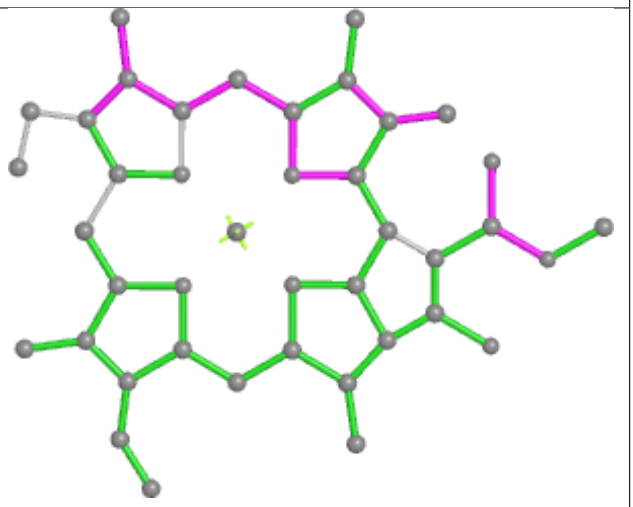


Rings

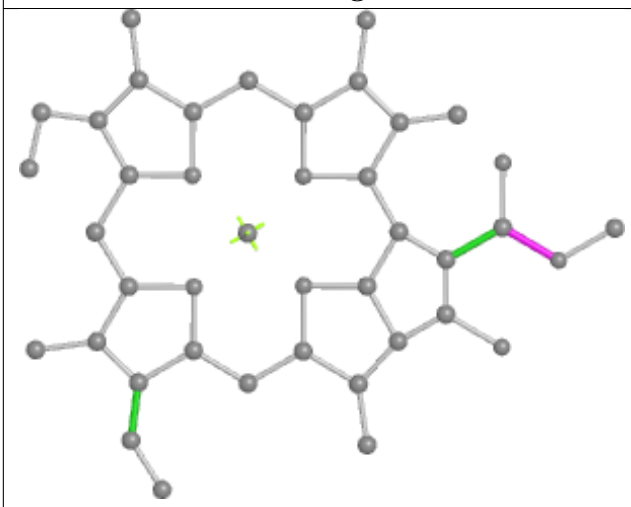
Ligand CLA b4 414



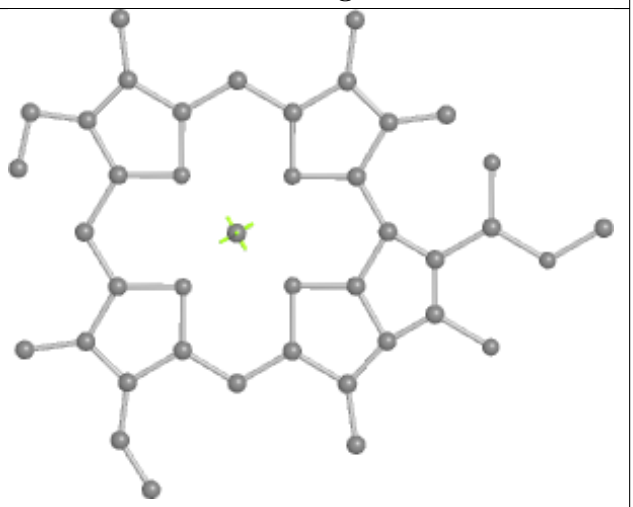
Bond lengths



Bond angles

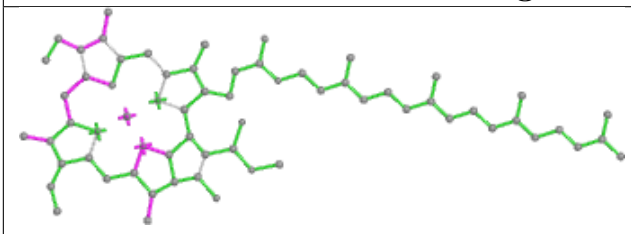


Torsions

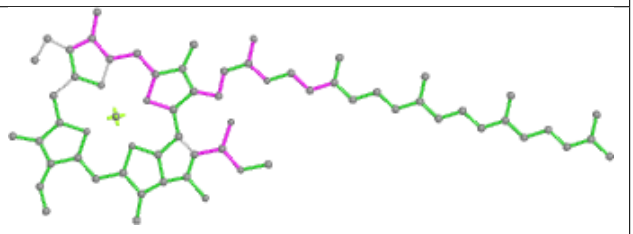


Rings

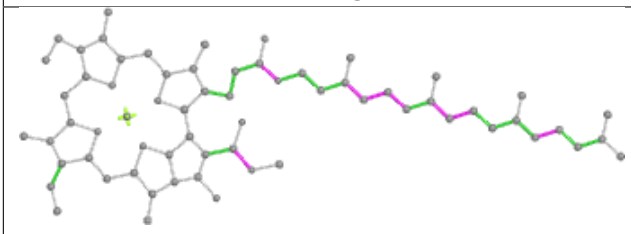
Ligand CLA cB 809



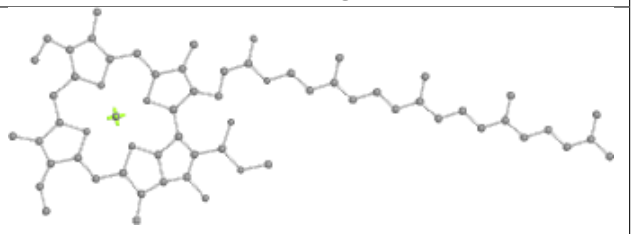
Bond lengths



Bond angles

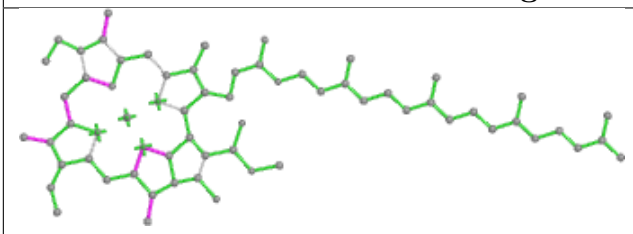


Torsions

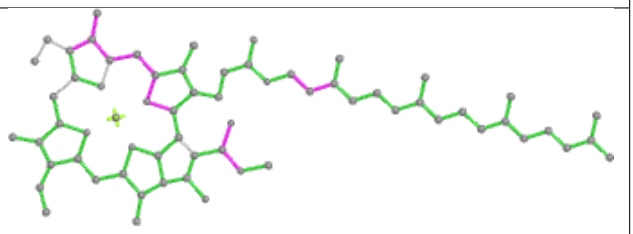


Rings

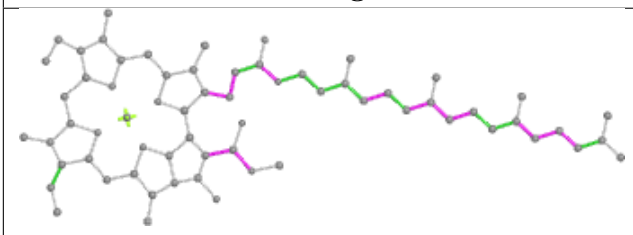
Ligand CLA c3 402



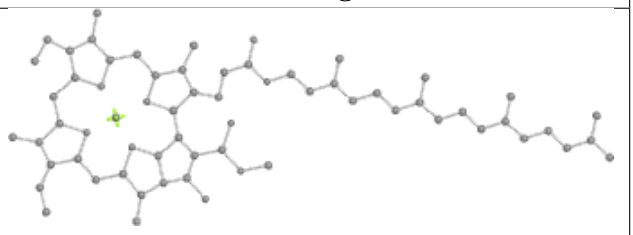
Bond lengths



Bond angles

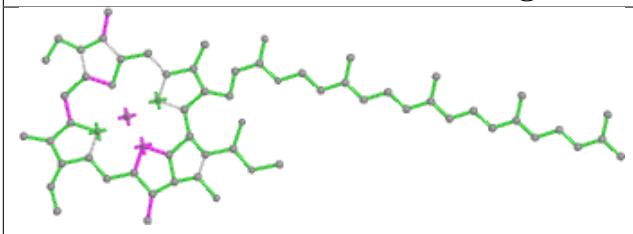


Torsions

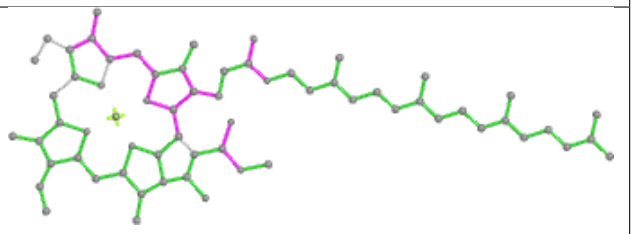


Rings

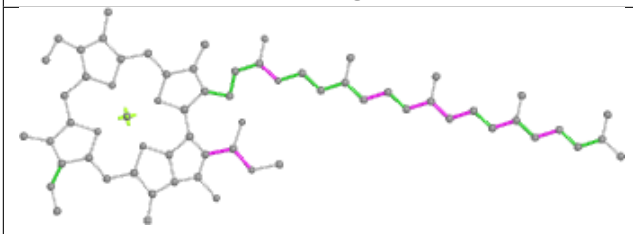
Ligand CLA b5 403



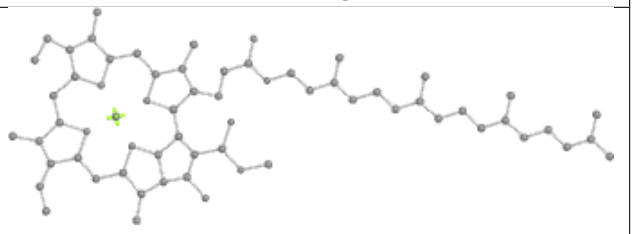
Bond lengths



Bond angles

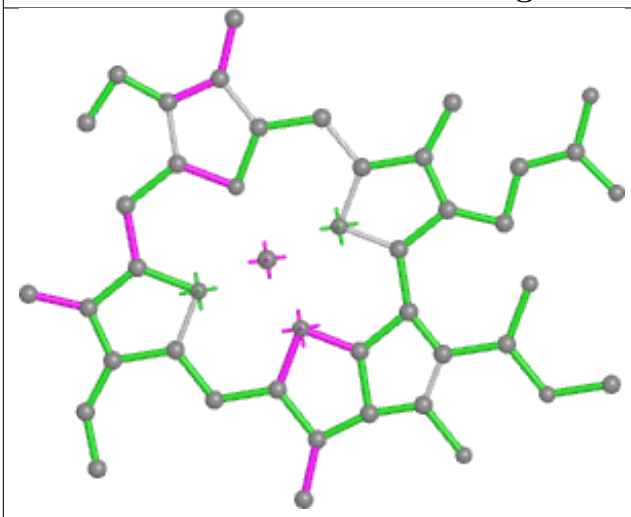


Torsions

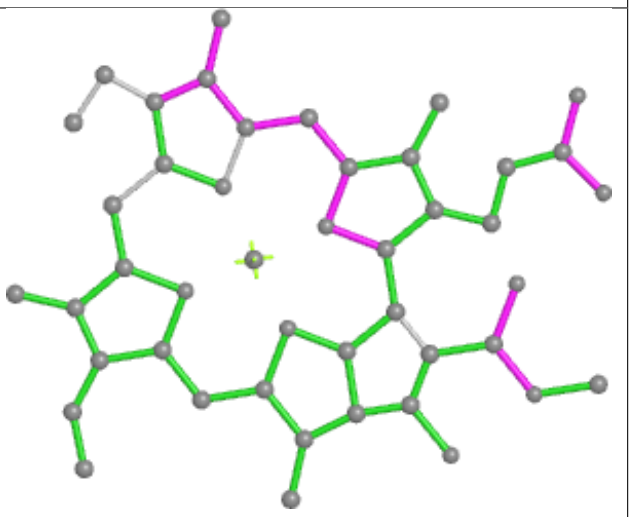


Rings

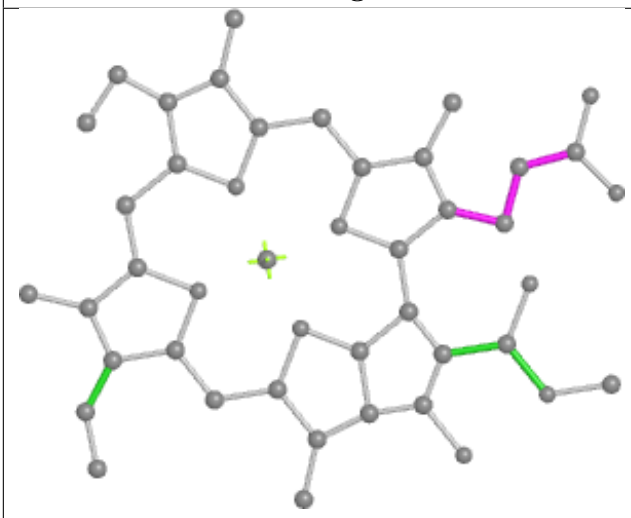
Ligand CLA aB 813



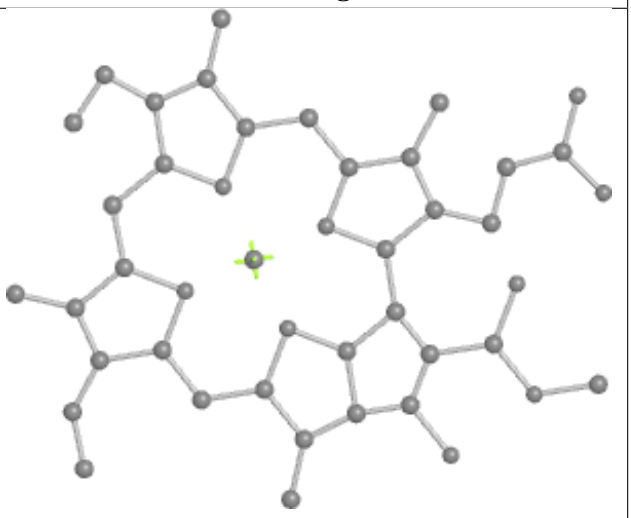
Bond lengths



Bond angles

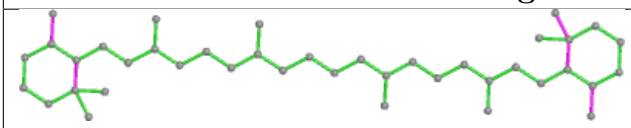


Torsions

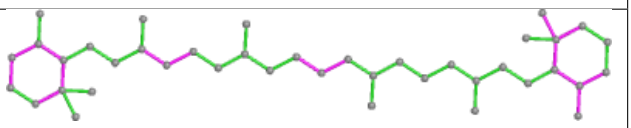


Rings

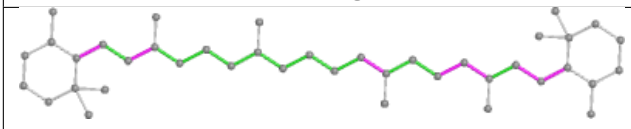
Ligand BCR a2 419



Bond lengths



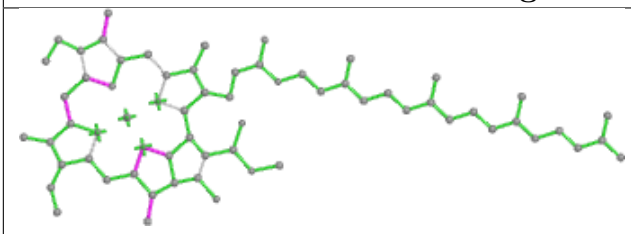
Bond angles



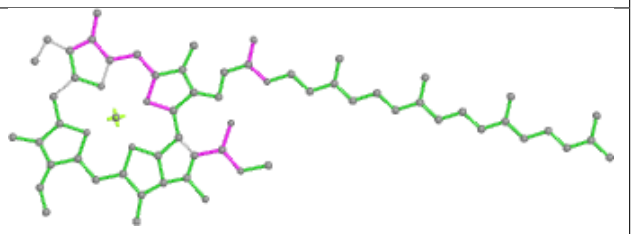
Torsions

Rings

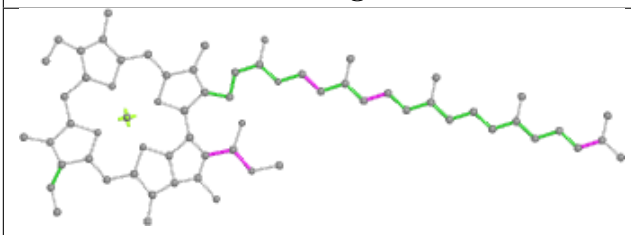
Ligand CLA a2 410



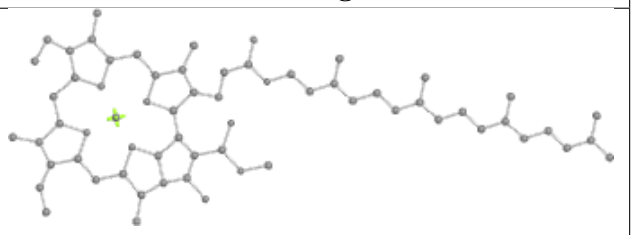
Bond lengths



Bond angles

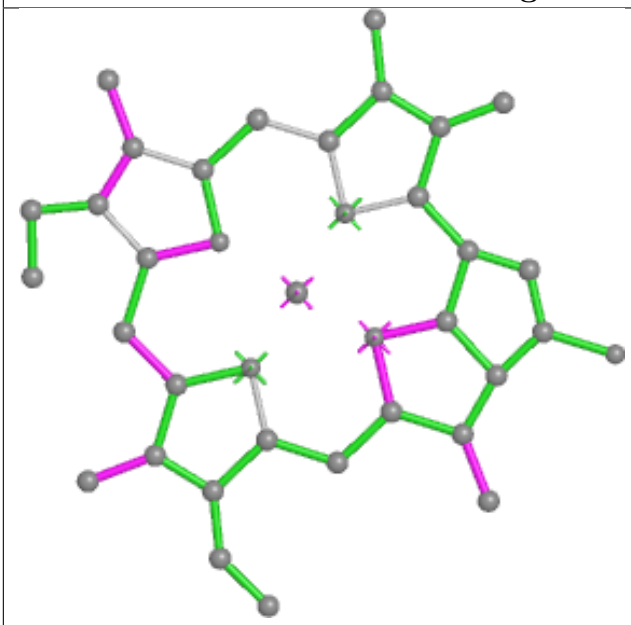


Torsions

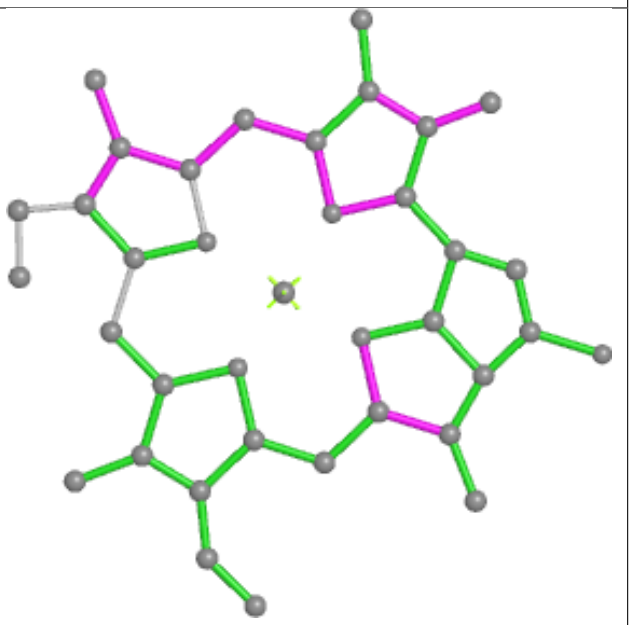


Rings

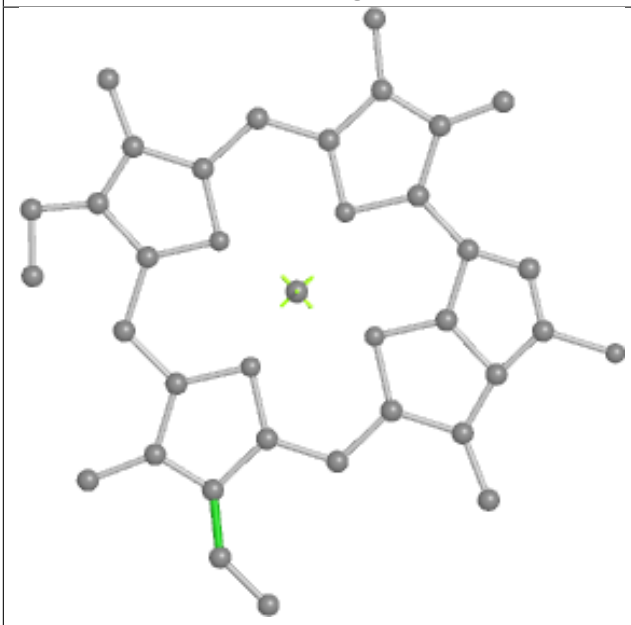
Ligand CLA cJ 102



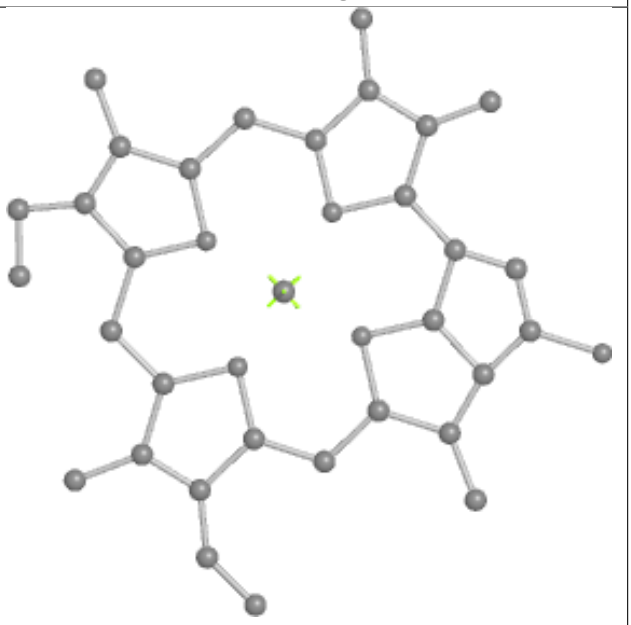
Bond lengths



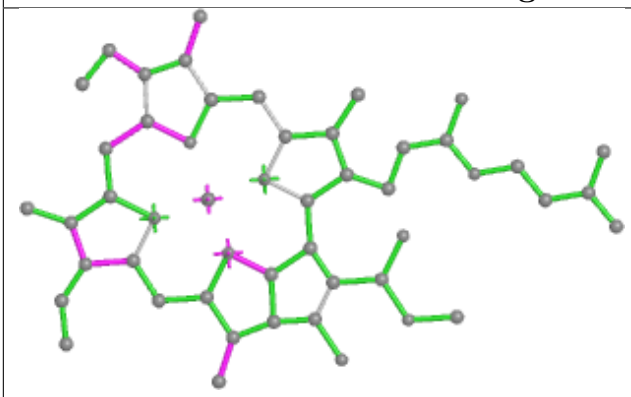
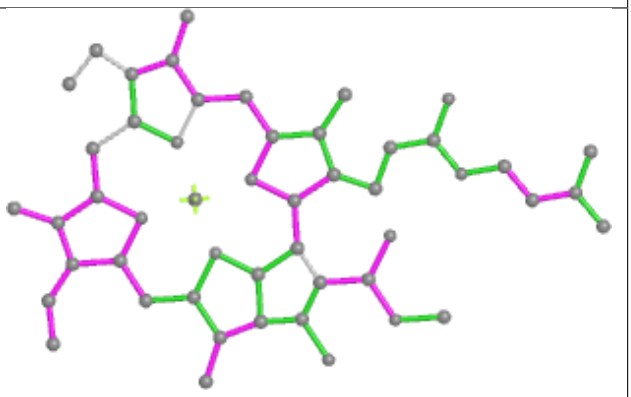
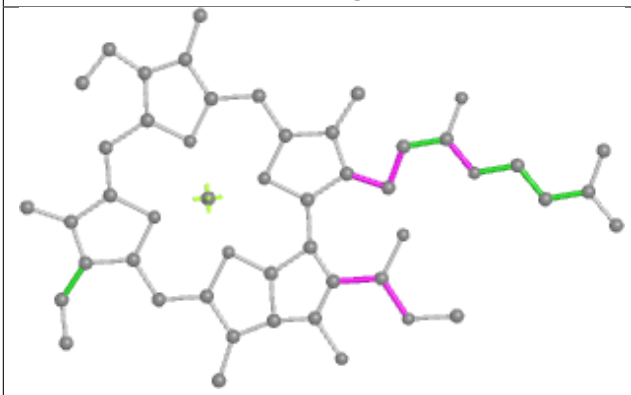
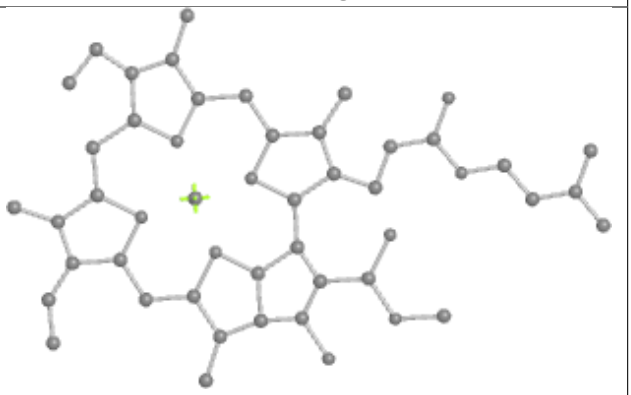
Bond angles

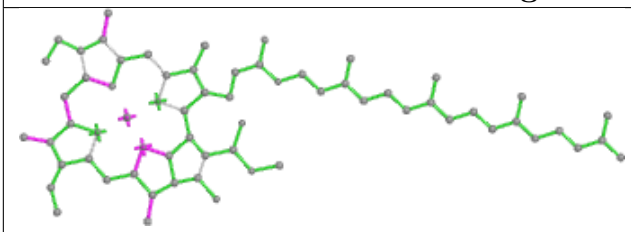
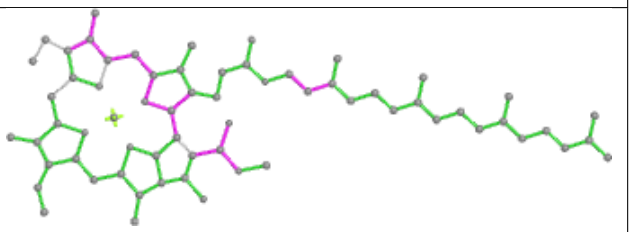
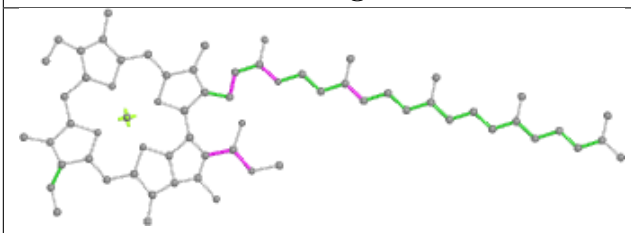
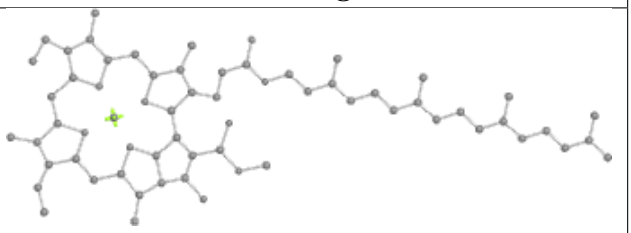


Torsions

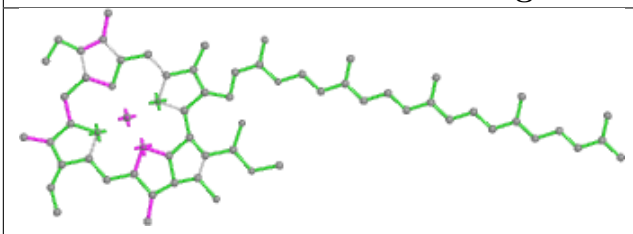


Rings

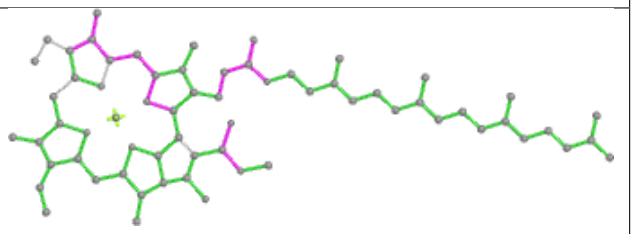
Ligand CLA b6 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c5 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

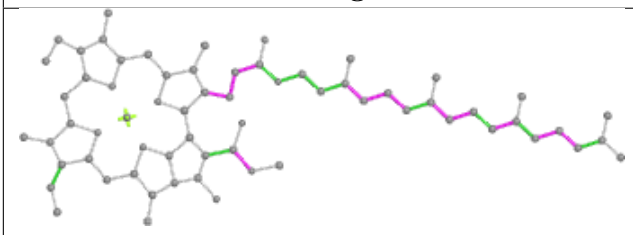
Ligand CLA cA 810



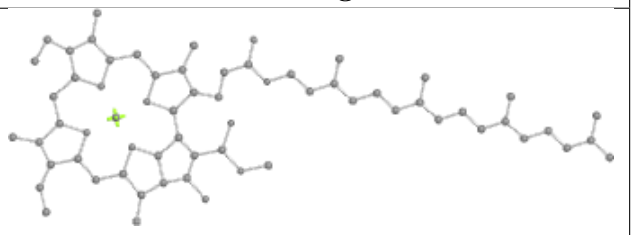
Bond lengths



Bond angles

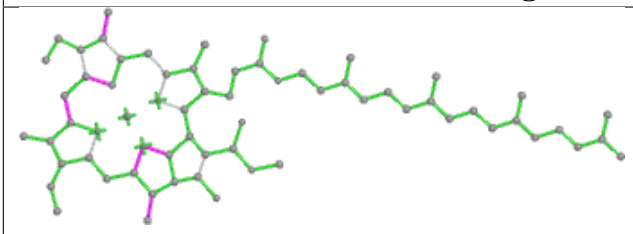


Torsions

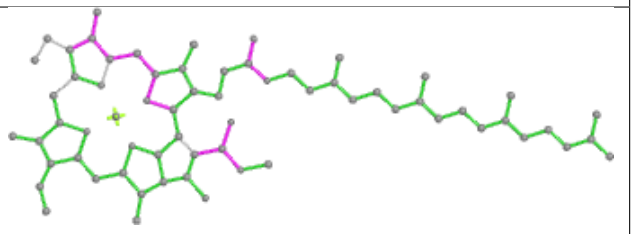


Rings

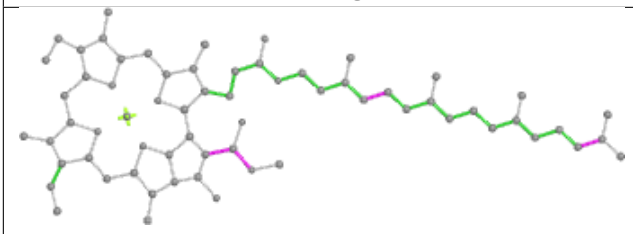
Ligand CLA c6 410



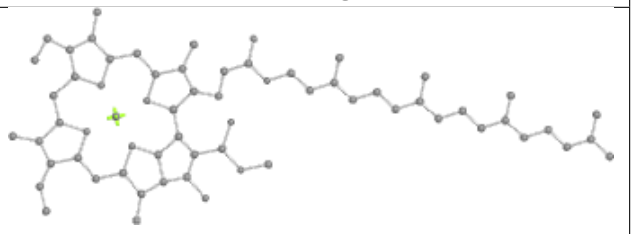
Bond lengths



Bond angles

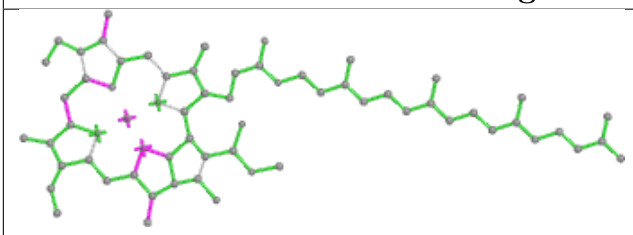


Torsions

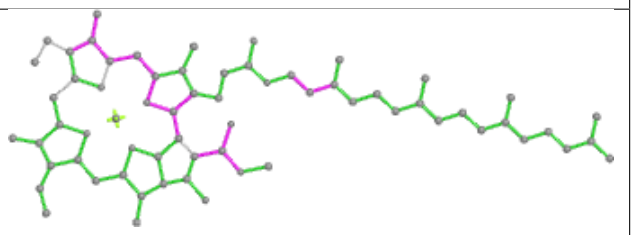


Rings

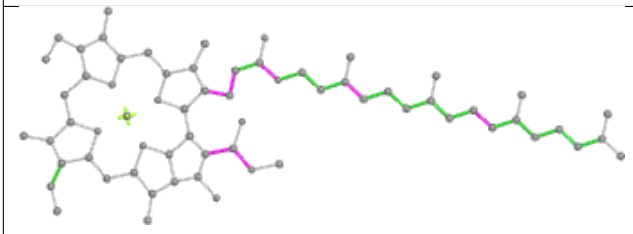
Ligand CLA b1 404



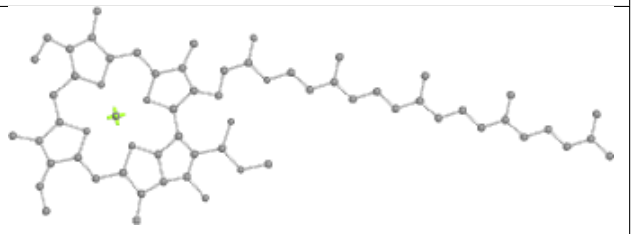
Bond lengths



Bond angles

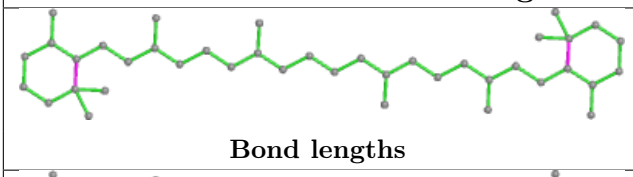


Torsions

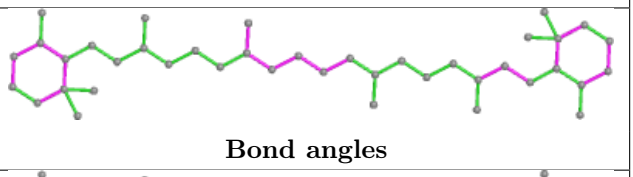


Rings

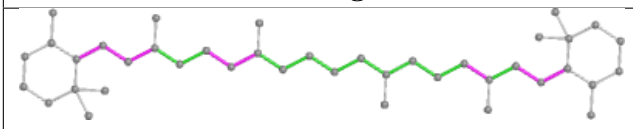
Ligand BCR b3 420



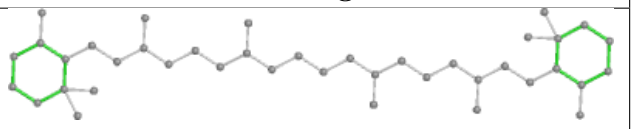
Bond lengths



Bond angles

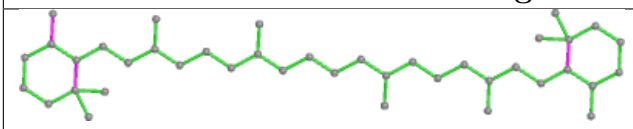


Torsions

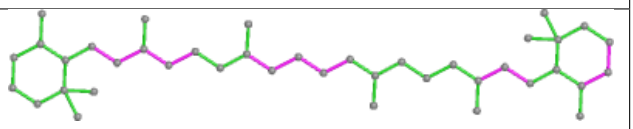


Rings

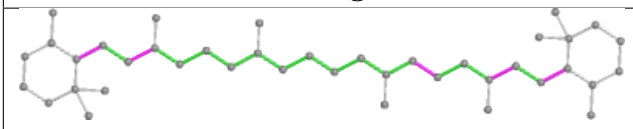
Ligand BCR cB 844



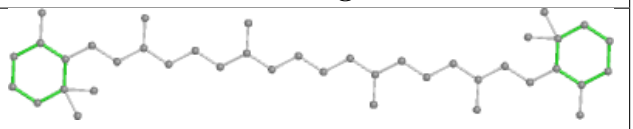
Bond lengths



Bond angles

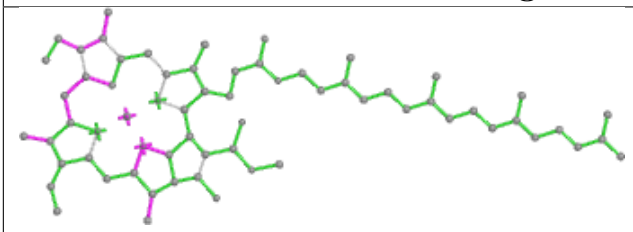


Torsions

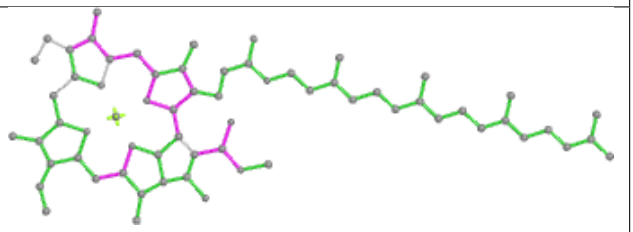


Rings

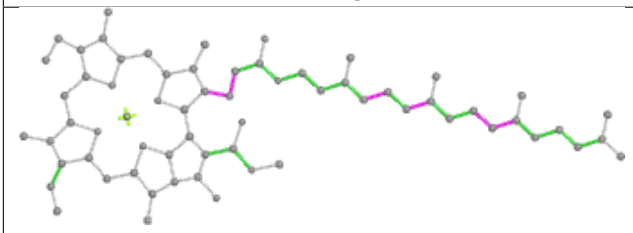
Ligand CLA cL 202



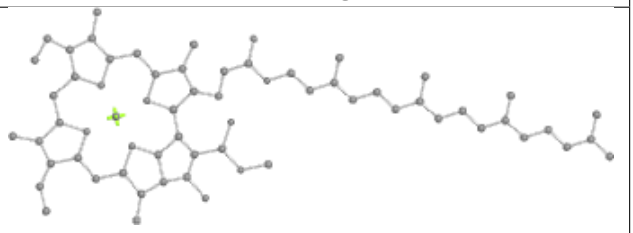
Bond lengths



Bond angles

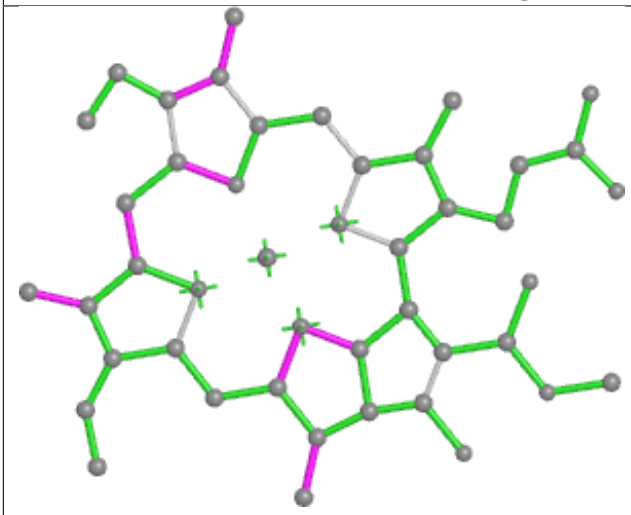


Torsions

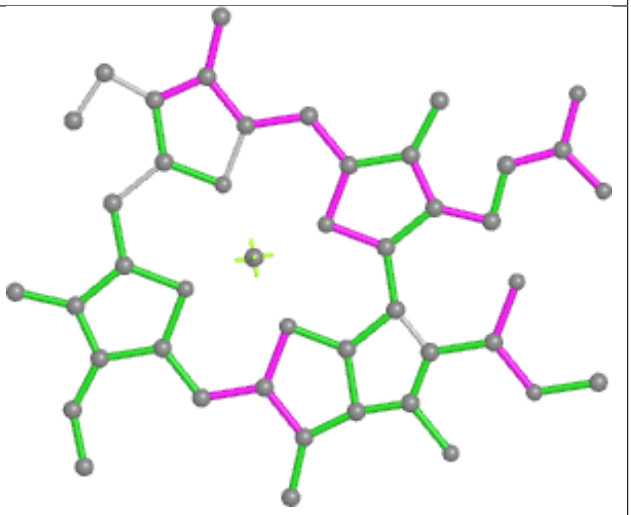


Rings

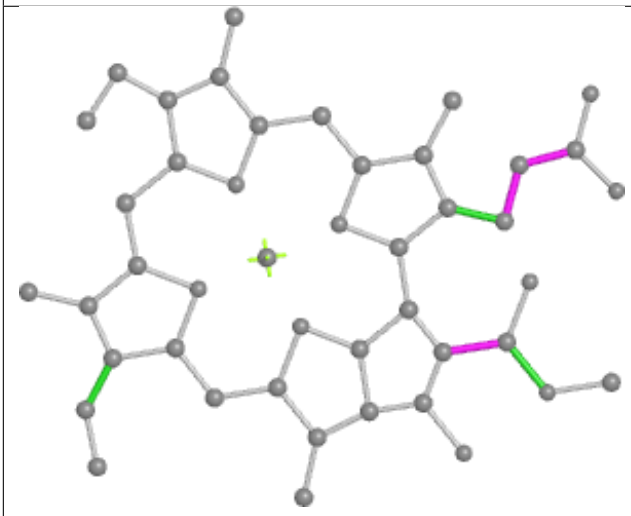
Ligand CLA aB 824



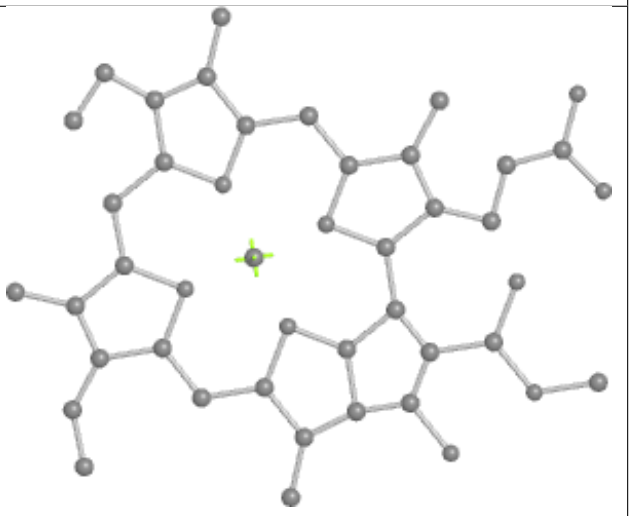
Bond lengths



Bond angles

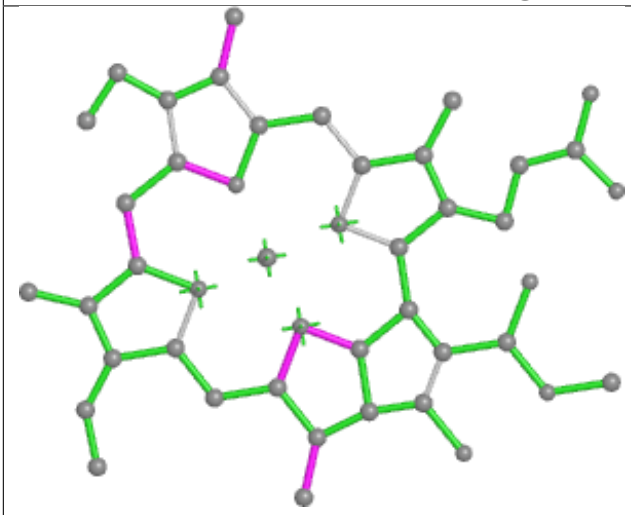


Torsions

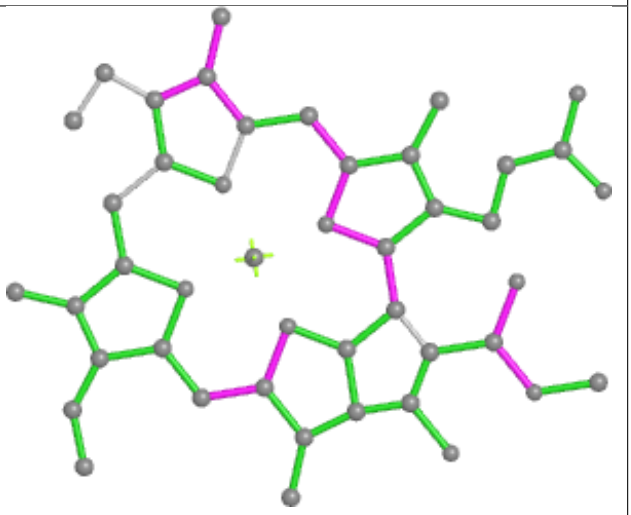


Rings

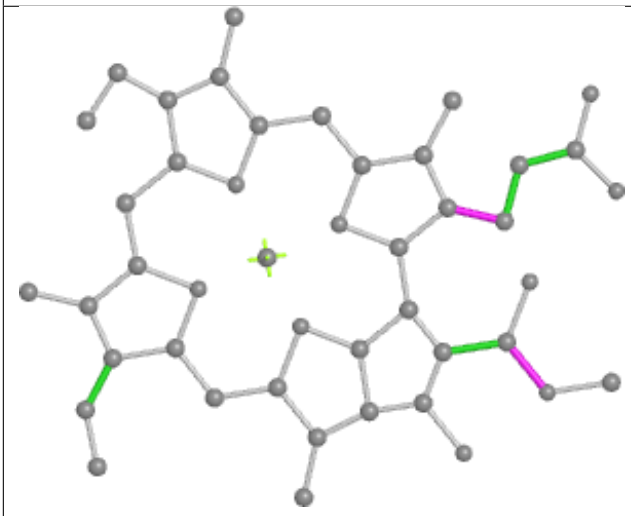
Ligand CLA cB 812



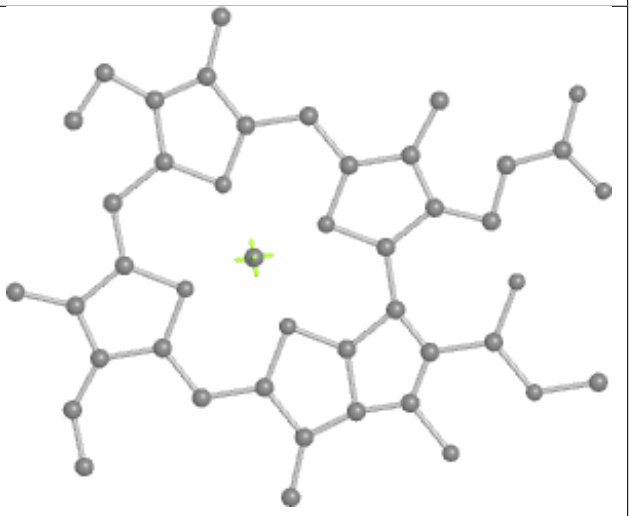
Bond lengths



Bond angles

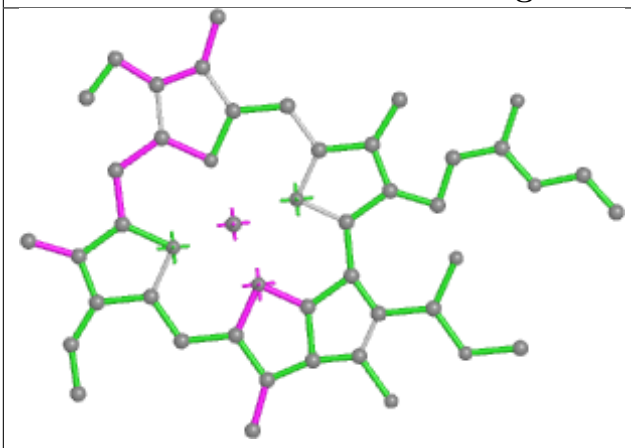


Torsions

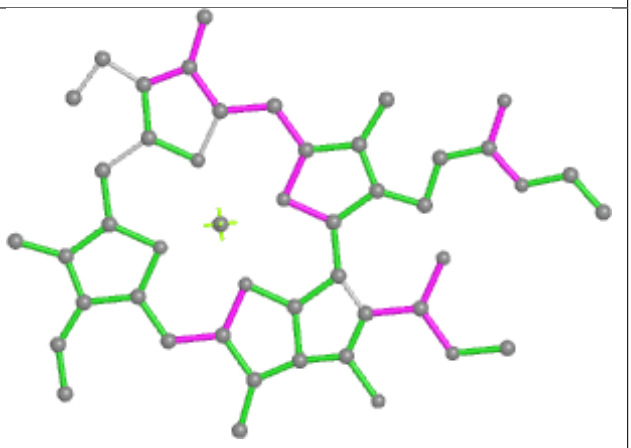


Rings

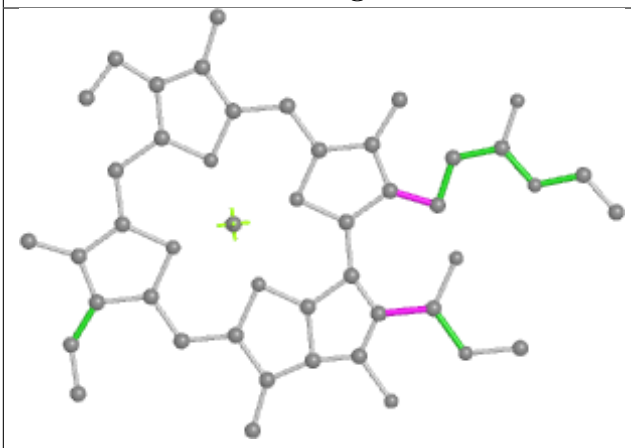
Ligand CLA aB 838



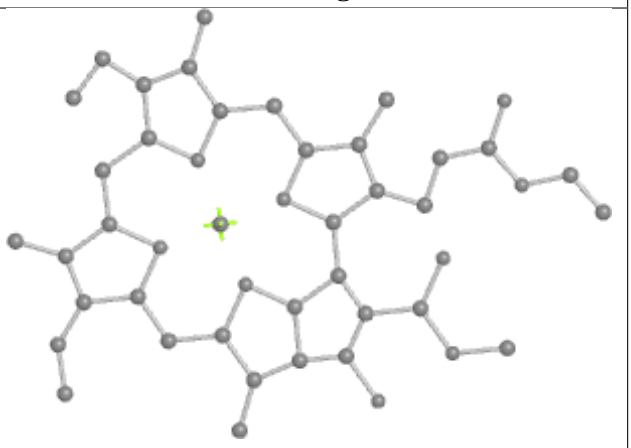
Bond lengths



Bond angles

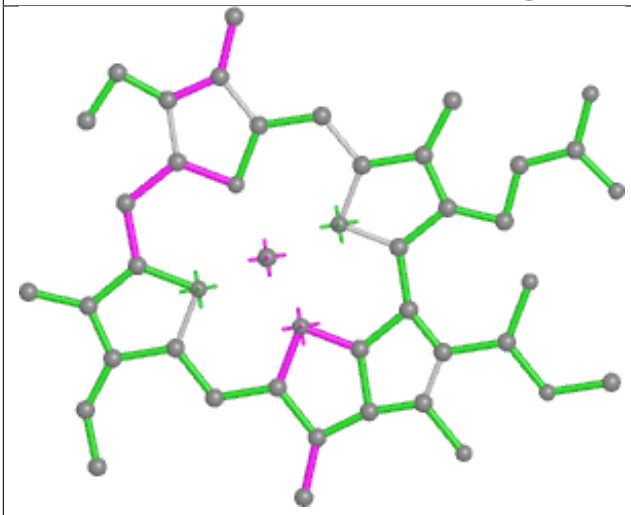


Torsions

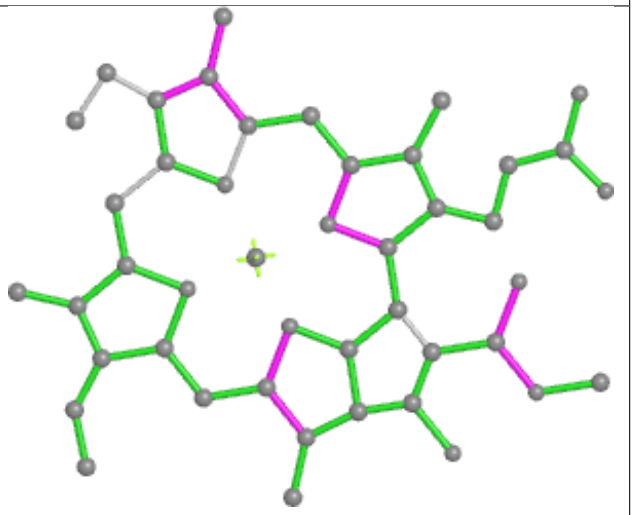


Rings

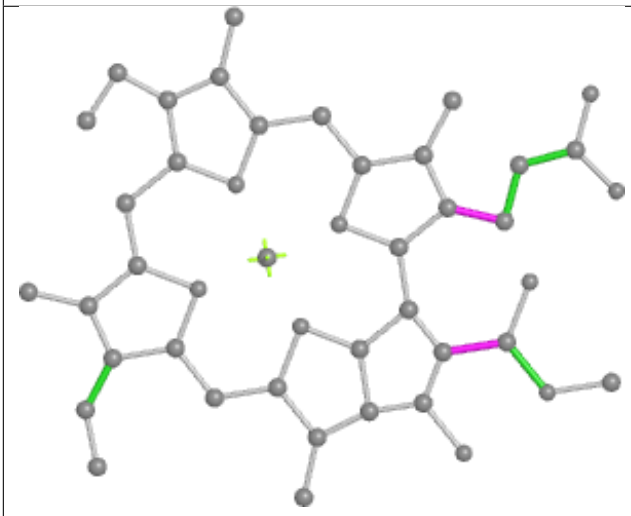
Ligand CLA c2 414



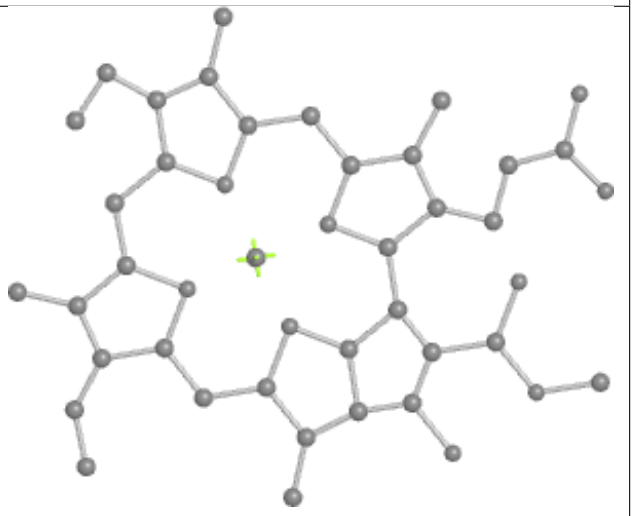
Bond lengths



Bond angles

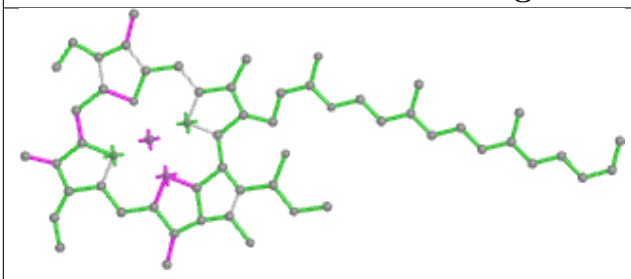


Torsions

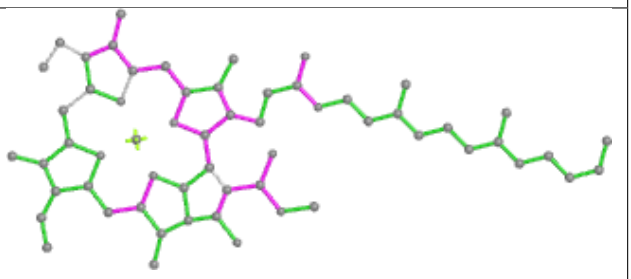


Rings

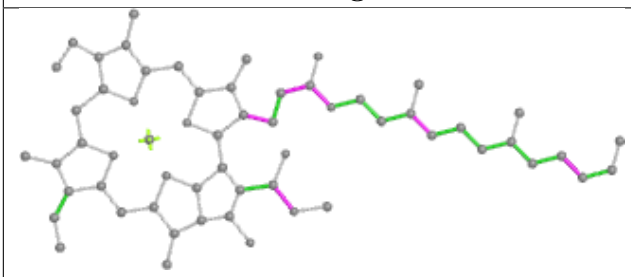
Ligand CLA bB 818



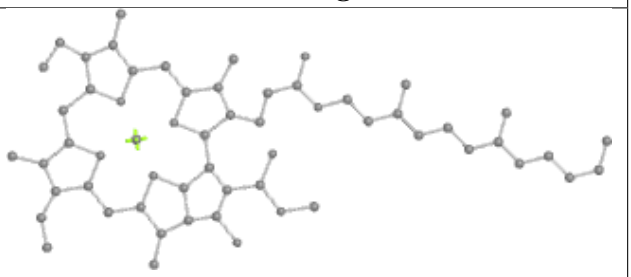
Bond lengths



Bond angles

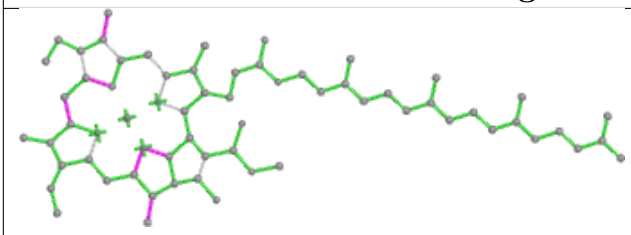


Torsions

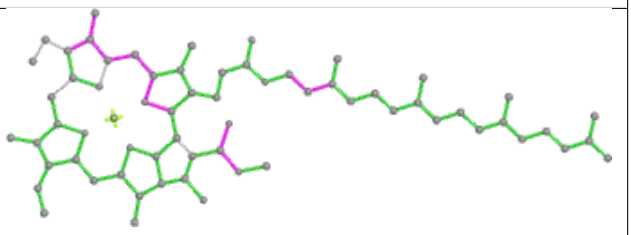


Rings

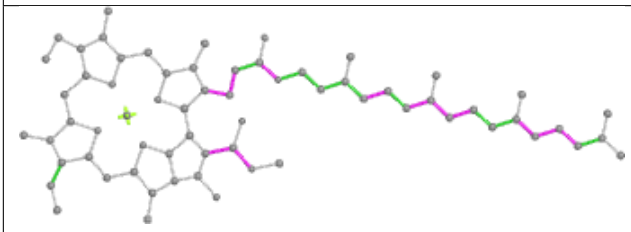
Ligand CLA b2 402



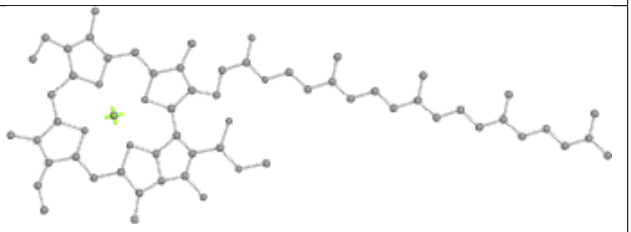
Bond lengths



Bond angles

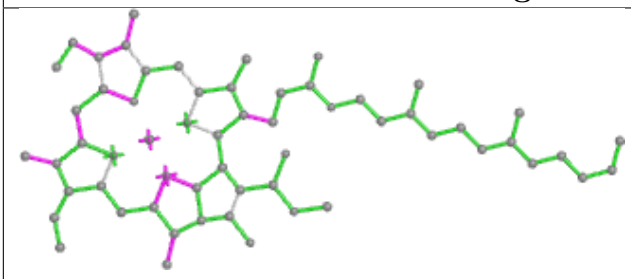


Torsions

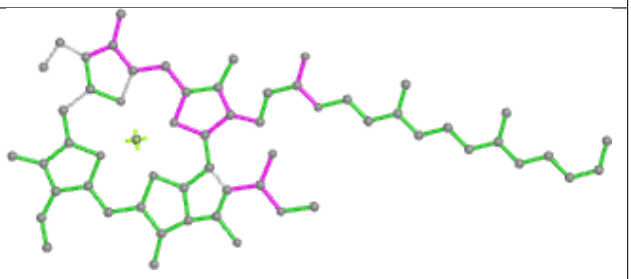


Rings

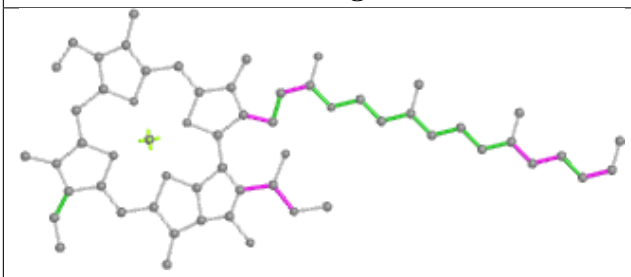
Ligand CLA bA 805



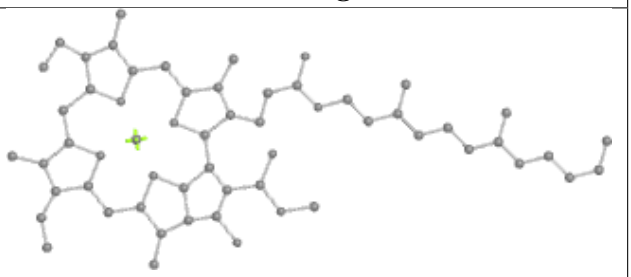
Bond lengths



Bond angles

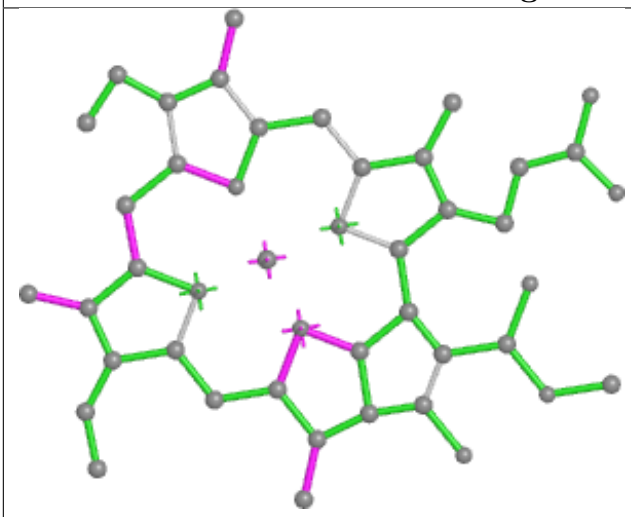


Torsions

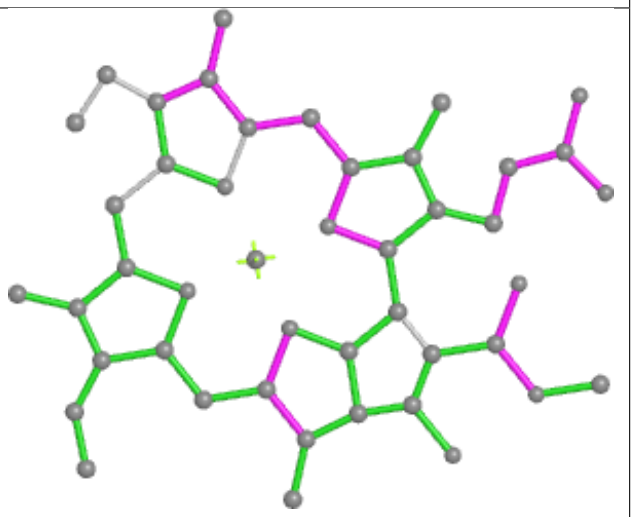


Rings

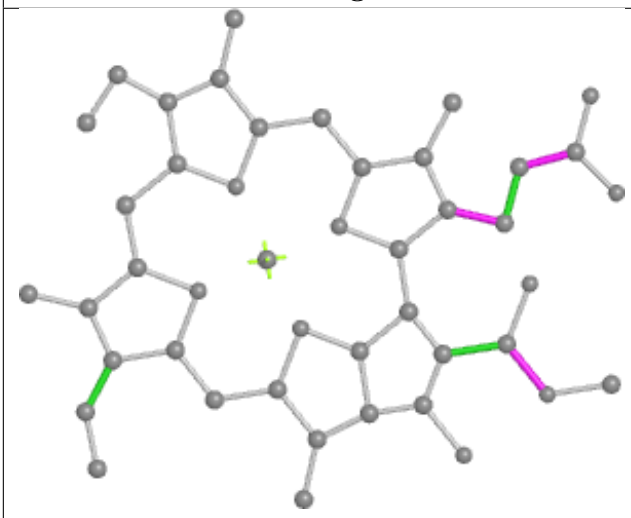
Ligand CLA c5 408



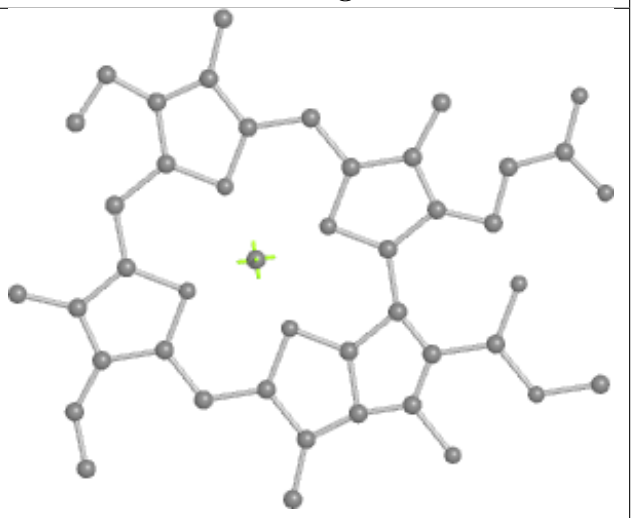
Bond lengths



Bond angles

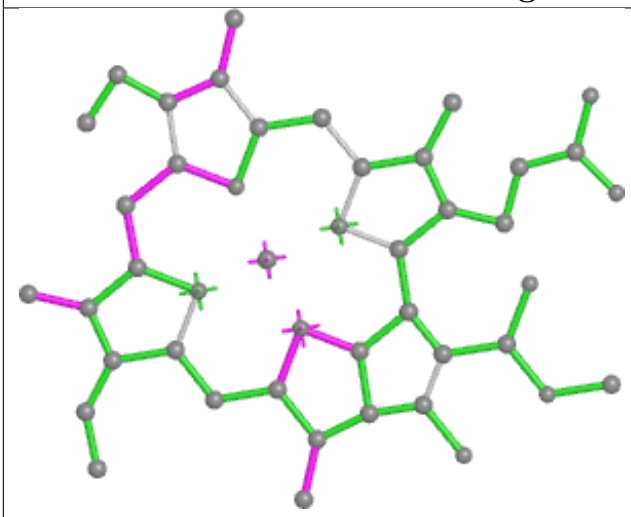


Torsions

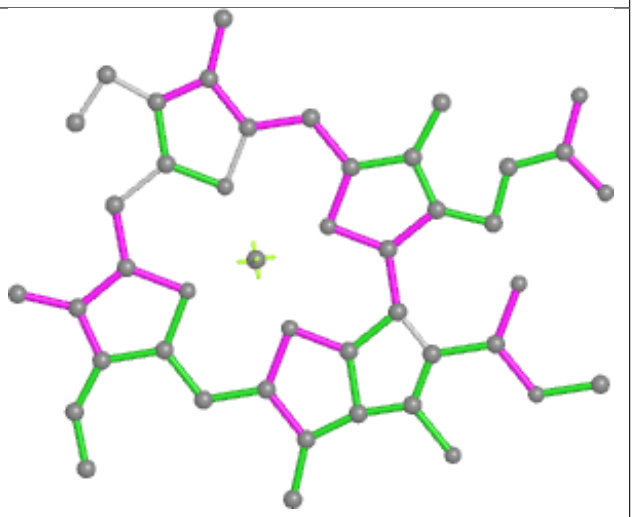


Rings

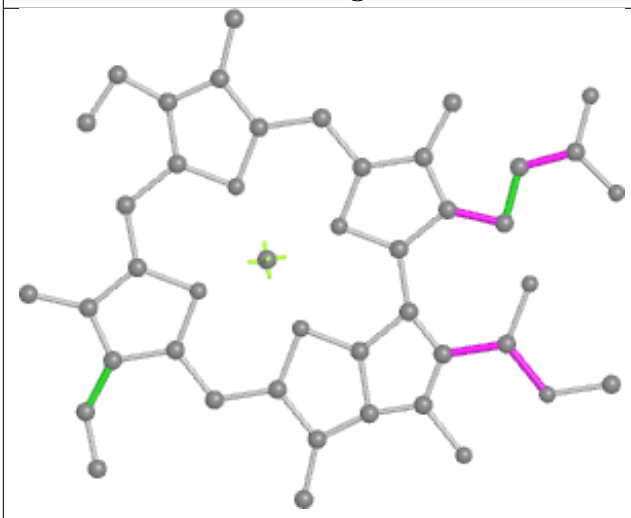
Ligand CLA b6 413



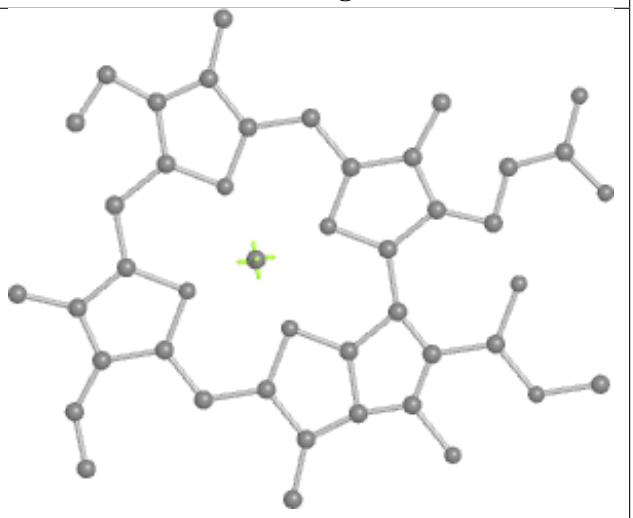
Bond lengths



Bond angles

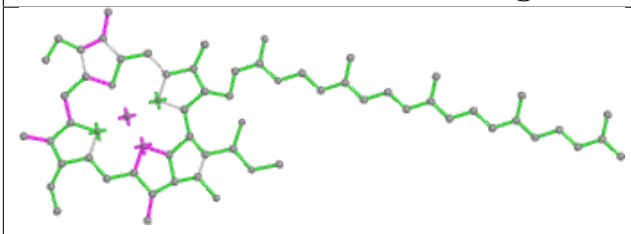


Torsions

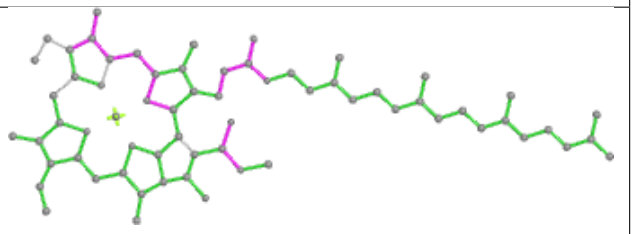


Rings

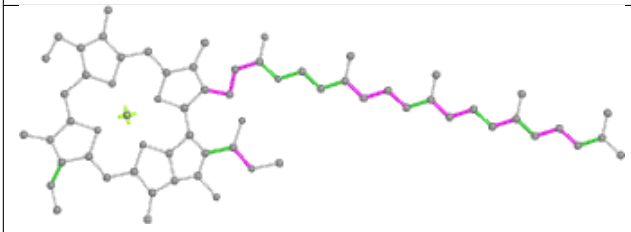
Ligand CLA aA 810



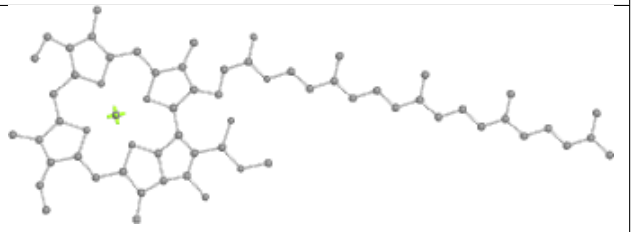
Bond lengths



Bond angles

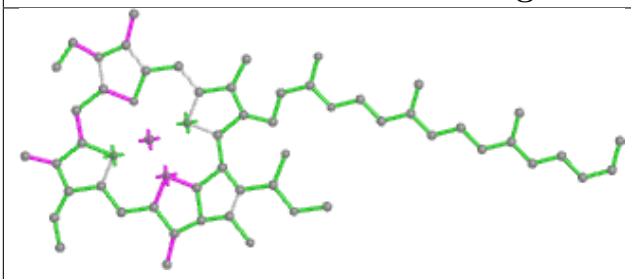


Torsions

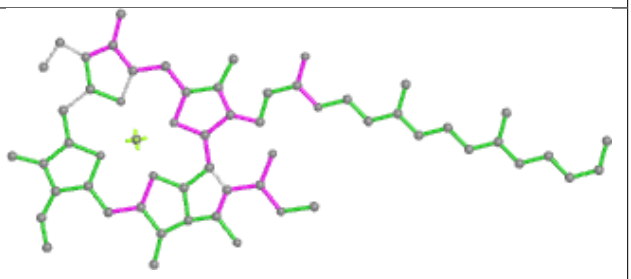


Rings

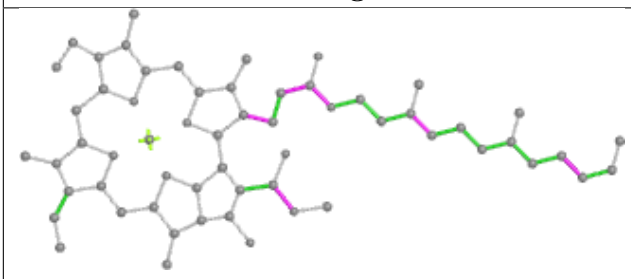
Ligand CLA cB 818



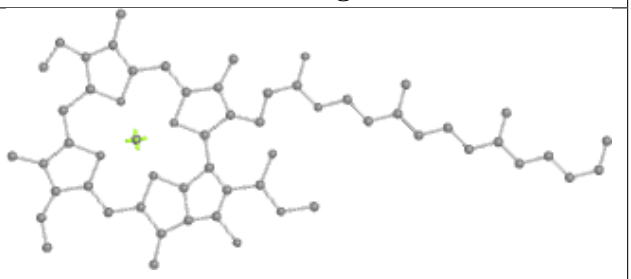
Bond lengths



Bond angles

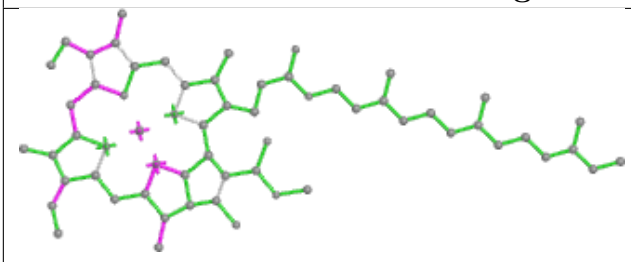


Torsions

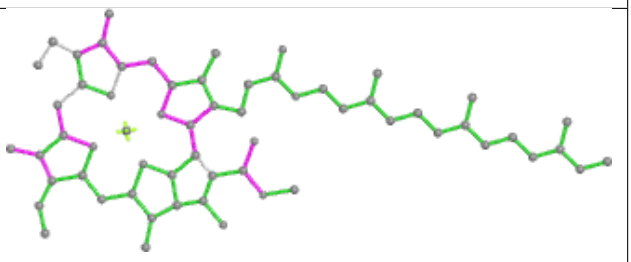


Rings

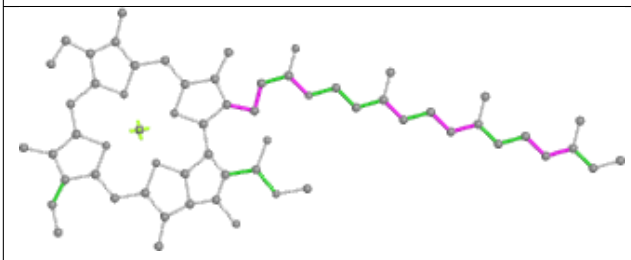
Ligand CLA bA 821



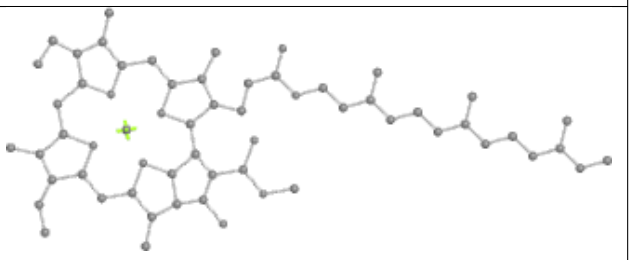
Bond lengths



Bond angles

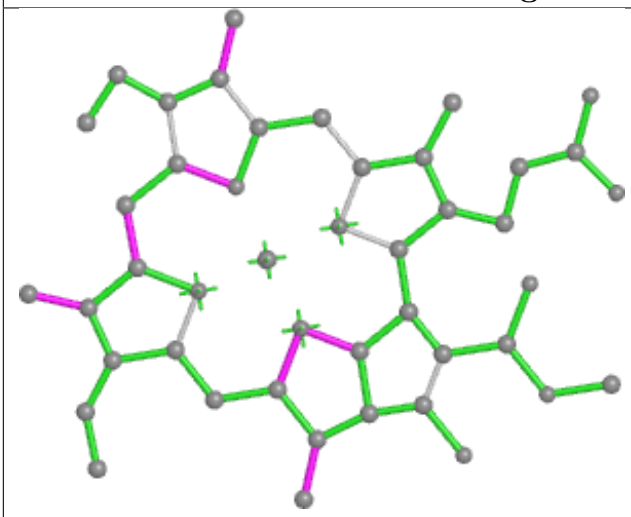


Torsions

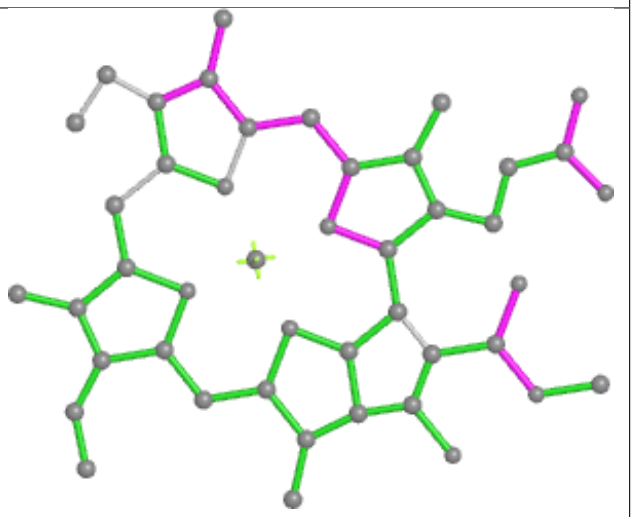


Rings

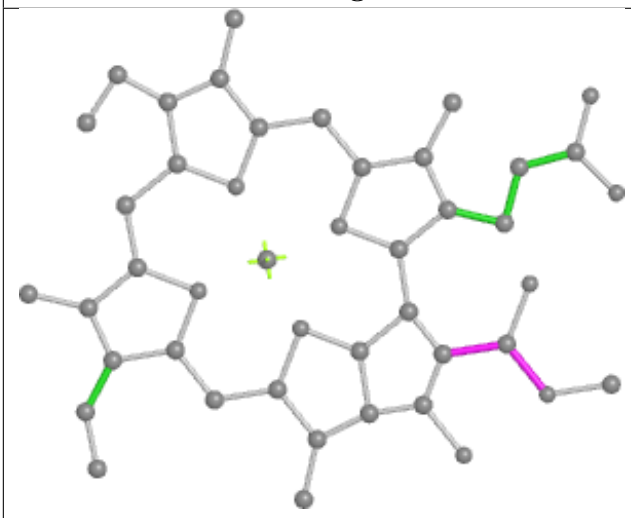
Ligand CLA c3 406



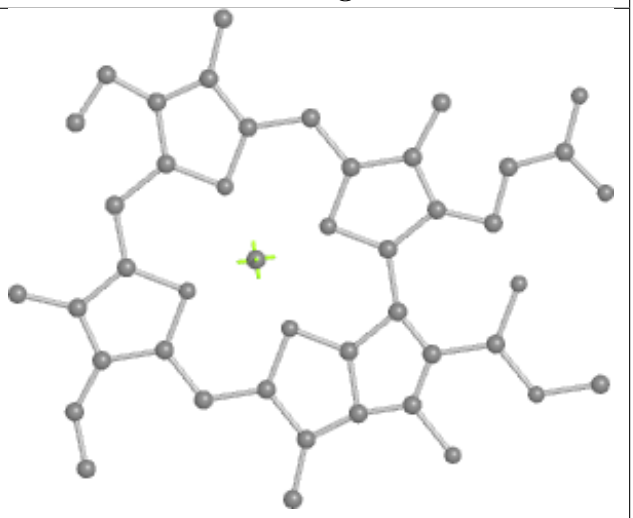
Bond lengths



Bond angles

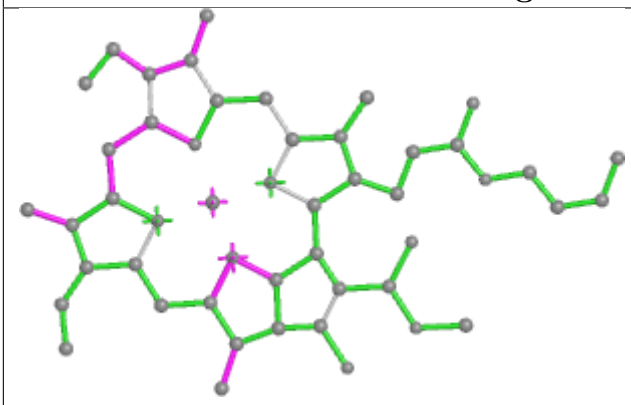


Torsions

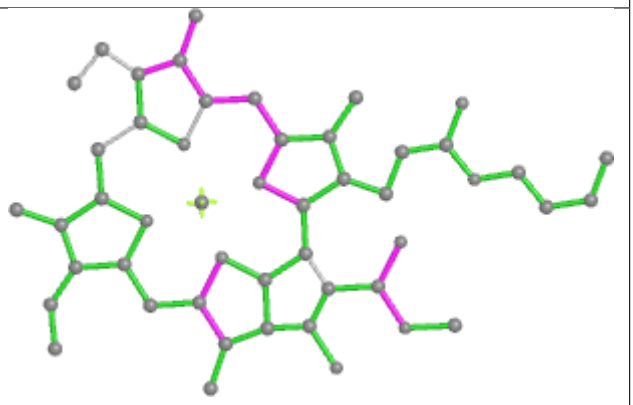


Rings

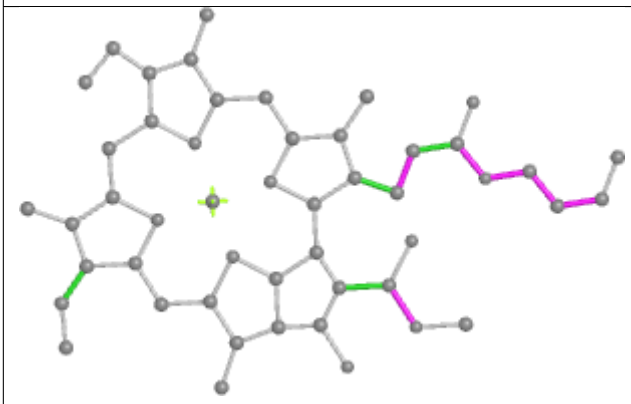
Ligand CLA aB 832



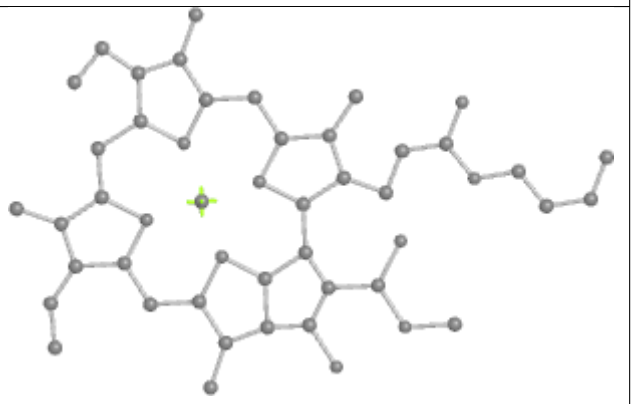
Bond lengths



Bond angles

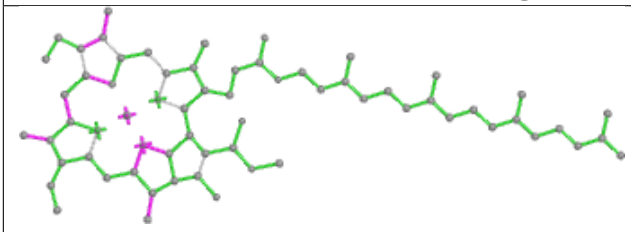


Torsions

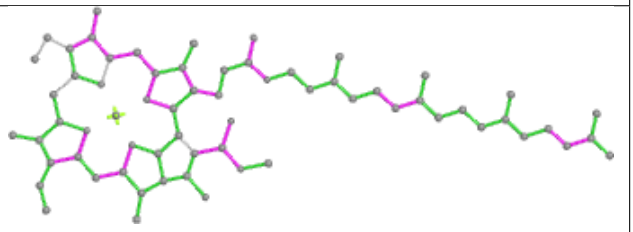


Rings

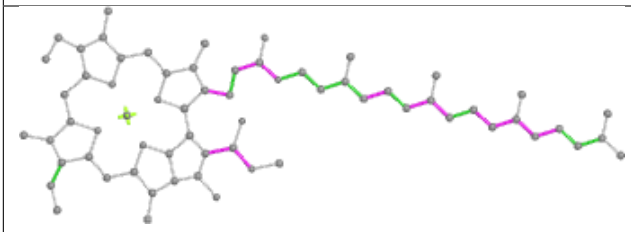
Ligand CLA aB 833



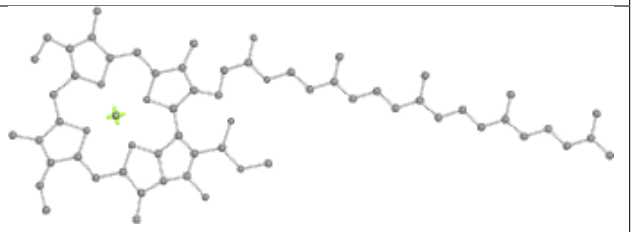
Bond lengths



Bond angles

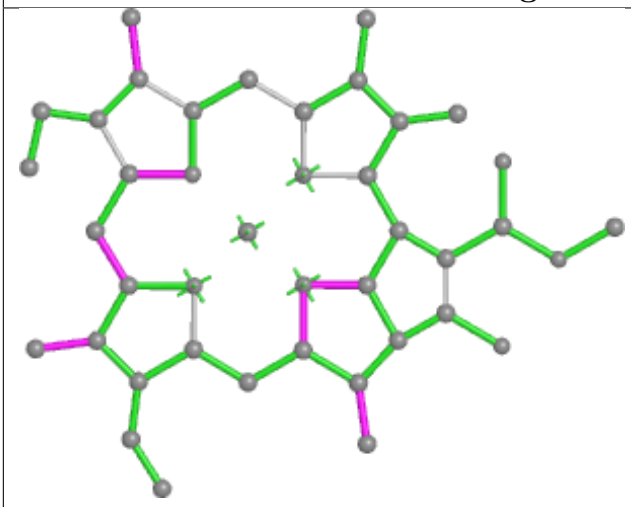


Torsions

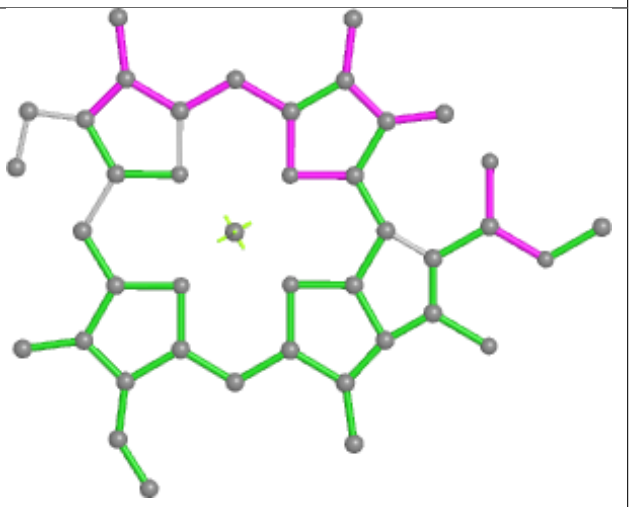


Rings

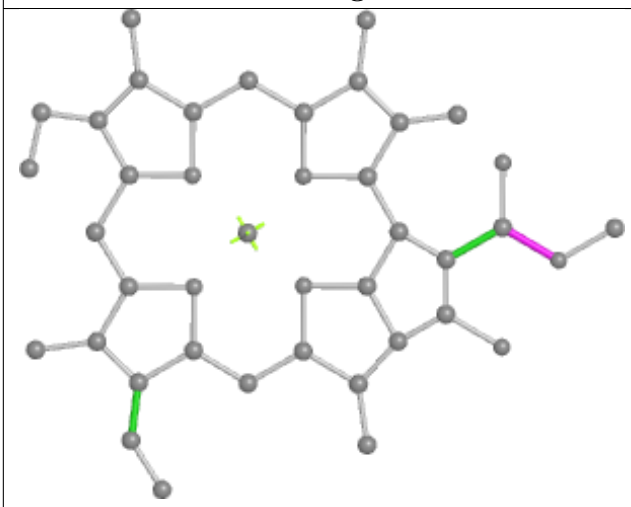
Ligand CLA a1 413



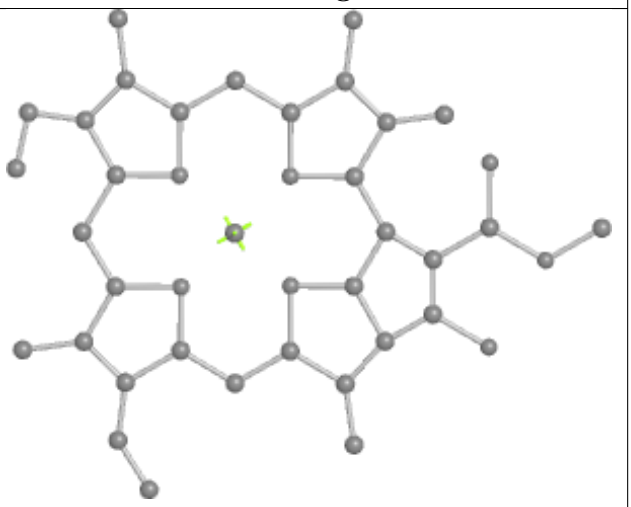
Bond lengths



Bond angles

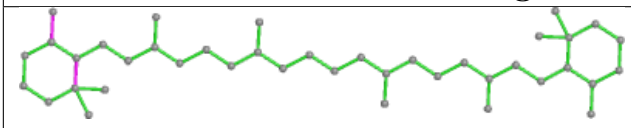


Torsions

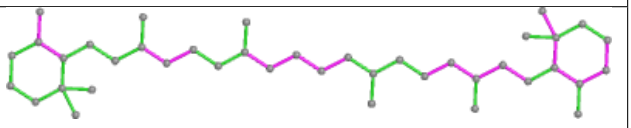


Rings

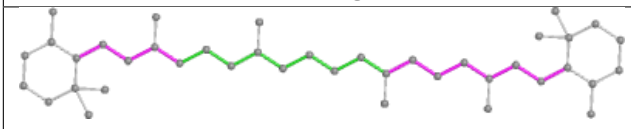
Ligand BCR cA 849



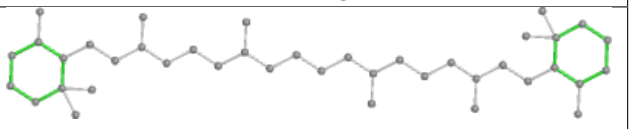
Bond lengths



Bond angles

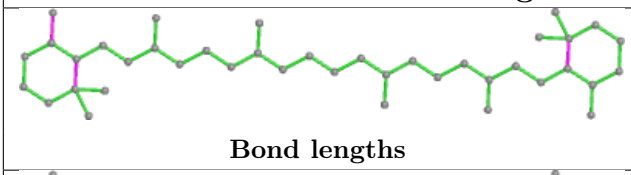


Torsions

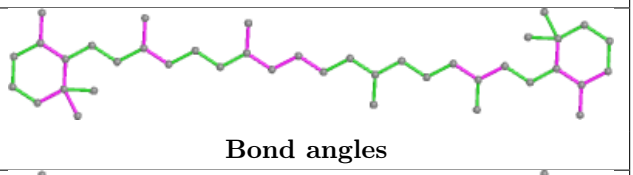


Rings

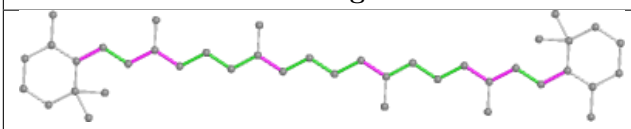
Ligand BCR cF 204



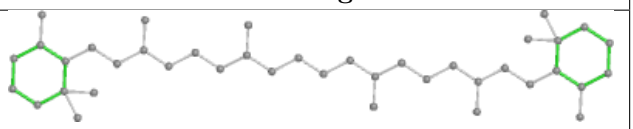
Bond lengths



Bond angles

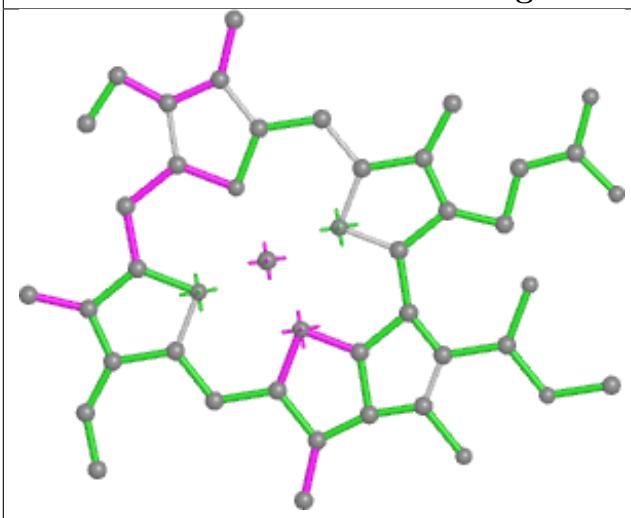


Torsions

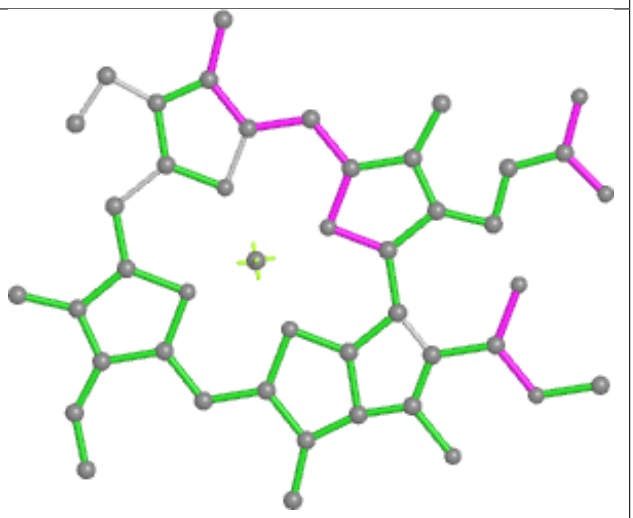


Rings

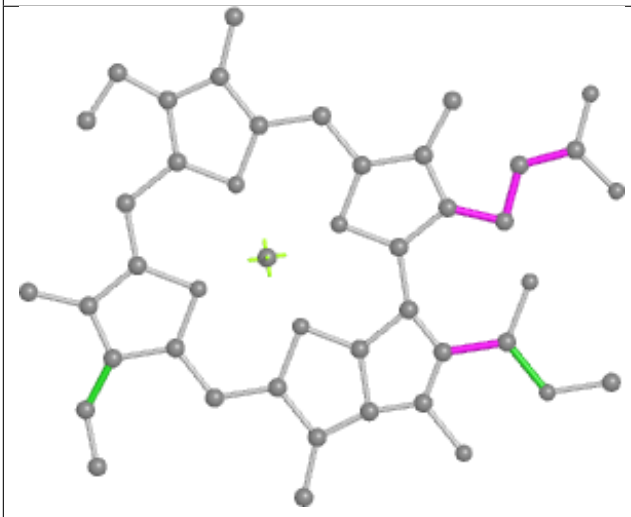
Ligand CLA aB 831



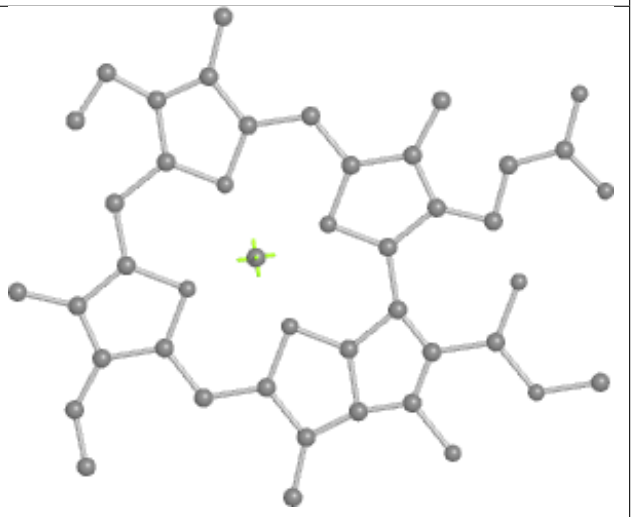
Bond lengths



Bond angles

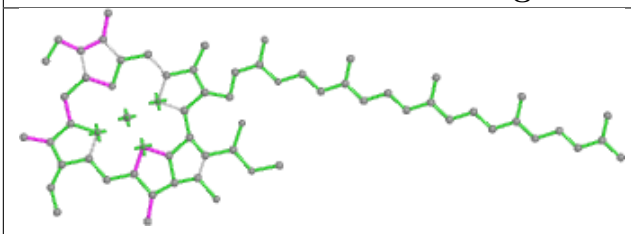


Torsions

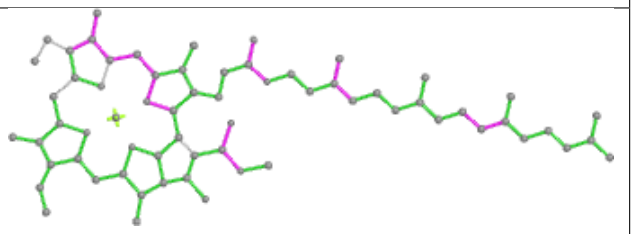


Rings

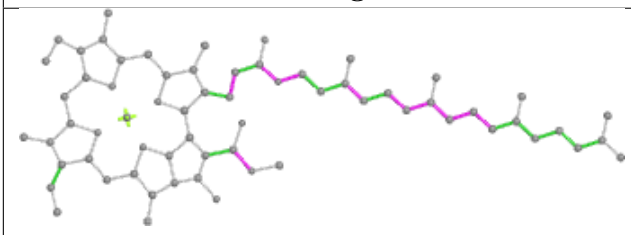
Ligand CLA bA 841



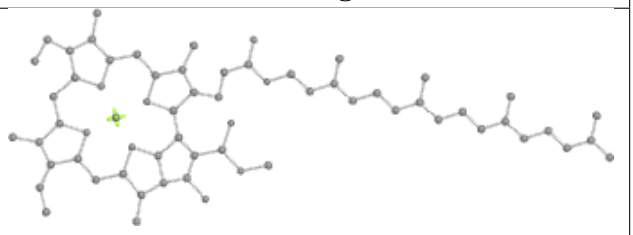
Bond lengths



Bond angles

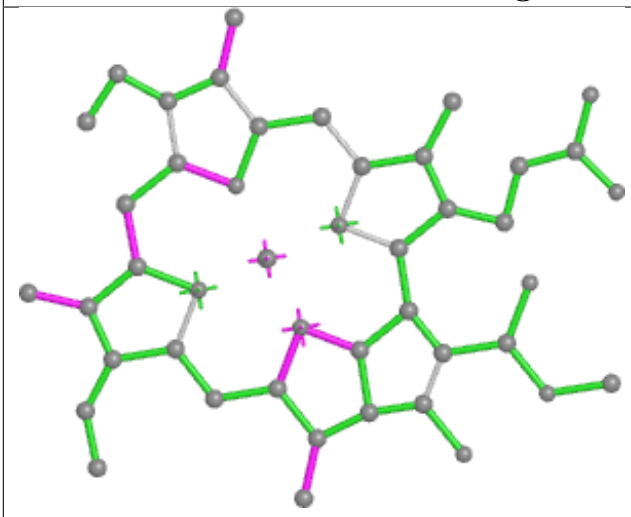


Torsions

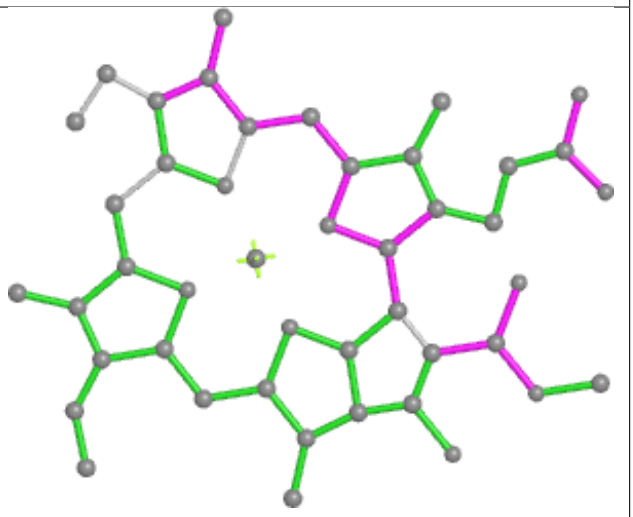


Rings

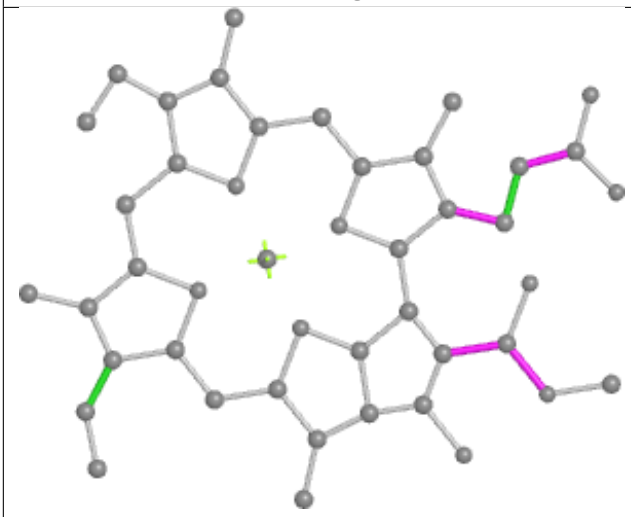
Ligand CLA aK 102



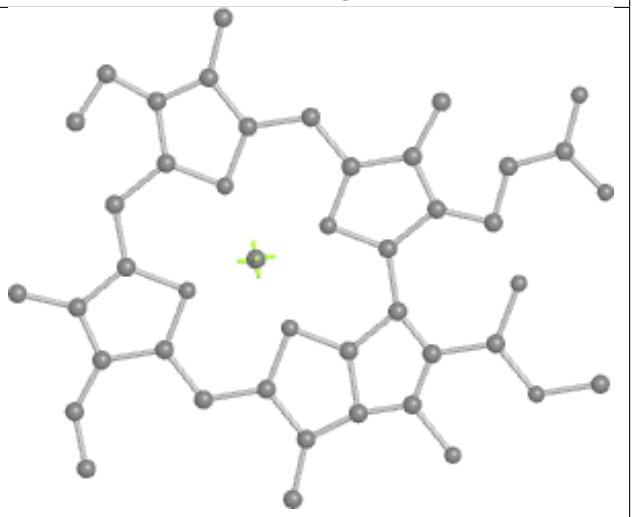
Bond lengths



Bond angles

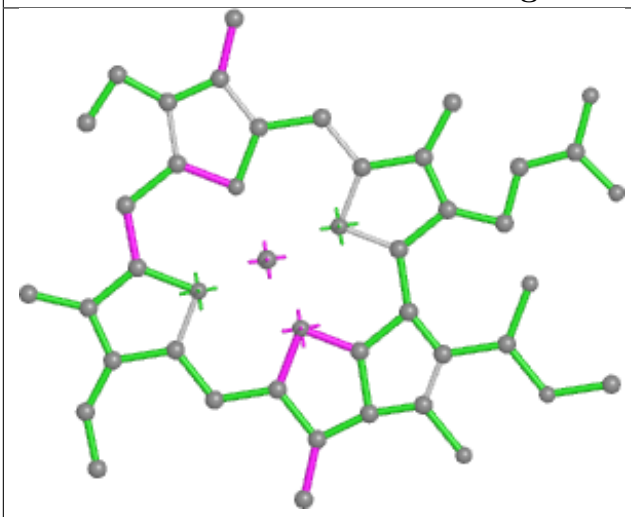


Torsions

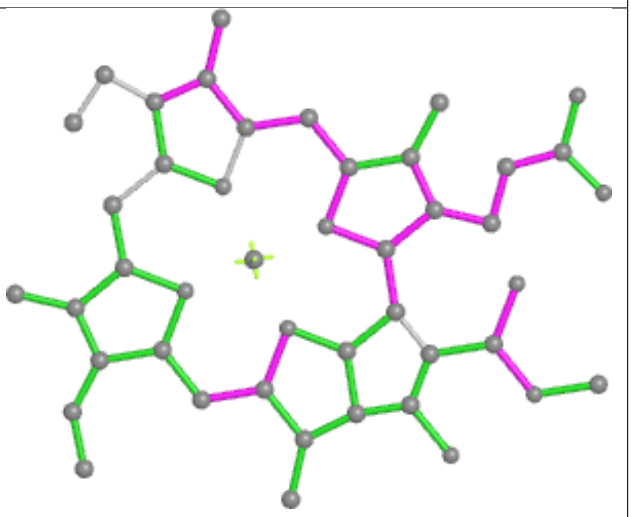


Rings

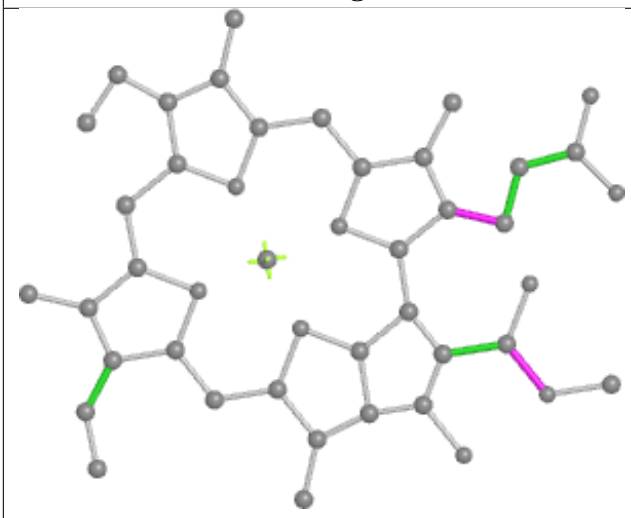
Ligand CLA c6 412



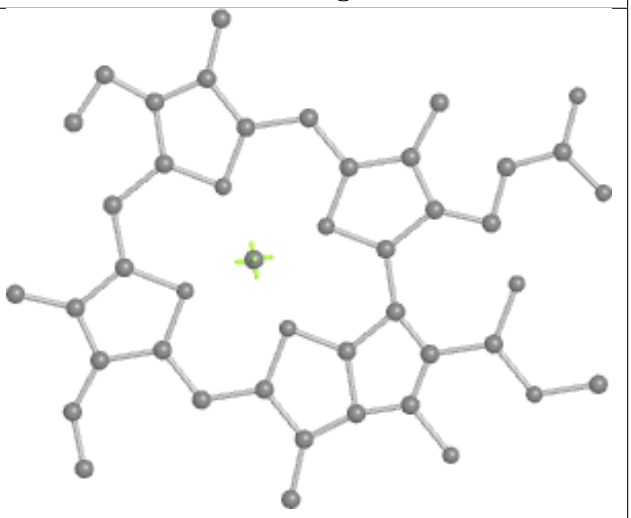
Bond lengths



Bond angles

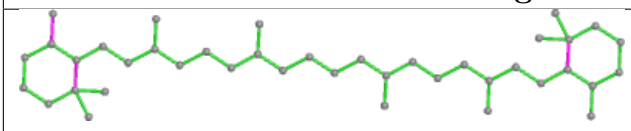


Torsions

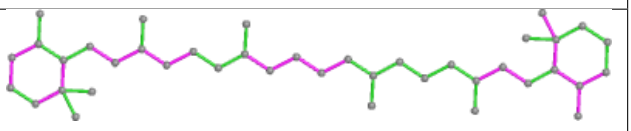


Rings

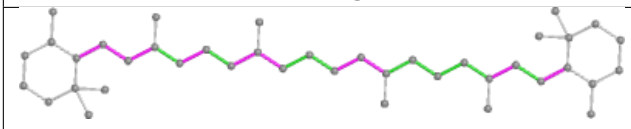
Ligand BCR bL 206



Bond lengths



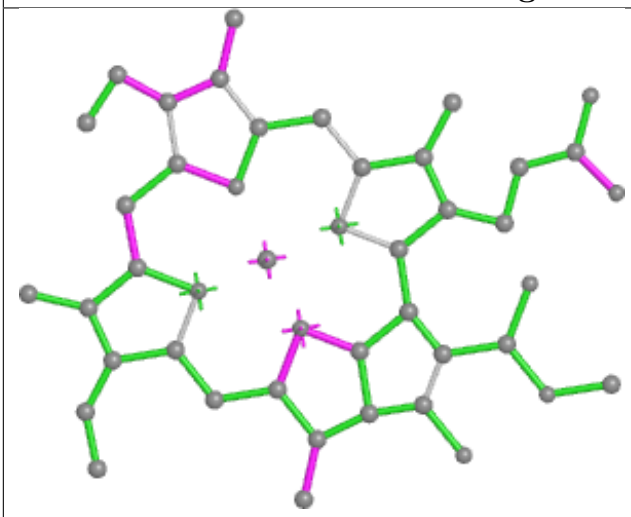
Bond angles



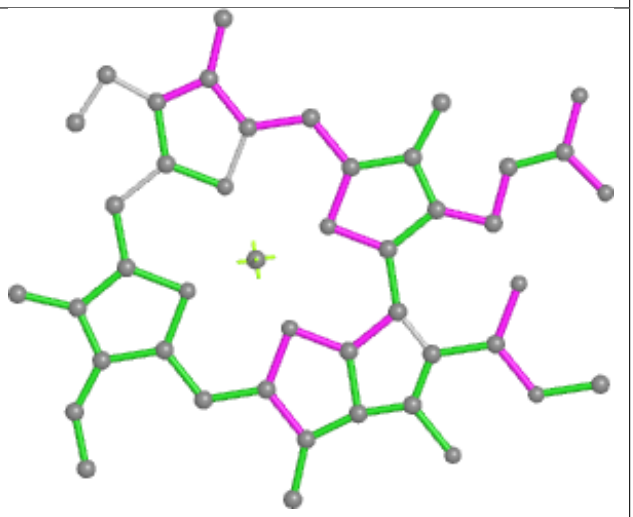
Torsions

Rings

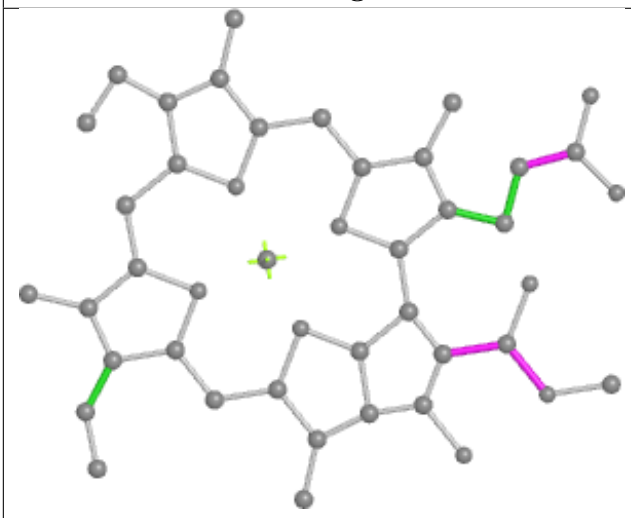
Ligand CLA b2 416



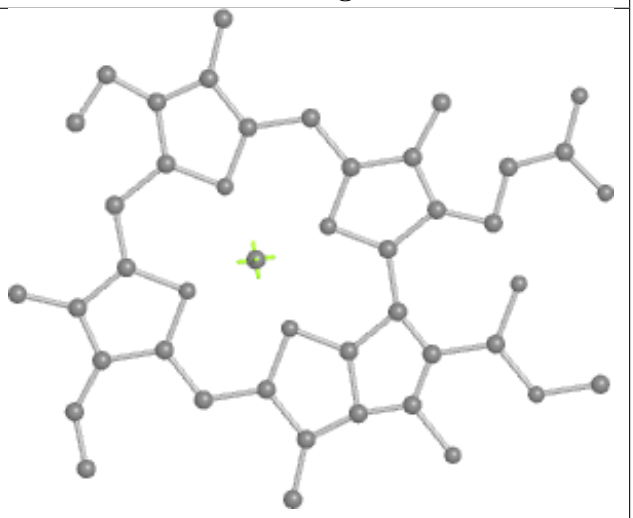
Bond lengths



Bond angles

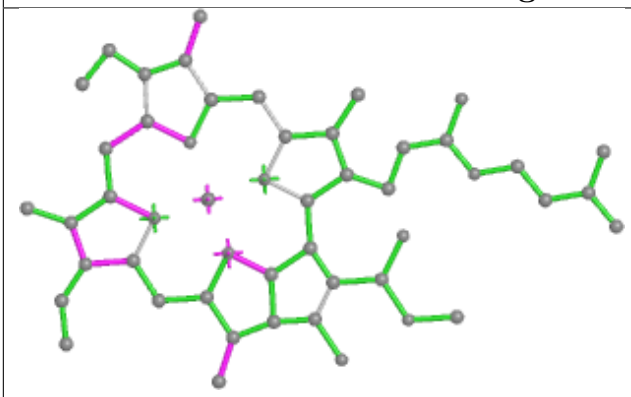


Torsions

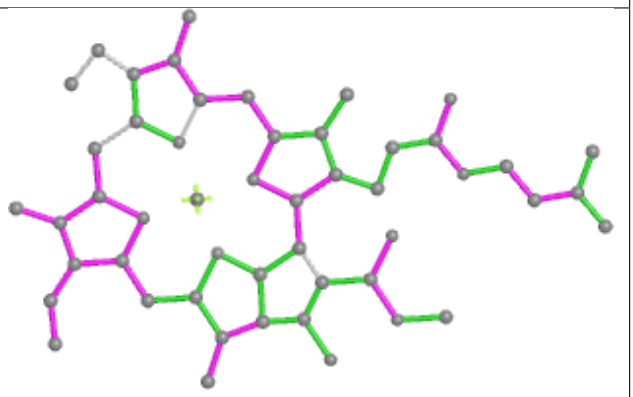


Rings

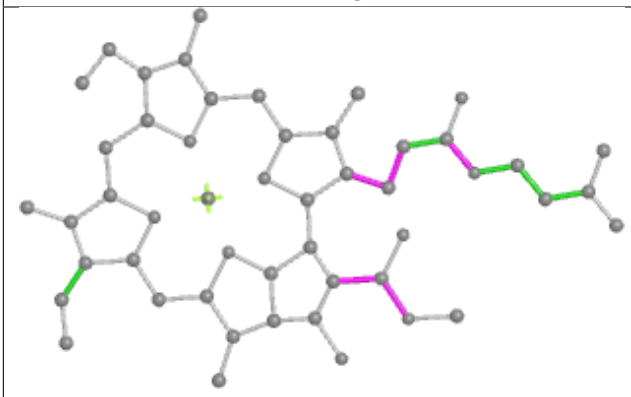
Ligand CLA b2 417



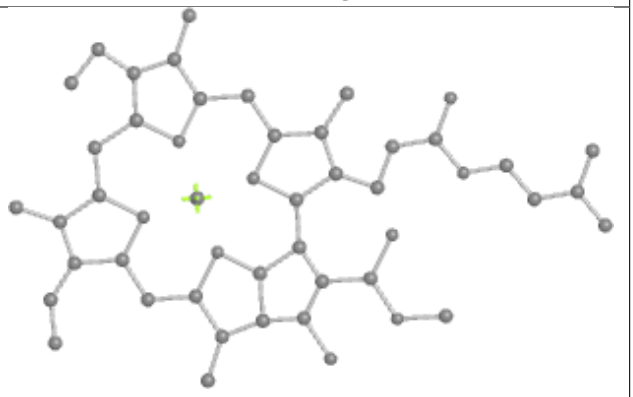
Bond lengths



Bond angles

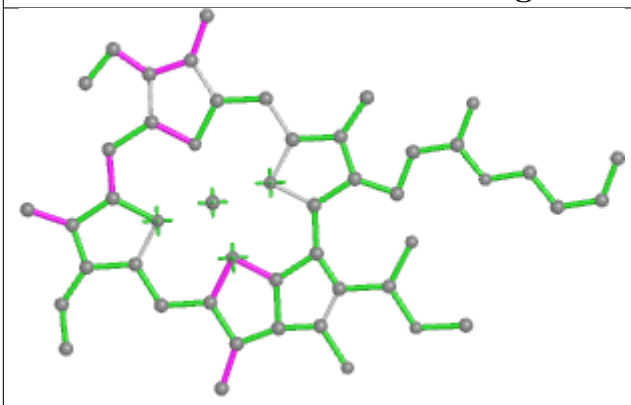


Torsions

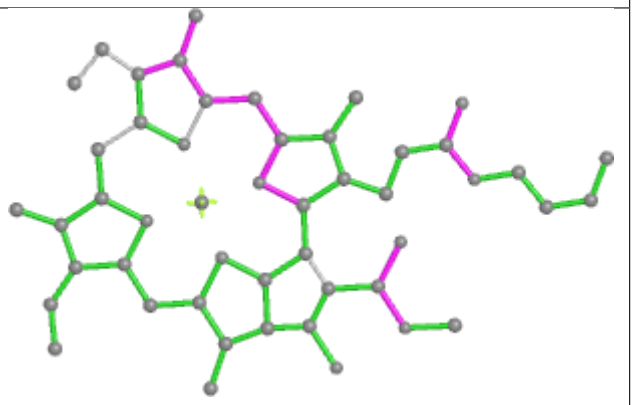


Rings

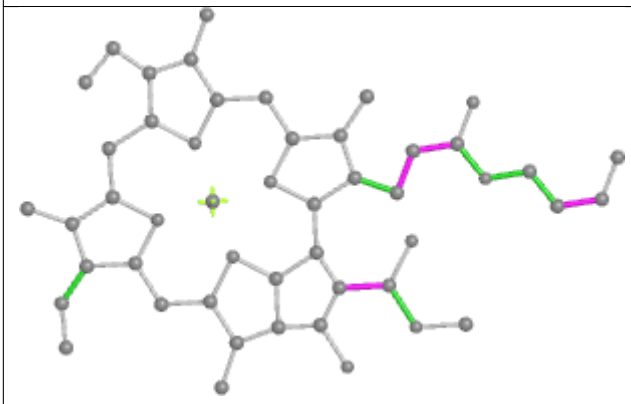
Ligand CLA aA 823



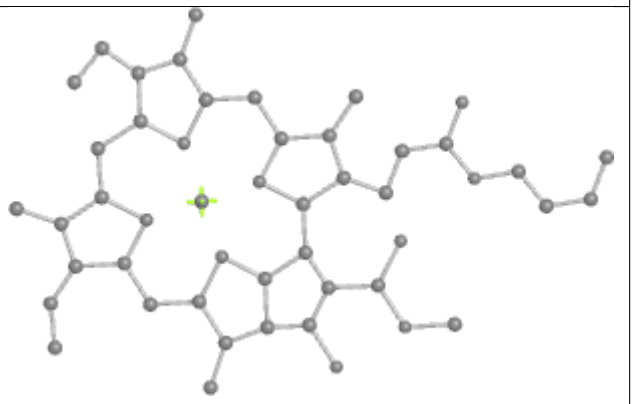
Bond lengths



Bond angles

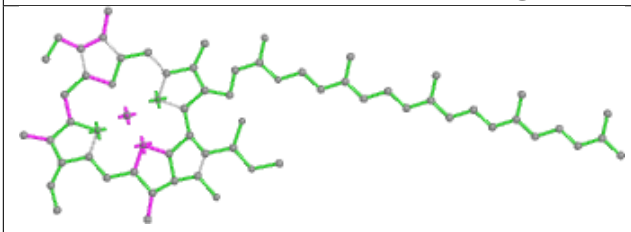


Torsions

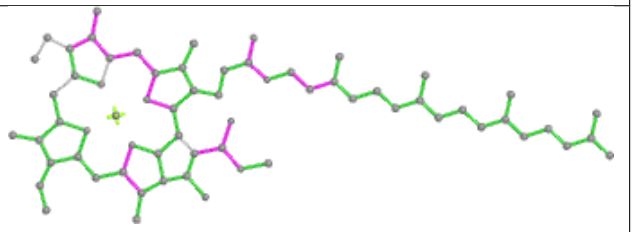


Rings

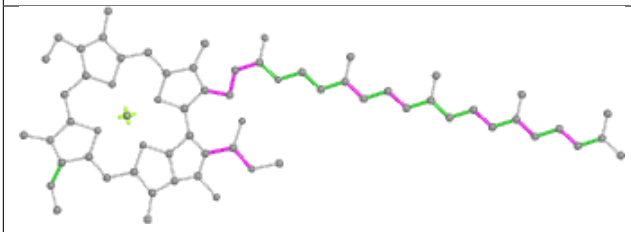
Ligand CLA bA 830



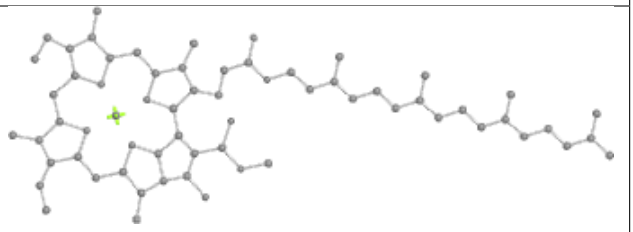
Bond lengths



Bond angles

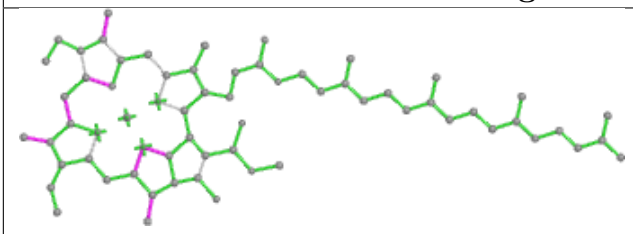


Torsions

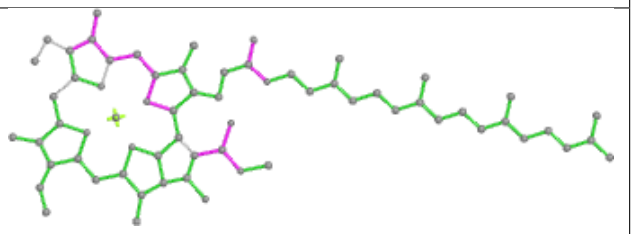


Rings

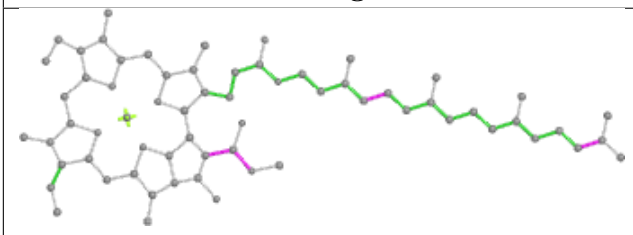
Ligand CLA b3 409



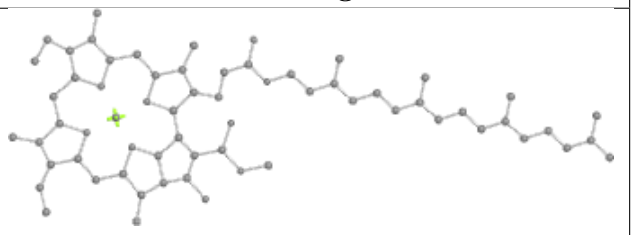
Bond lengths



Bond angles

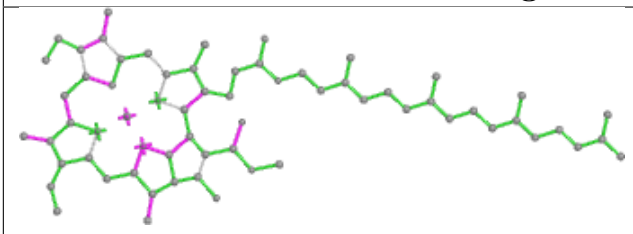


Torsions

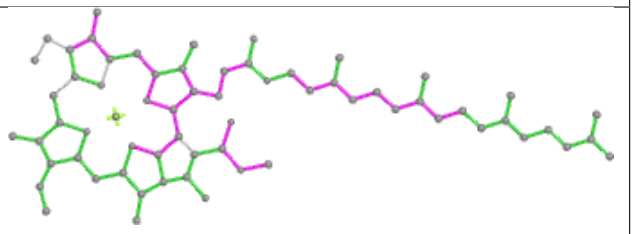


Rings

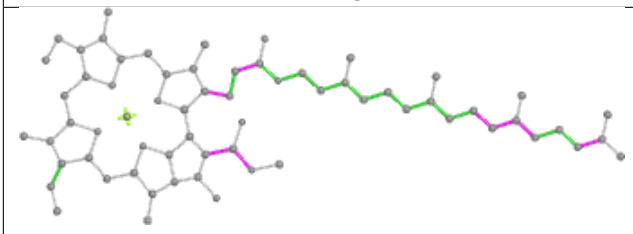
Ligand CLA c4 421



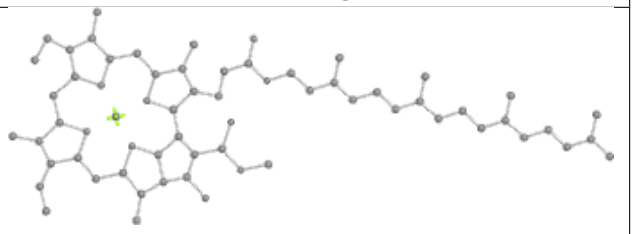
Bond lengths



Bond angles

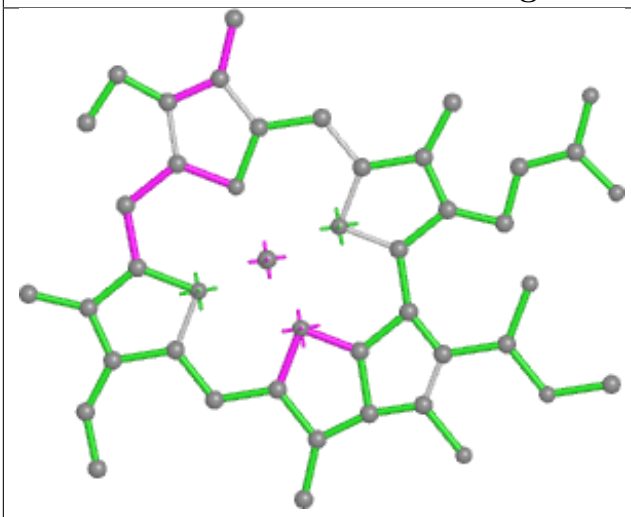


Torsions

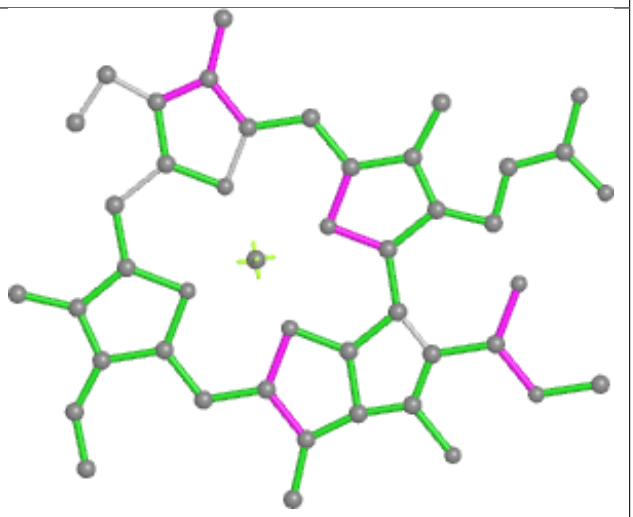


Rings

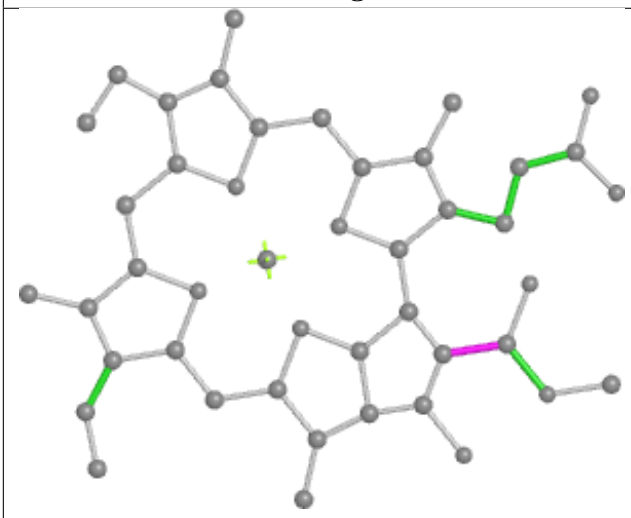
Ligand CLA a2 414



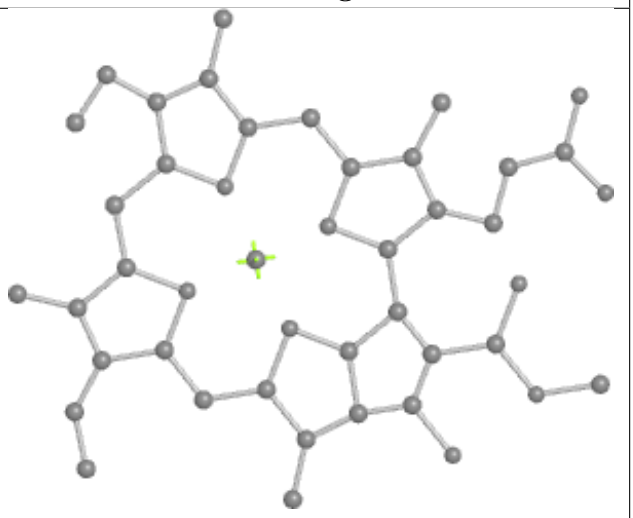
Bond lengths



Bond angles

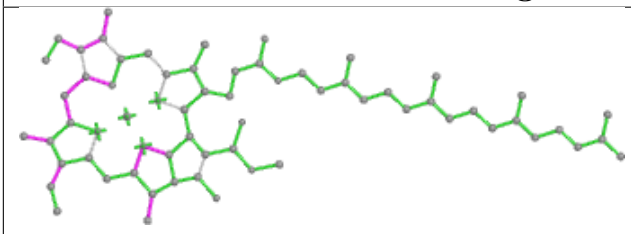


Torsions

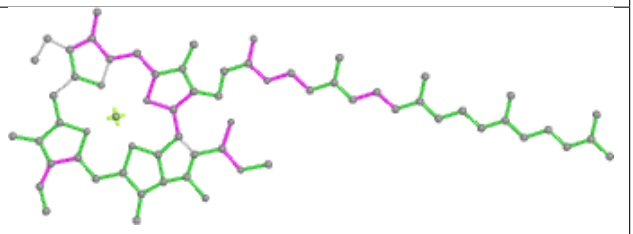


Rings

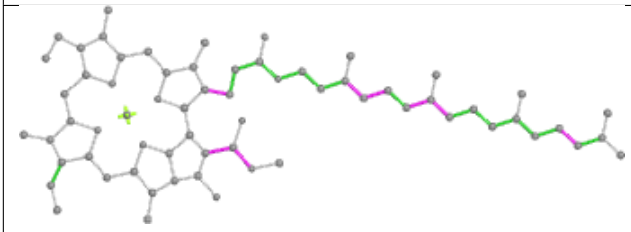
Ligand CLA cB 811



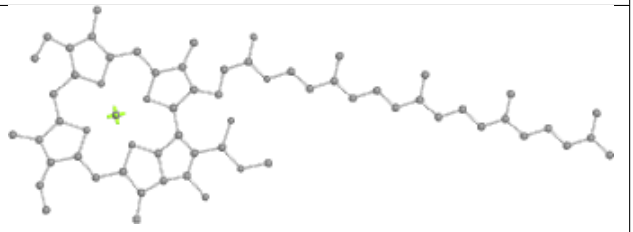
Bond lengths



Bond angles

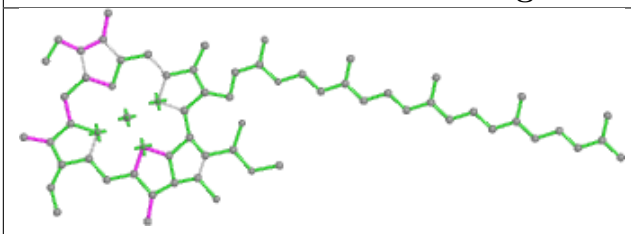


Torsions

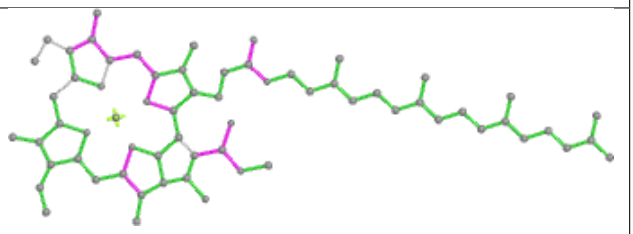


Rings

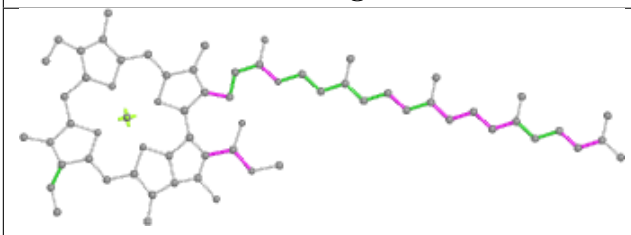
Ligand CLA cB 815



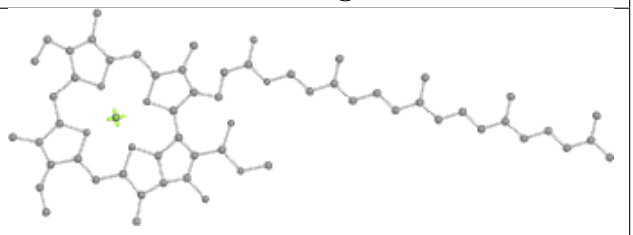
Bond lengths



Bond angles

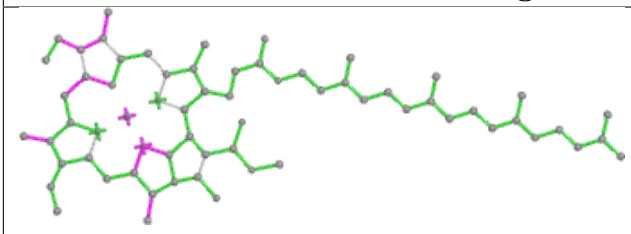


Torsions

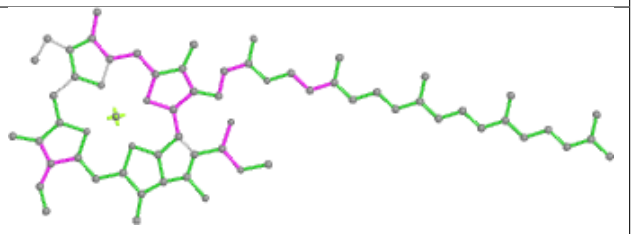


Rings

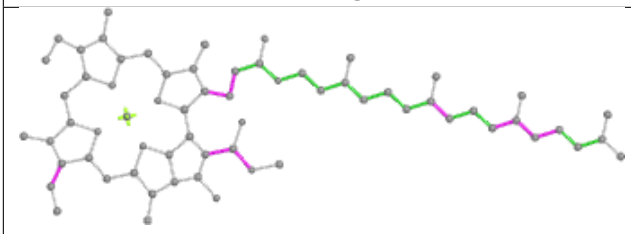
Ligand CLA cB 840



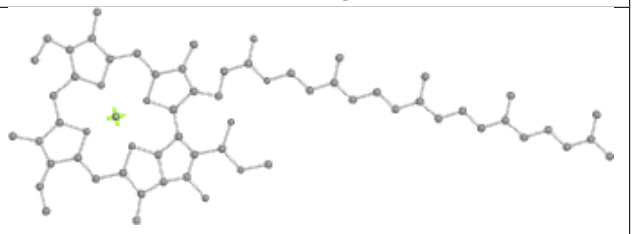
Bond lengths



Bond angles

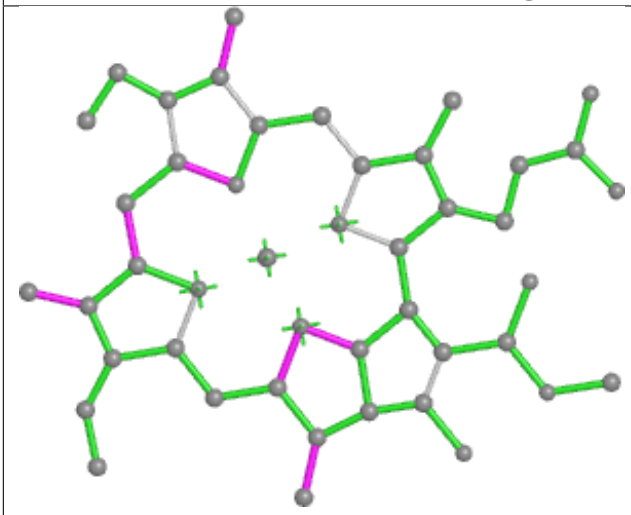


Torsions

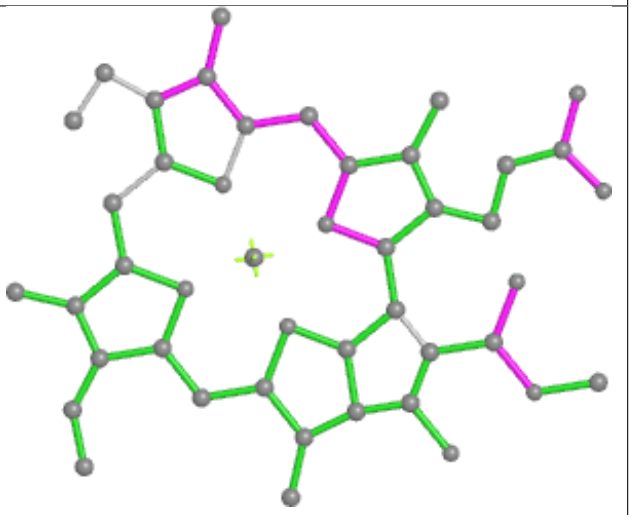


Rings

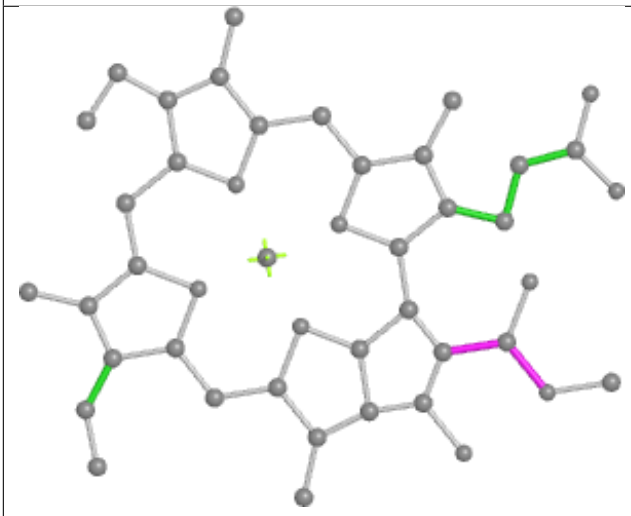
Ligand CLA c4 406



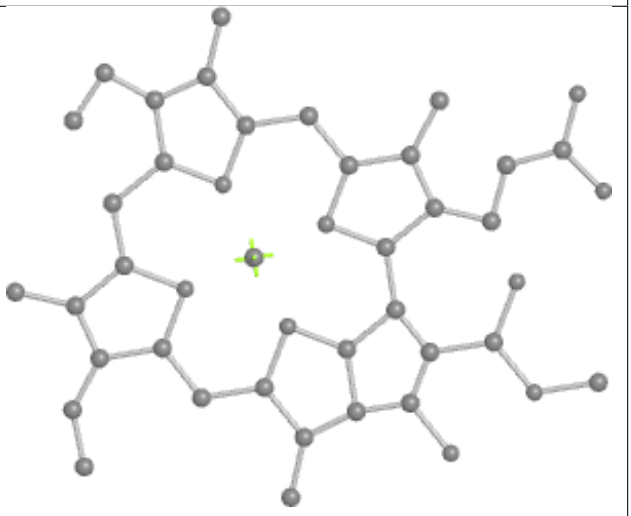
Bond lengths



Bond angles

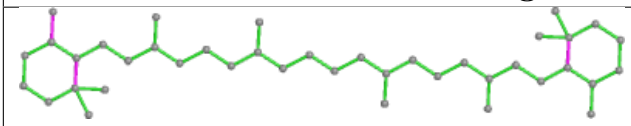


Torsions

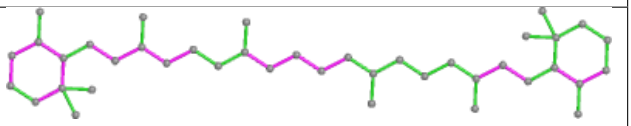


Rings

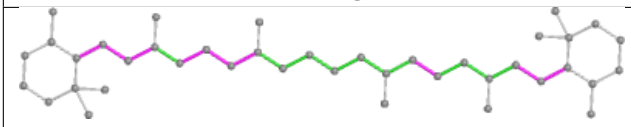
Ligand BCR c4 401



Bond lengths



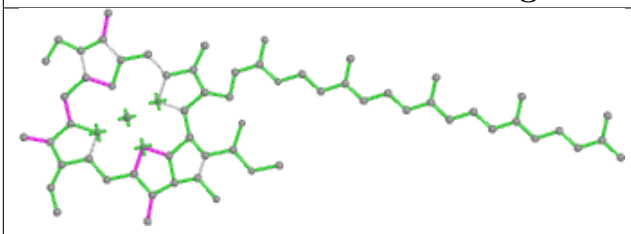
Bond angles



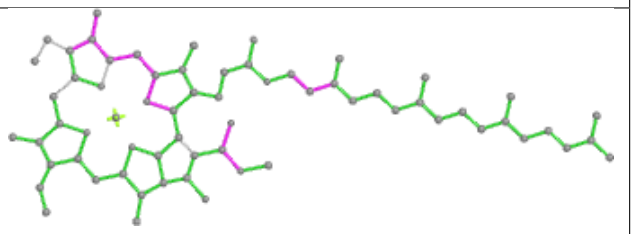
Torsions

Rings

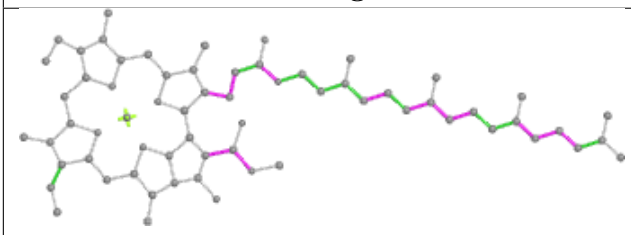
Ligand CLA a3 402



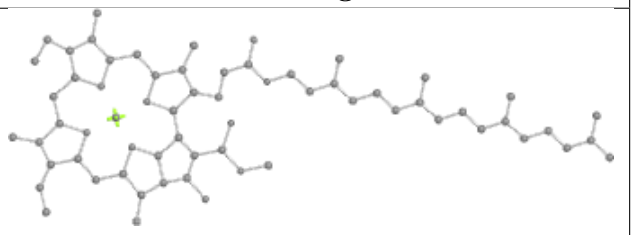
Bond lengths



Bond angles

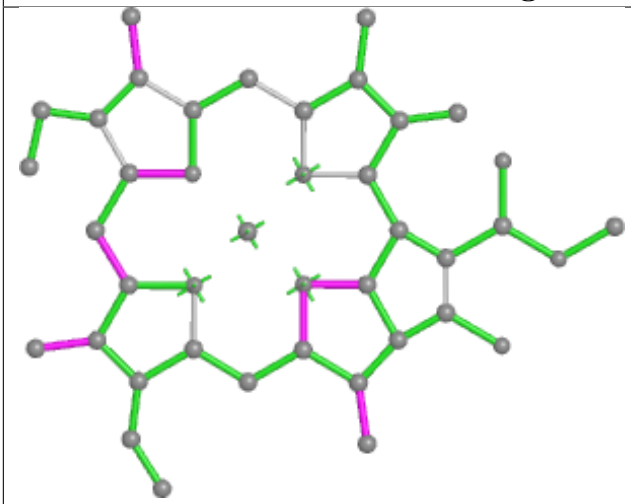


Torsions

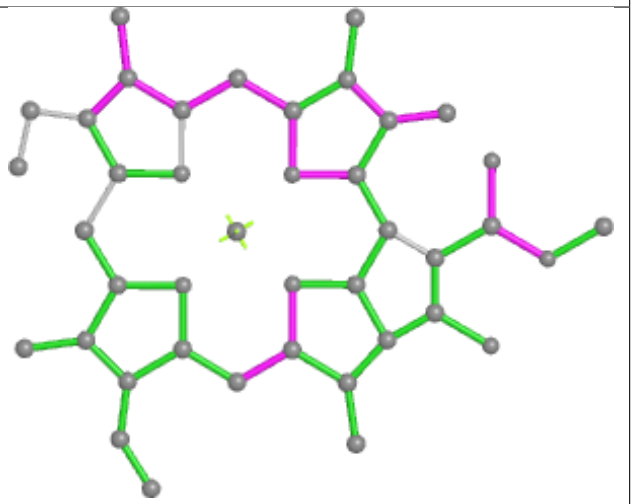


Rings

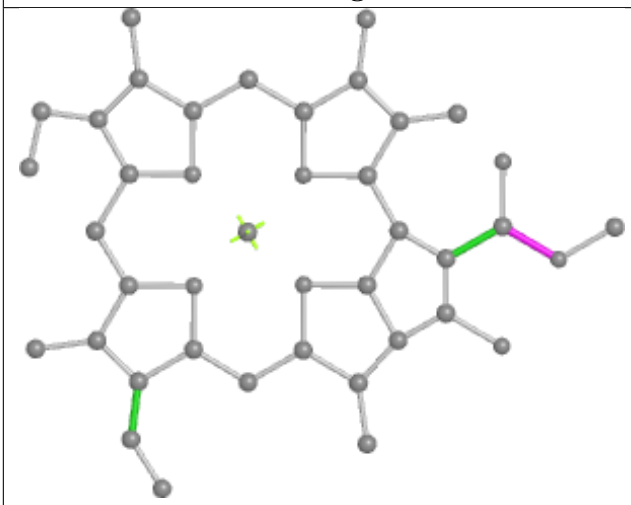
Ligand CLA a5 414



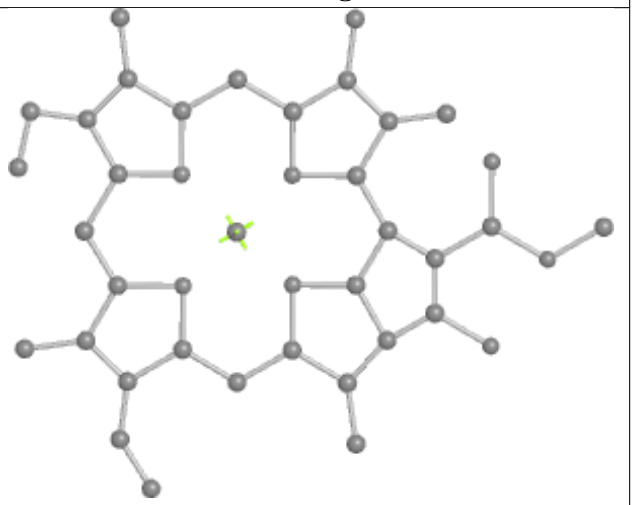
Bond lengths



Bond angles

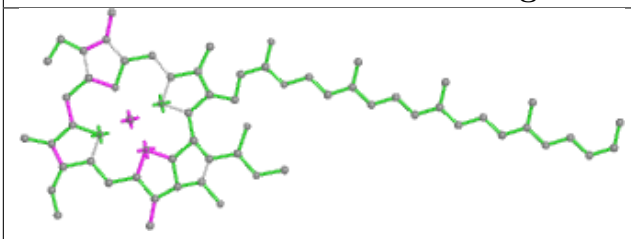


Torsions

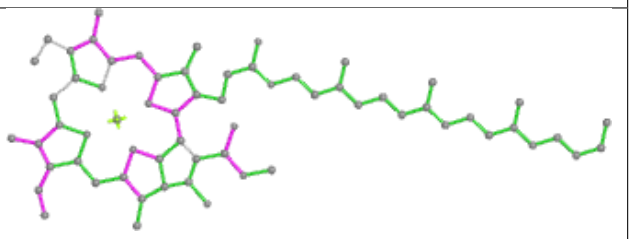


Rings

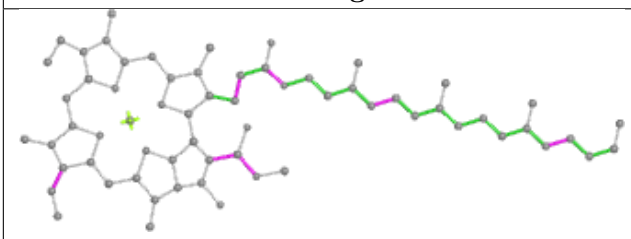
Ligand CLA a3 410



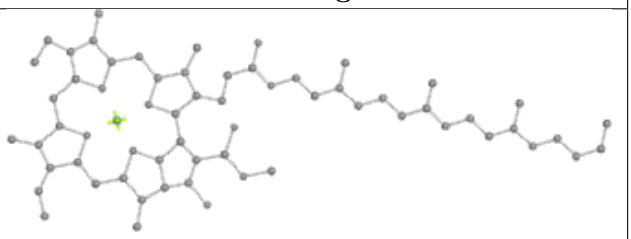
Bond lengths



Bond angles

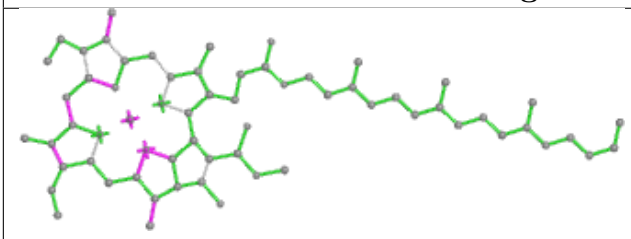


Torsions

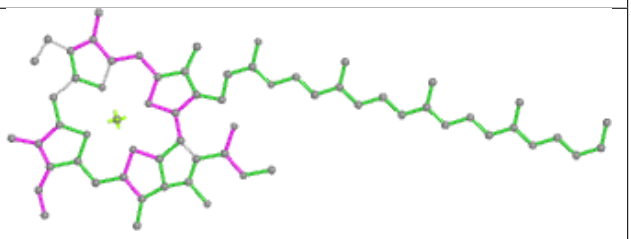


Rings

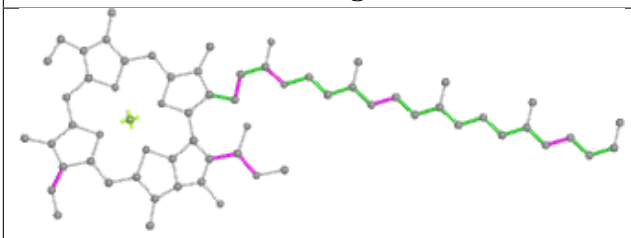
Ligand CLA c2 411



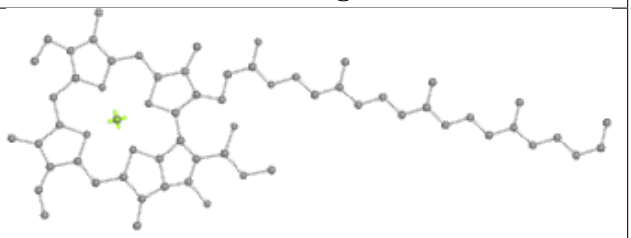
Bond lengths



Bond angles

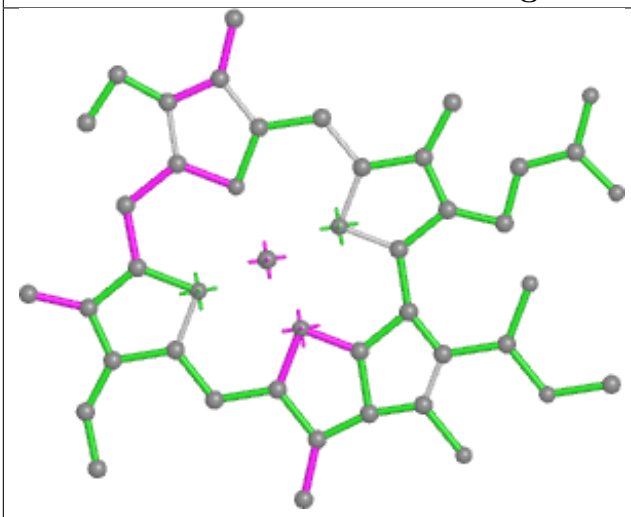


Torsions

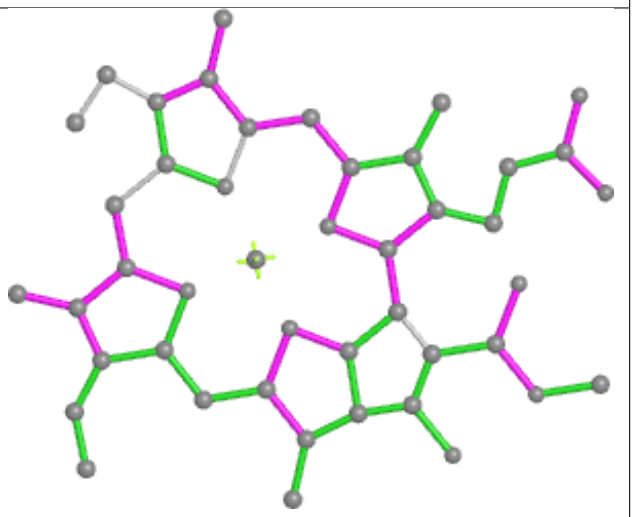


Rings

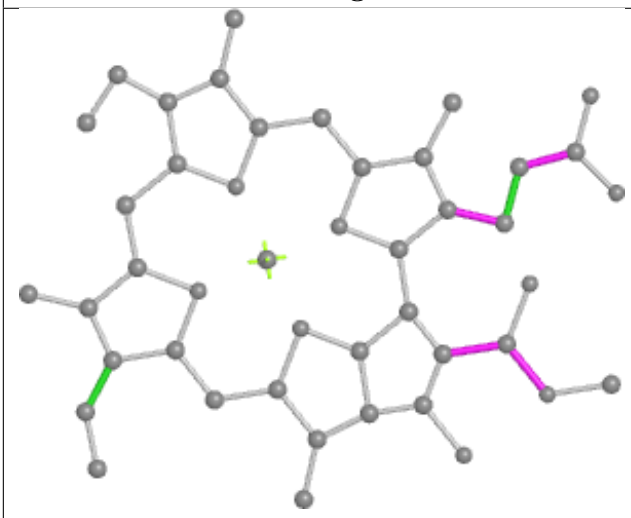
Ligand CLA c6 413



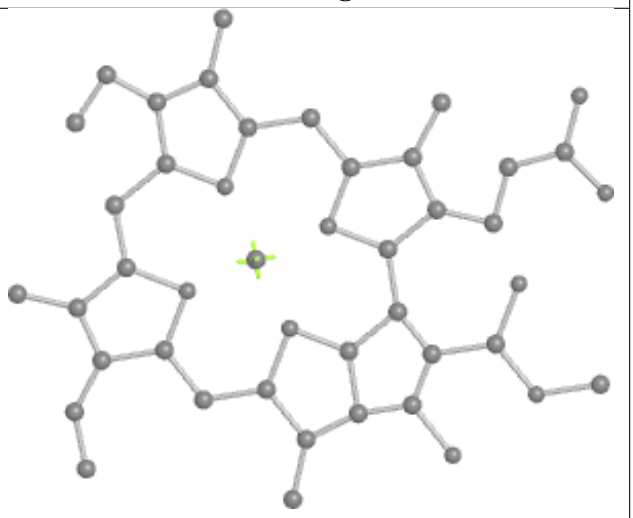
Bond lengths



Bond angles

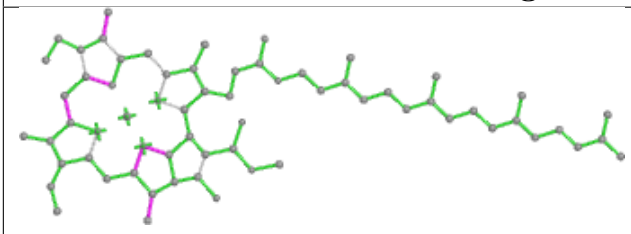


Torsions

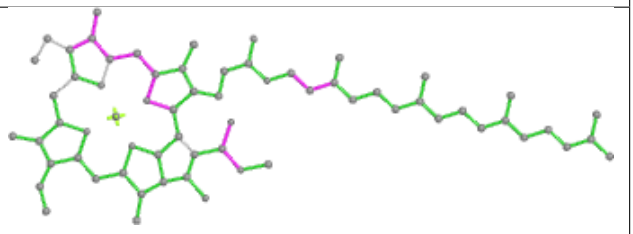


Rings

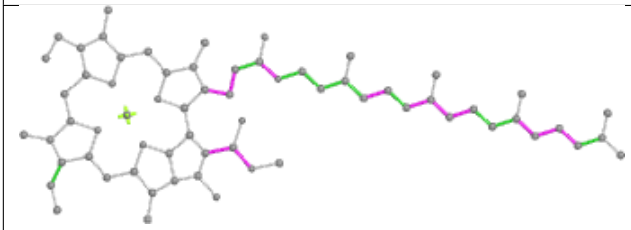
Ligand CLA a6 403



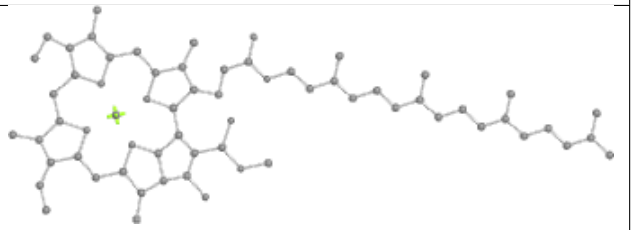
Bond lengths



Bond angles

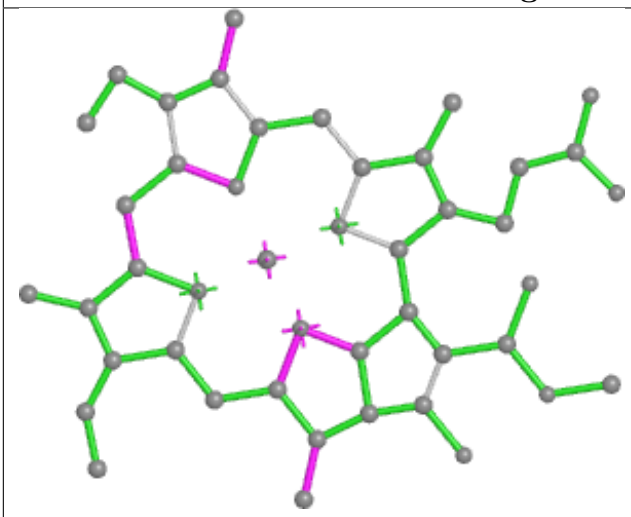


Torsions

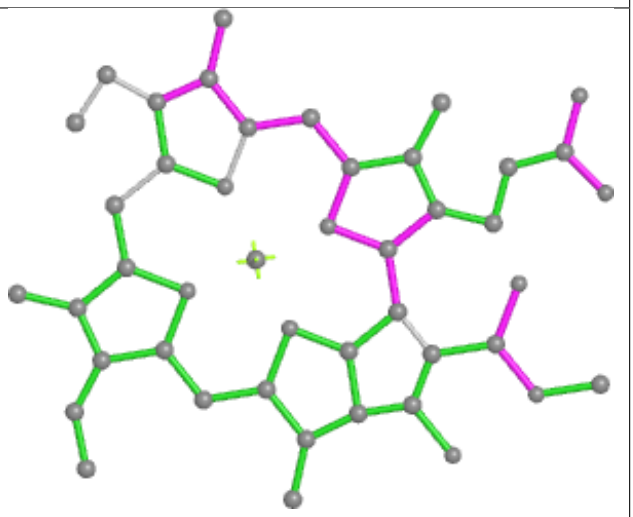


Rings

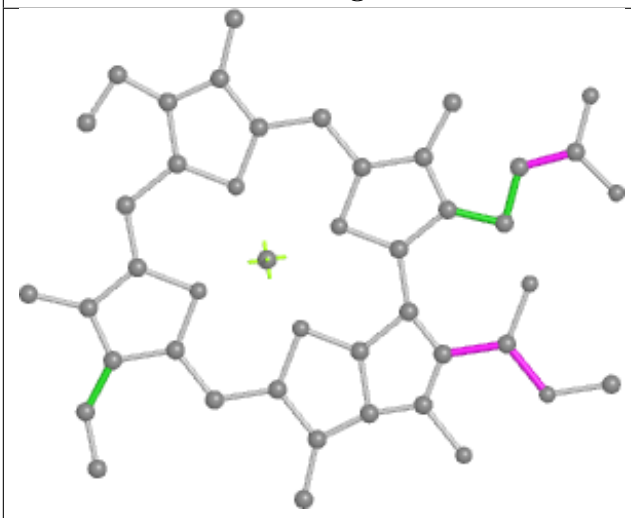
Ligand CLA c5 407



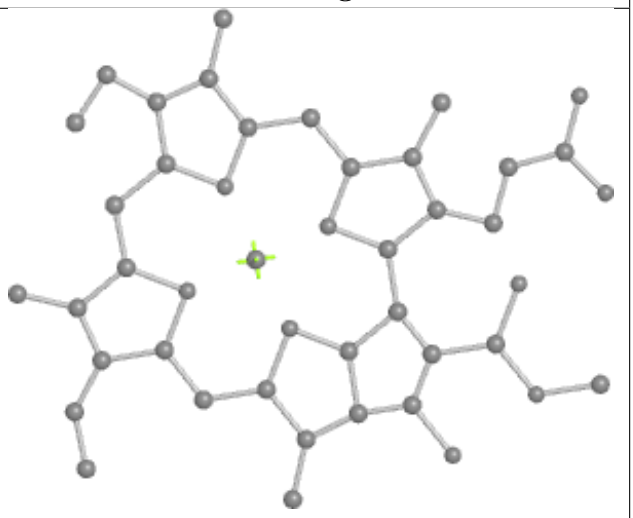
Bond lengths



Bond angles

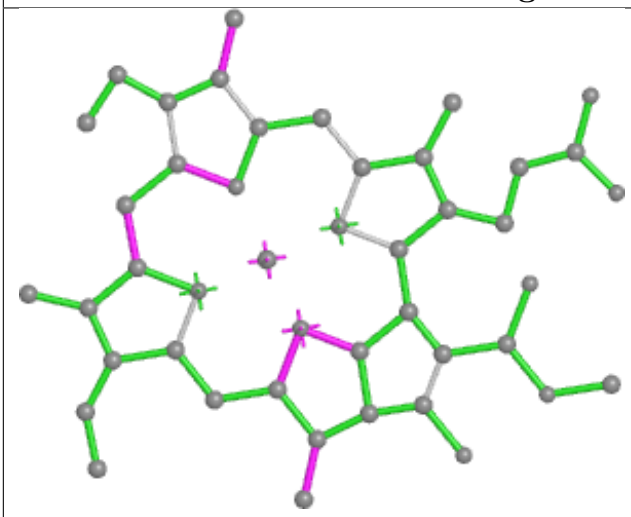


Torsions

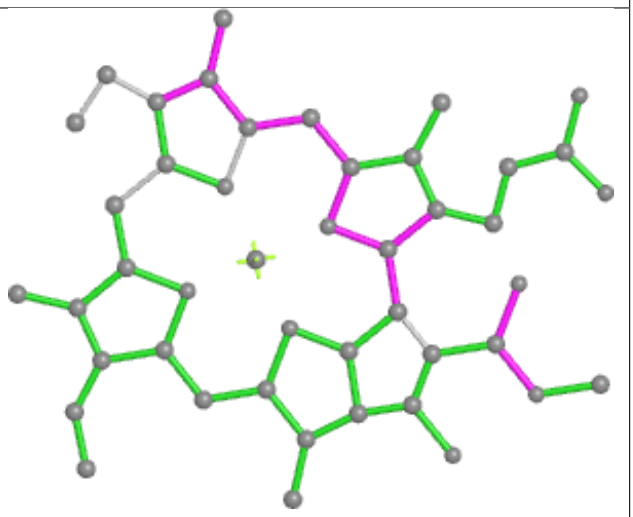


Rings

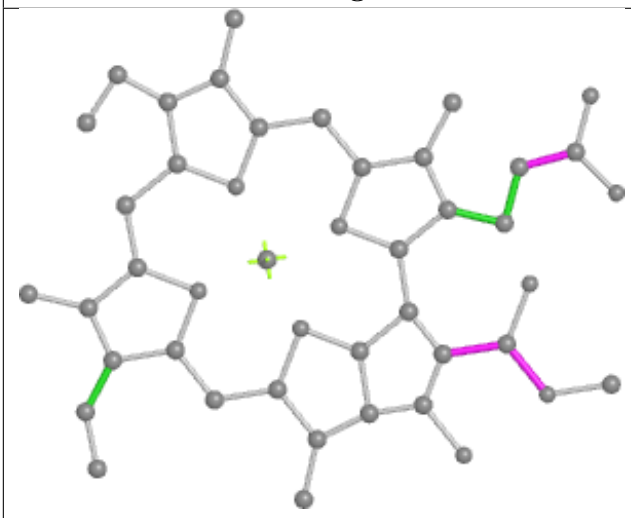
Ligand CLA b1 407



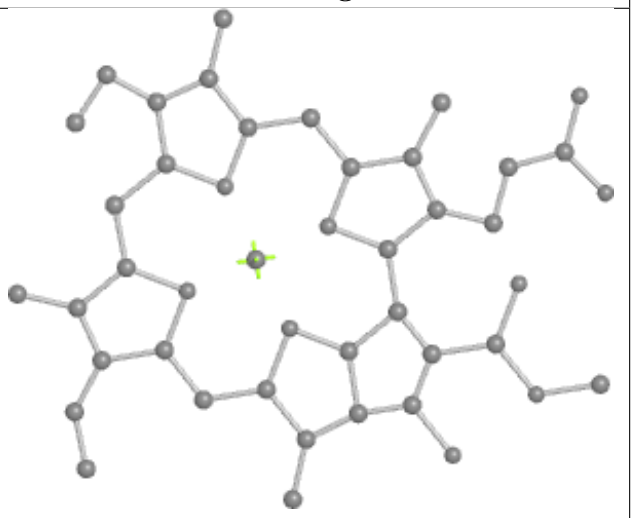
Bond lengths



Bond angles

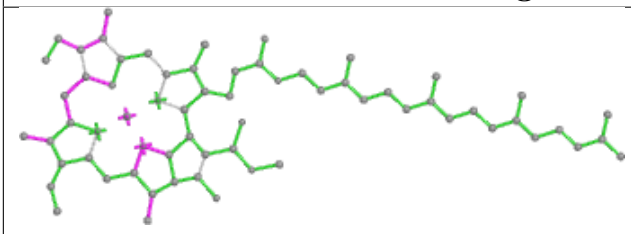


Torsions

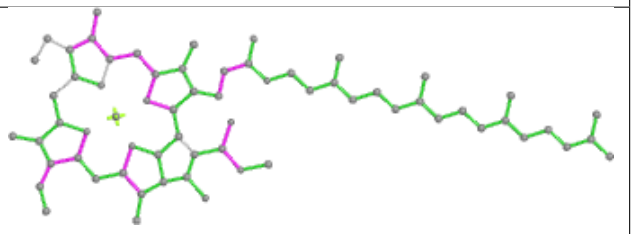


Rings

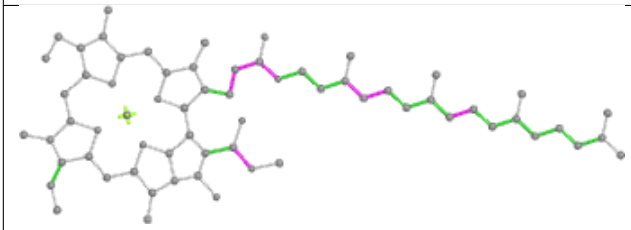
Ligand CLA aB 801



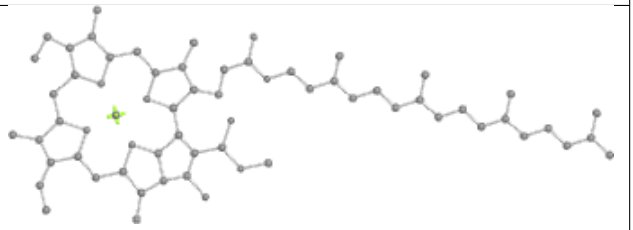
Bond lengths



Bond angles

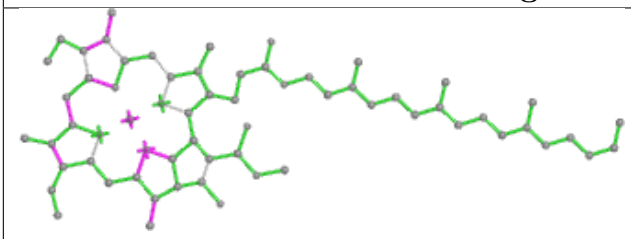


Torsions

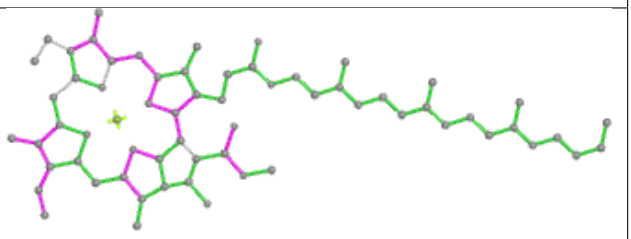


Rings

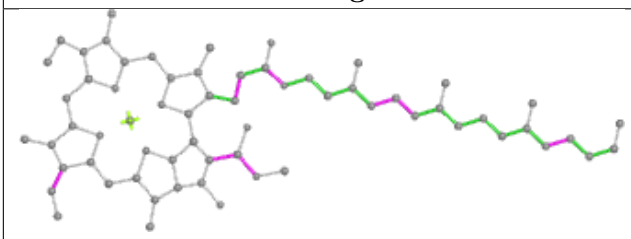
Ligand CLA c4 410



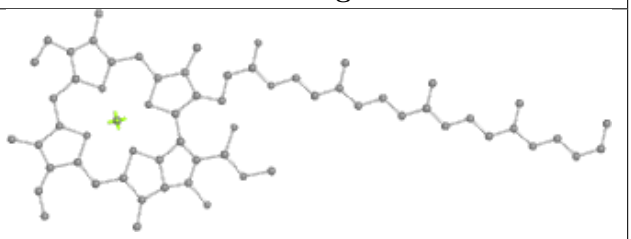
Bond lengths



Bond angles

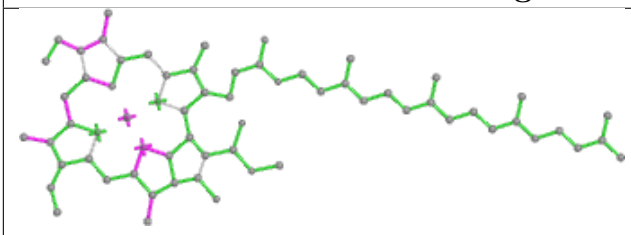


Torsions

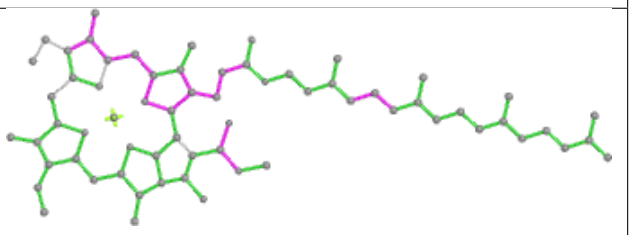


Rings

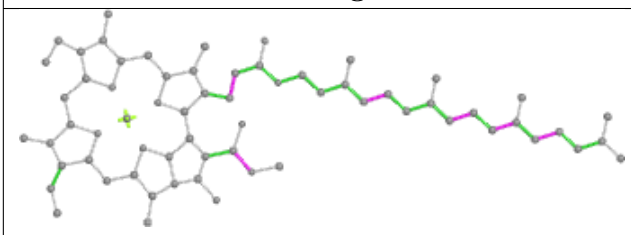
Ligand CLA bB 839



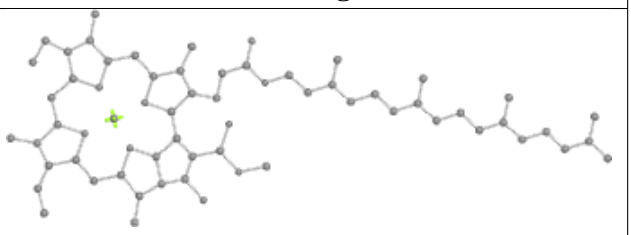
Bond lengths



Bond angles

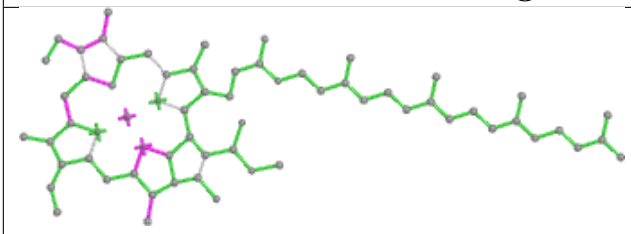


Torsions

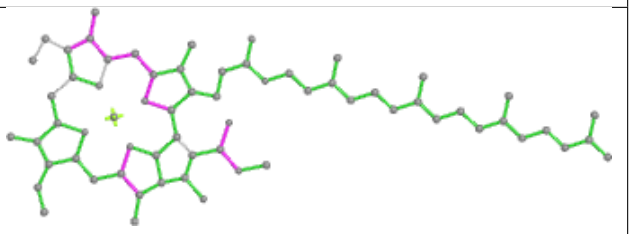


Rings

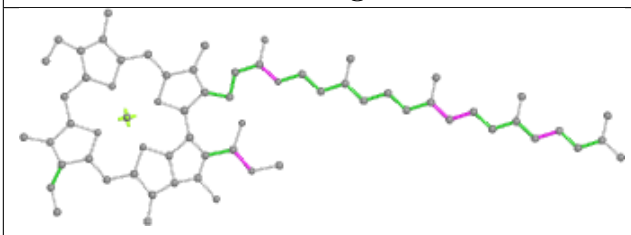
Ligand CLA cB 820



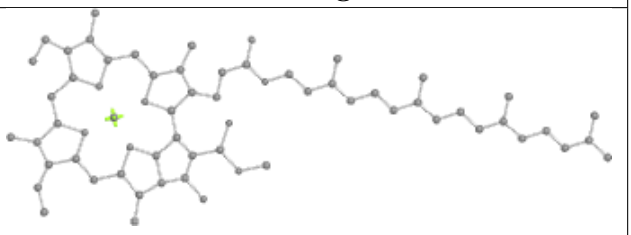
Bond lengths



Bond angles

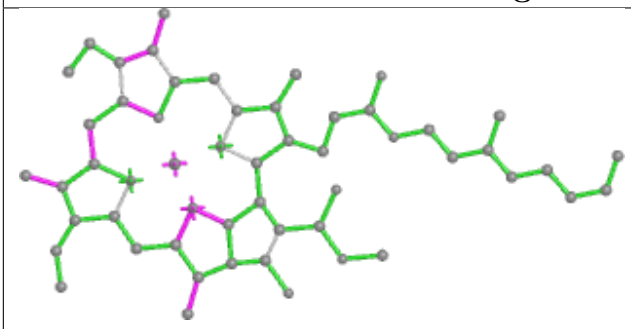


Torsions

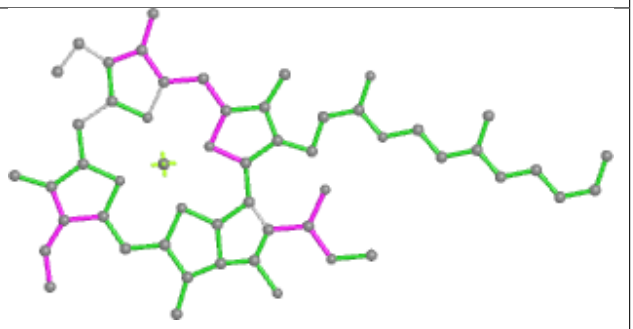


Rings

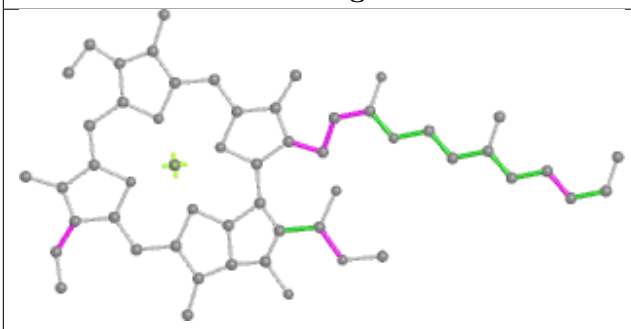
Ligand CLA bA 819



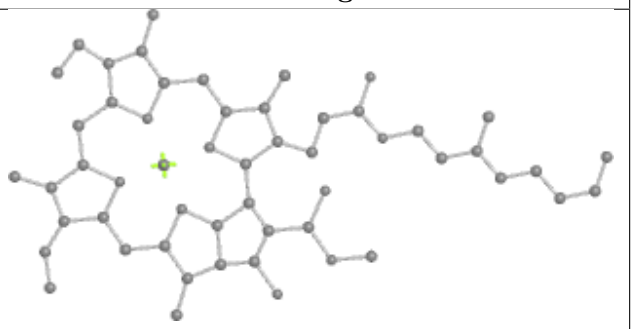
Bond lengths



Bond angles

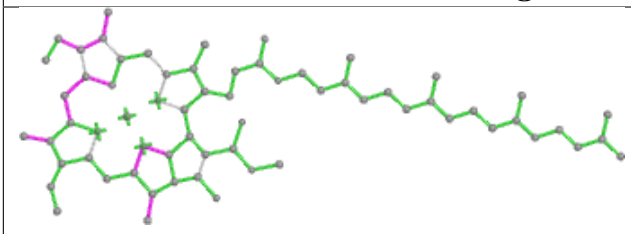


Torsions

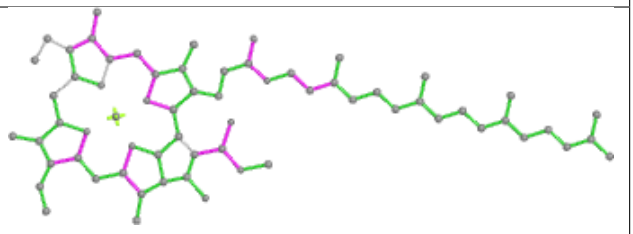


Rings

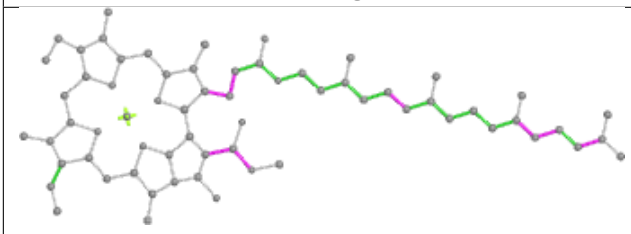
Ligand CLA cA 835



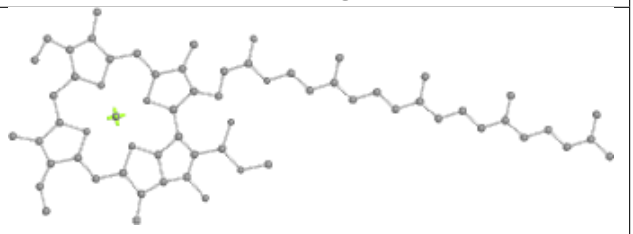
Bond lengths



Bond angles

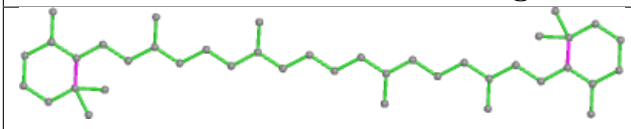


Torsions

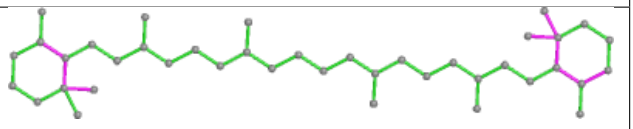


Rings

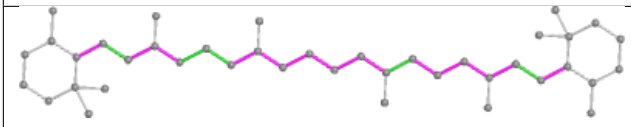
Ligand BCR bA 853



Bond lengths



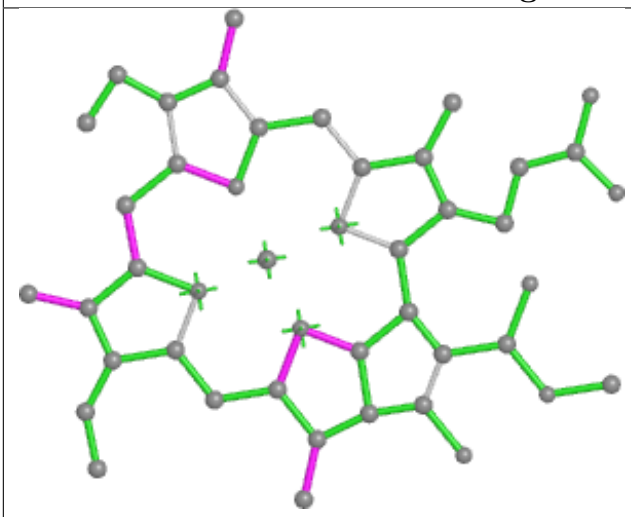
Bond angles



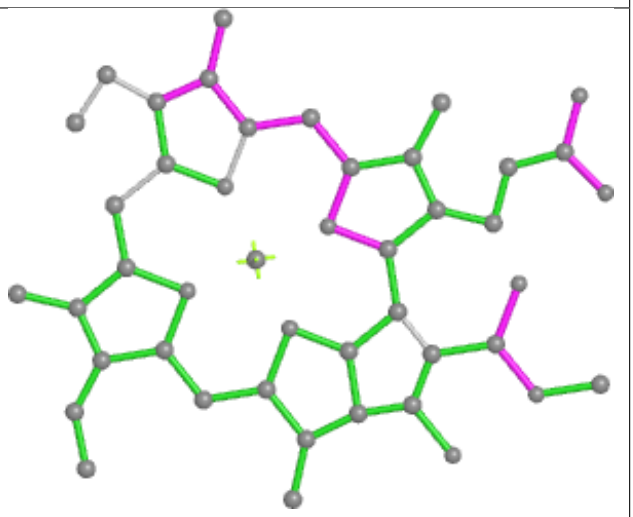
Torsions

Rings

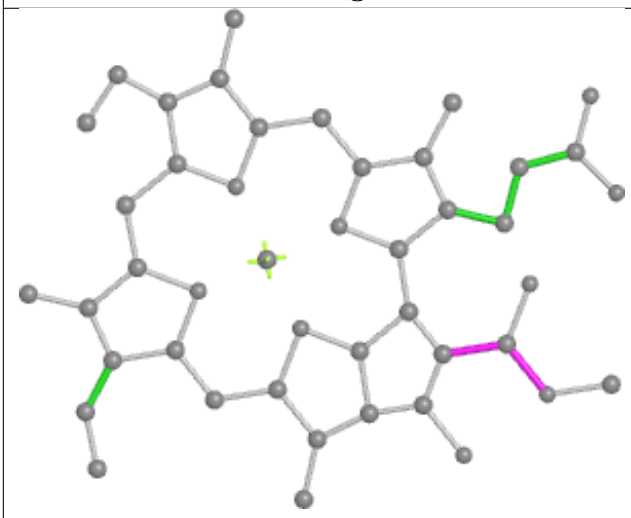
Ligand CLA a3 406



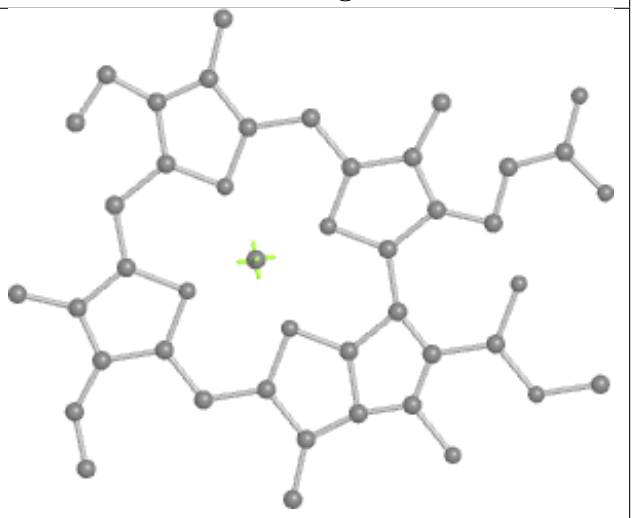
Bond lengths



Bond angles

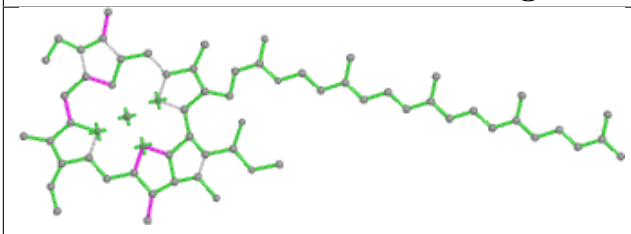


Torsions

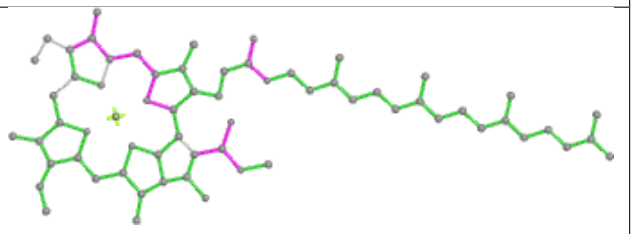


Rings

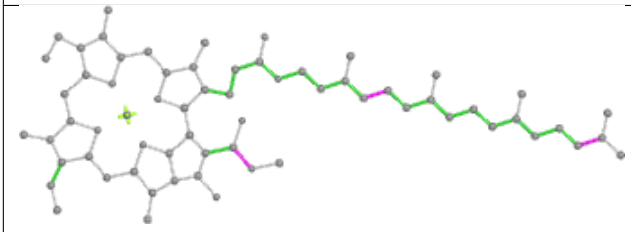
Ligand CLA a4 409



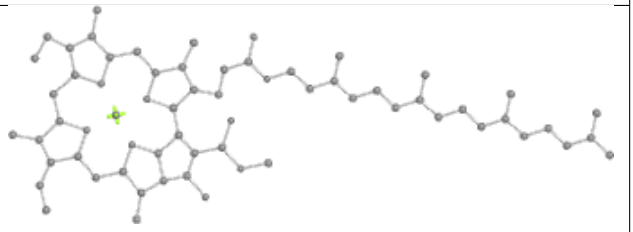
Bond lengths



Bond angles

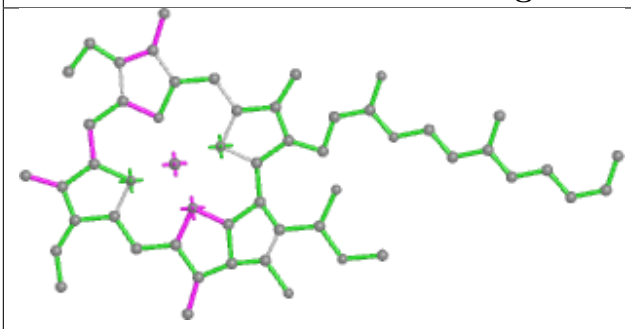


Torsions

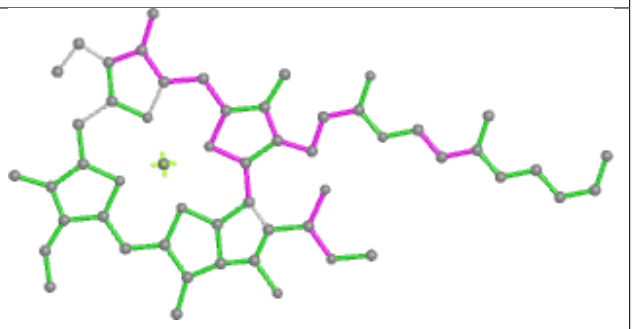


Rings

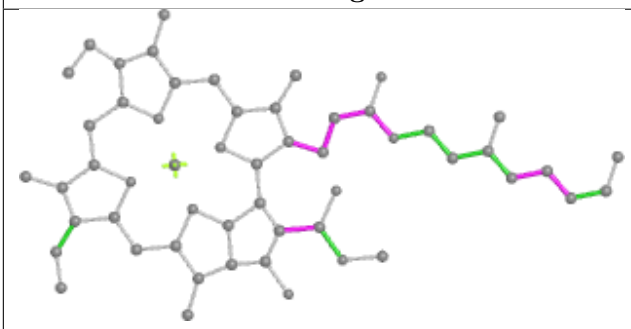
Ligand CLA aA 813



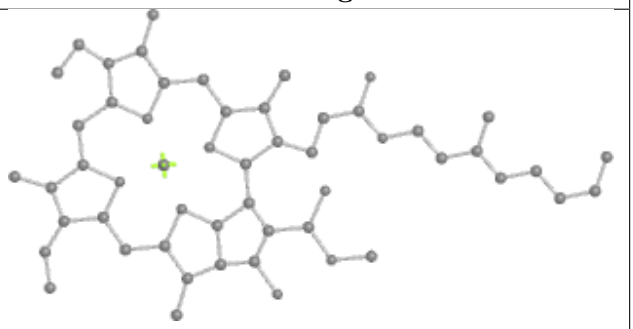
Bond lengths



Bond angles

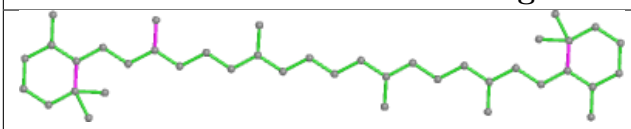


Torsions

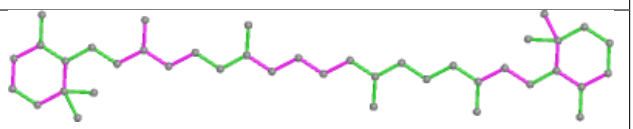


Rings

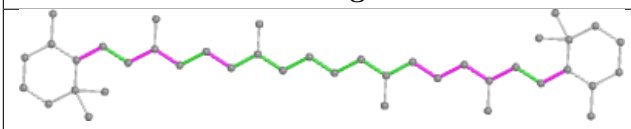
Ligand BCR a1 420



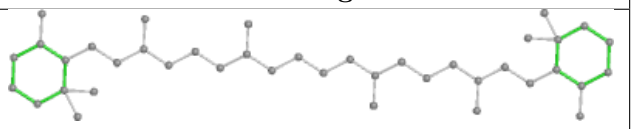
Bond lengths



Bond angles

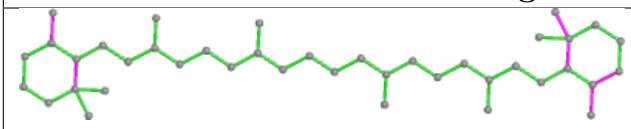


Torsions

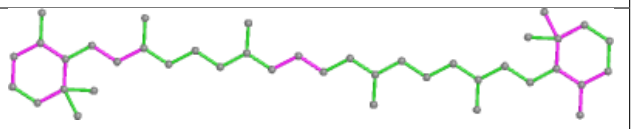


Rings

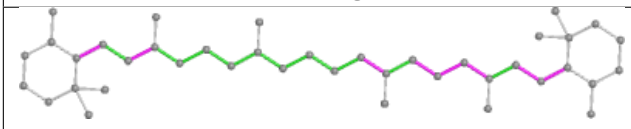
Ligand BCR c3 418



Bond lengths



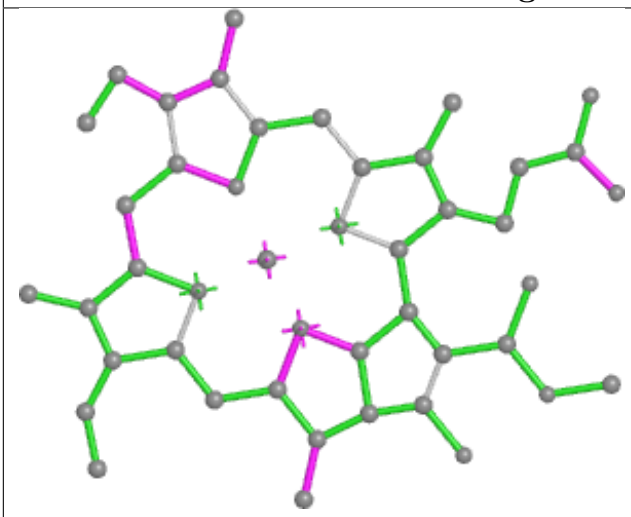
Bond angles



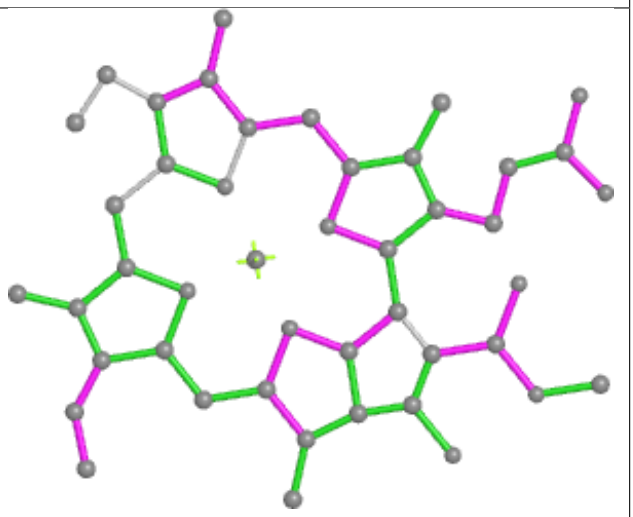
Torsions

Rings

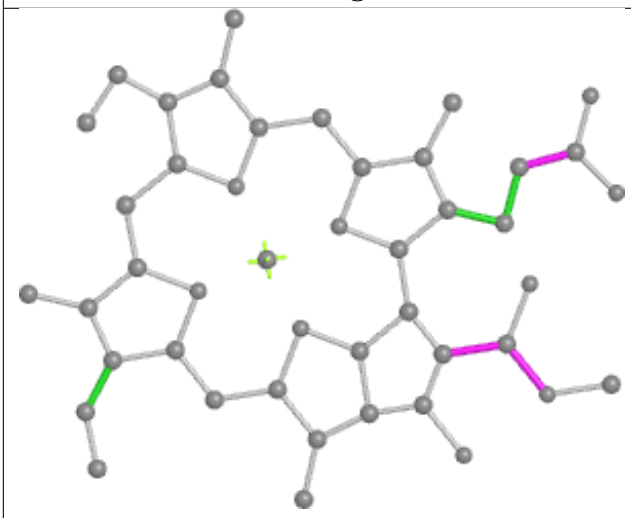
Ligand CLA b4 415



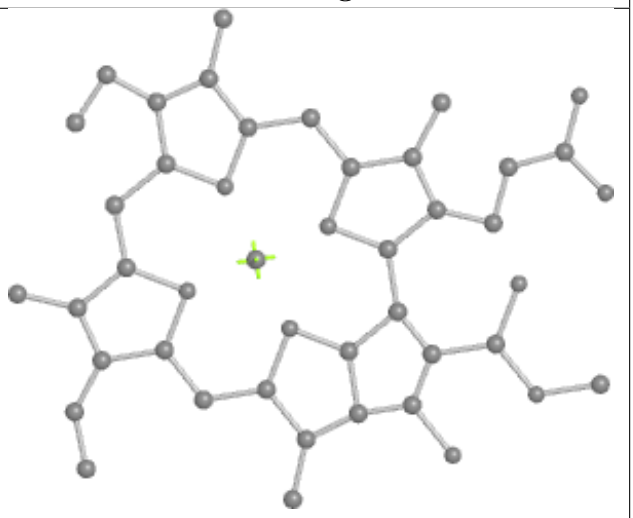
Bond lengths



Bond angles

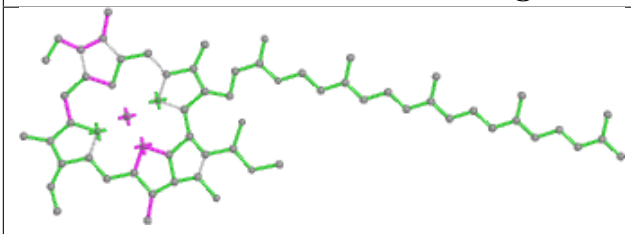


Torsions

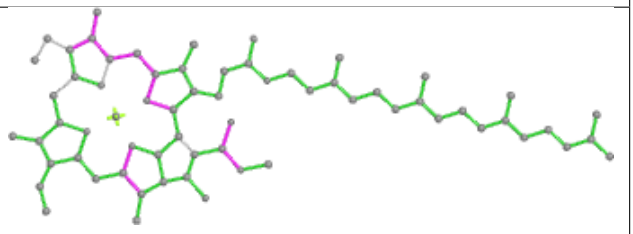


Rings

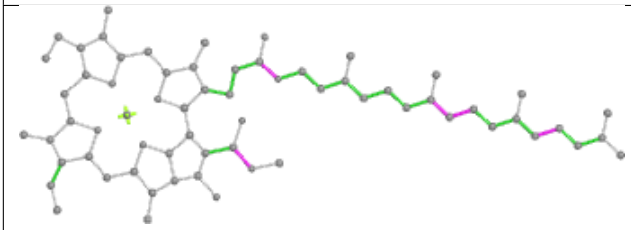
Ligand CLA bB 820



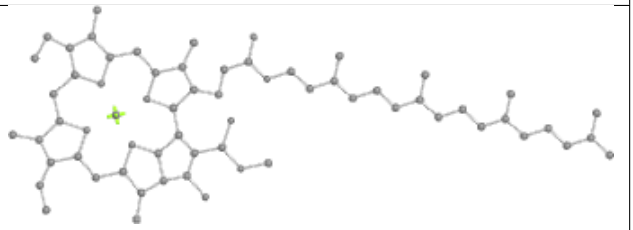
Bond lengths



Bond angles

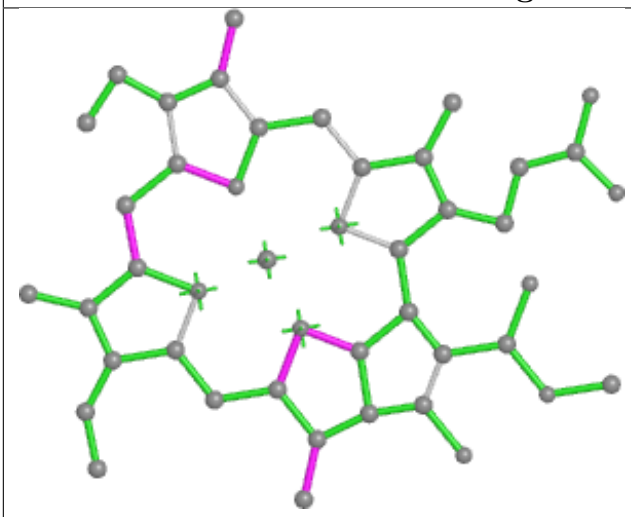


Torsions

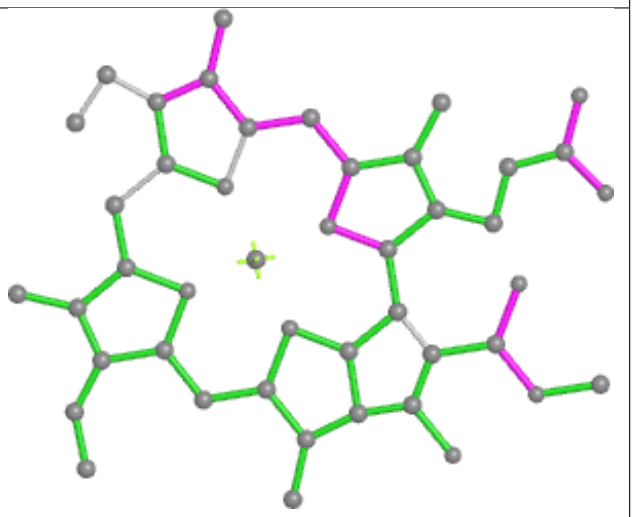


Rings

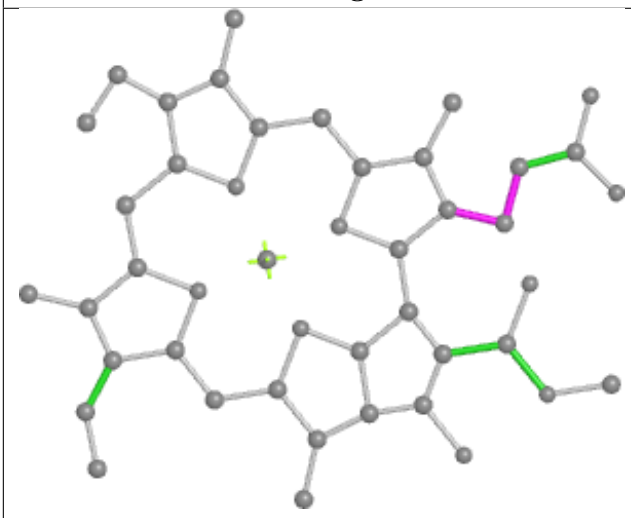
Ligand CLA cB 822



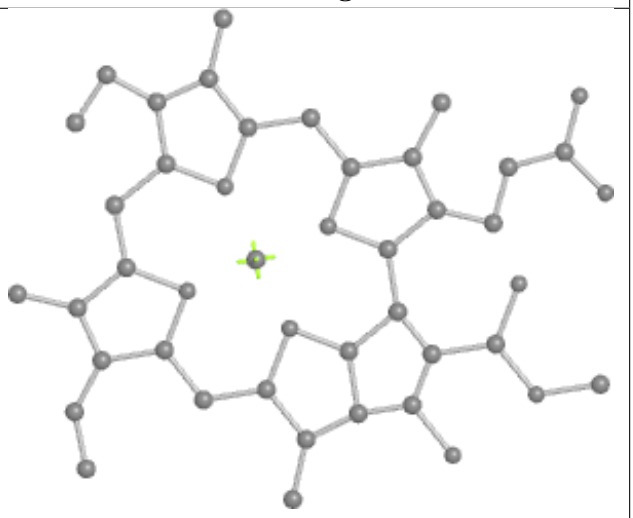
Bond lengths



Bond angles

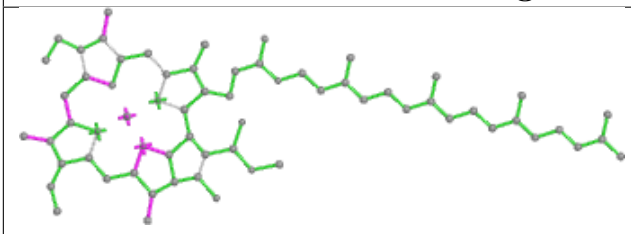


Torsions

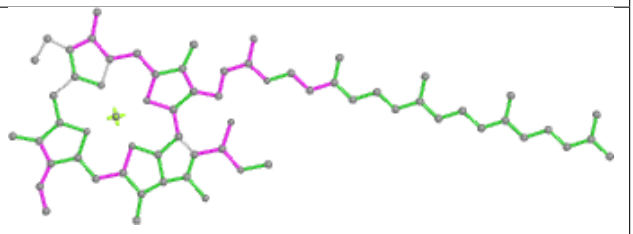


Rings

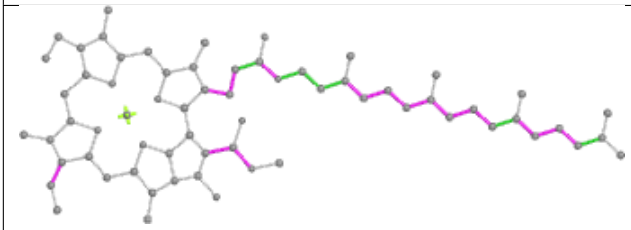
Ligand CLA cB 814



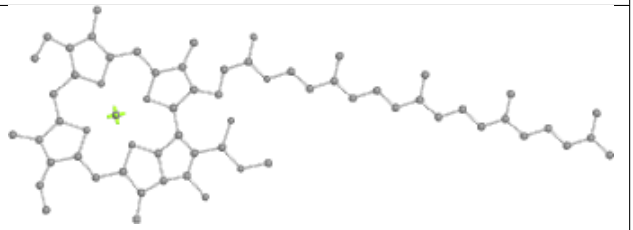
Bond lengths



Bond angles

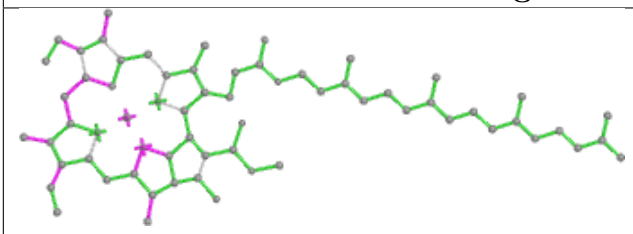


Torsions

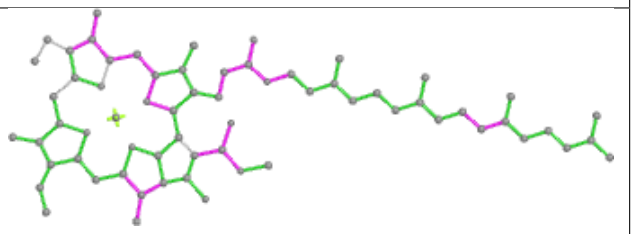


Rings

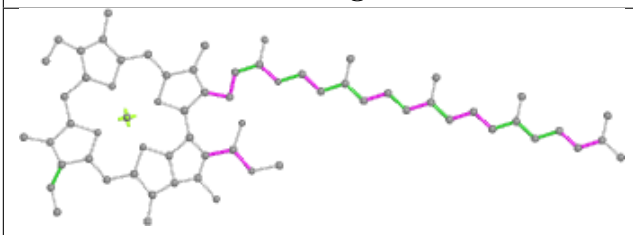
Ligand CLA bA 803



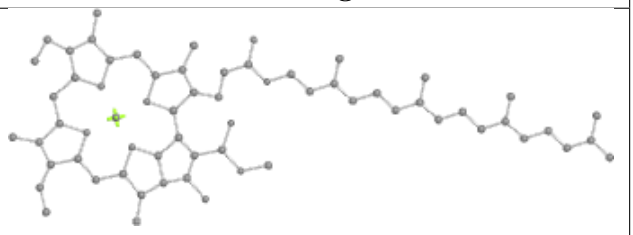
Bond lengths



Bond angles

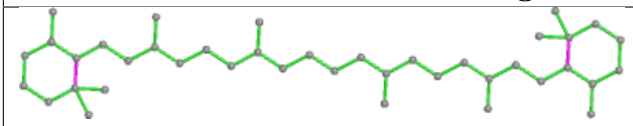


Torsions

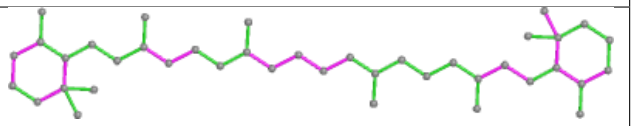


Rings

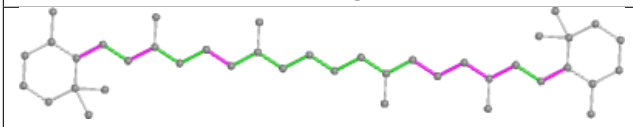
Ligand BCR b4 419



Bond lengths



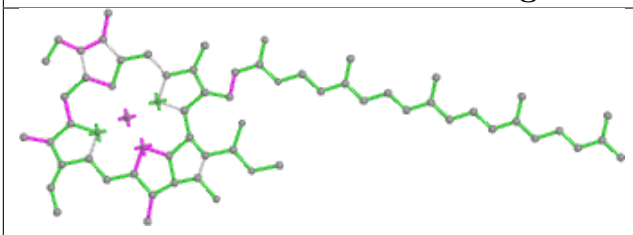
Bond angles



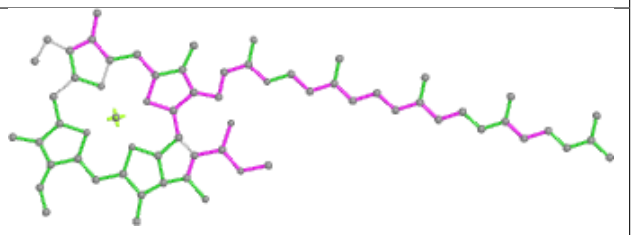
Torsions

Rings

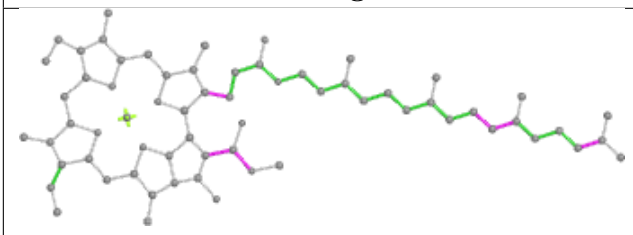
Ligand CLA a2 406



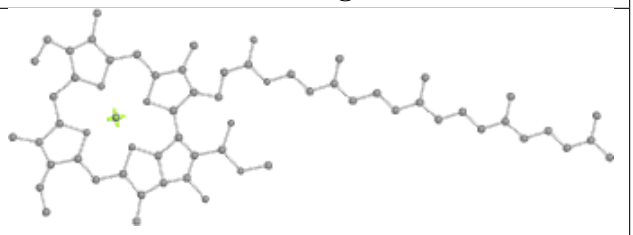
Bond lengths



Bond angles

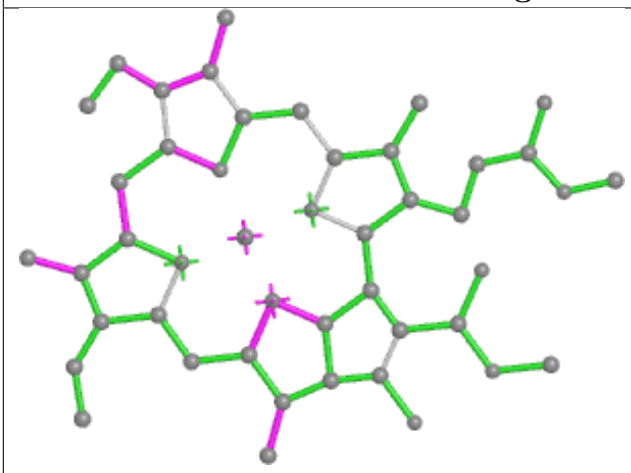


Torsions

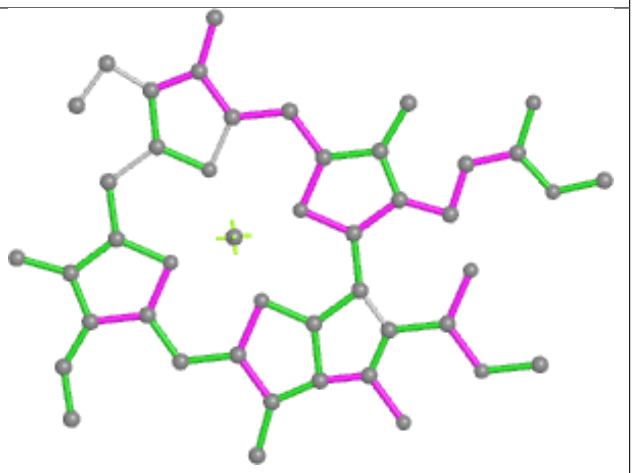


Rings

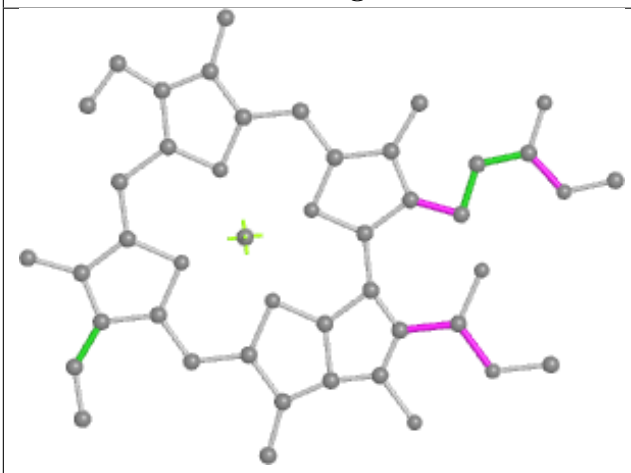
Ligand CLA bB 826



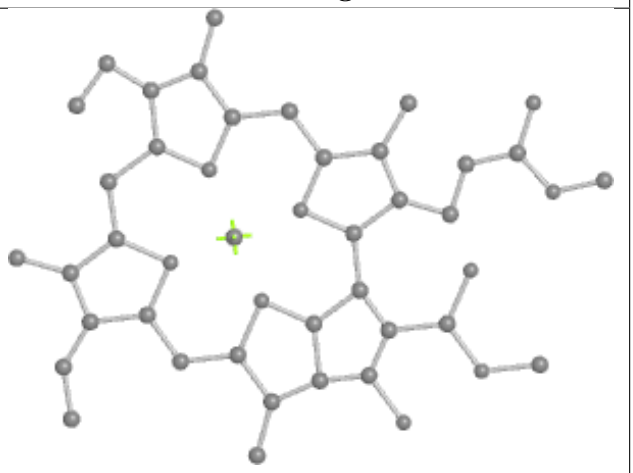
Bond lengths



Bond angles

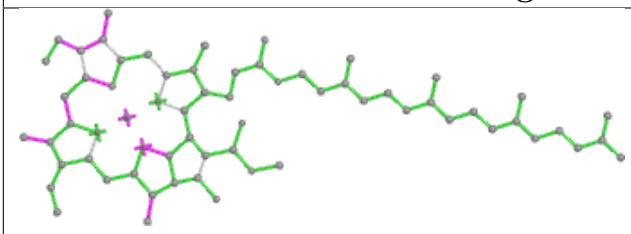


Torsions

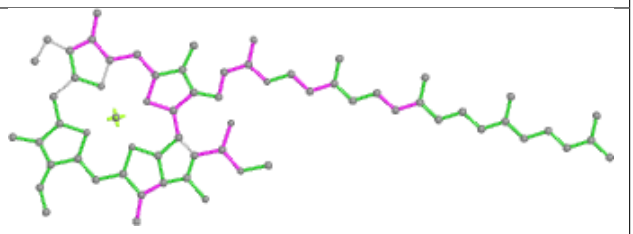


Rings

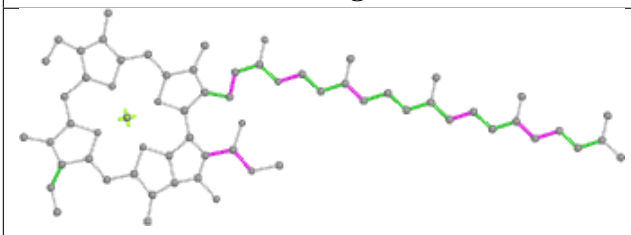
Ligand CLA cB 803



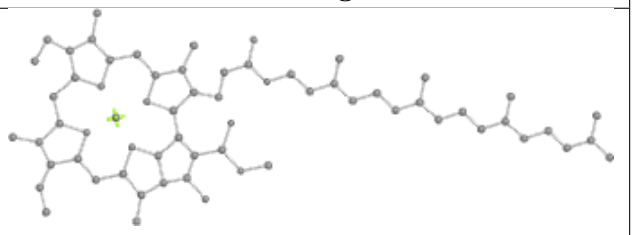
Bond lengths



Bond angles

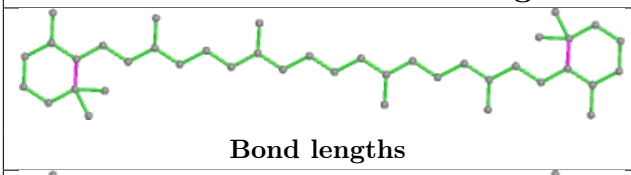


Torsions

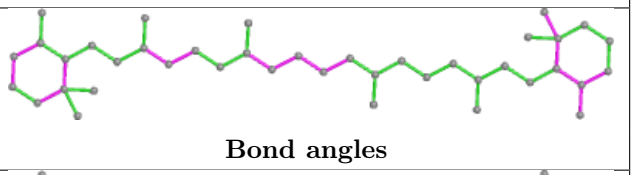


Rings

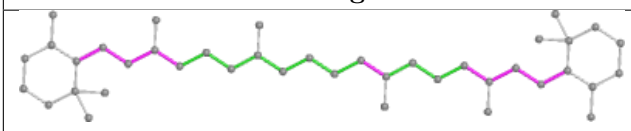
Ligand BCR cA 848



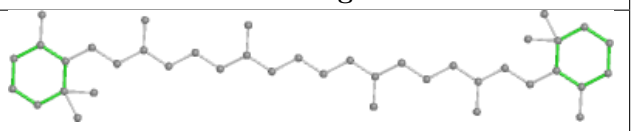
Bond lengths



Bond angles

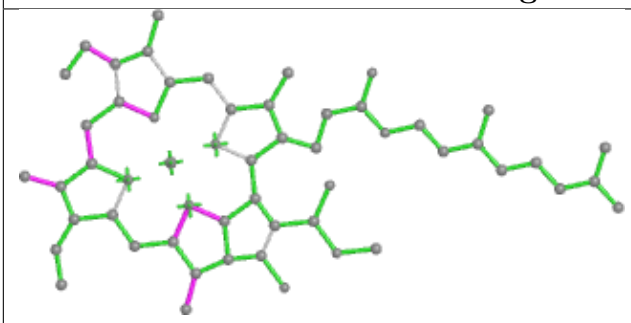


Torsions

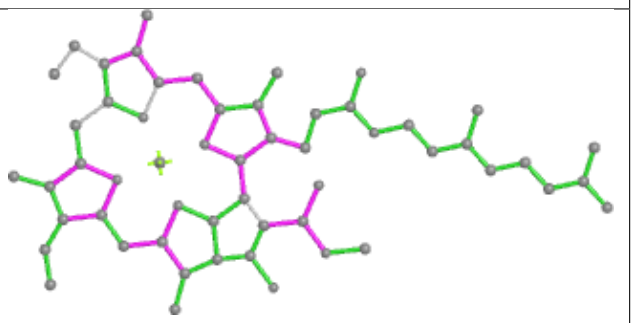


Rings

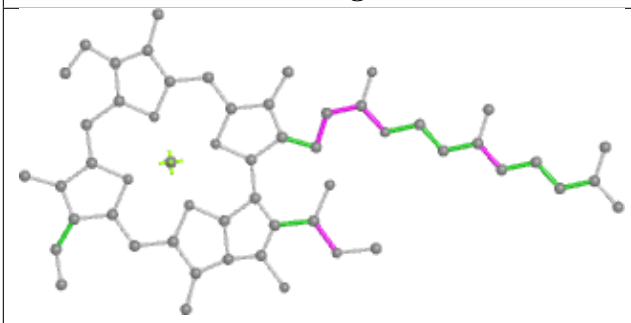
Ligand CLA a1 416



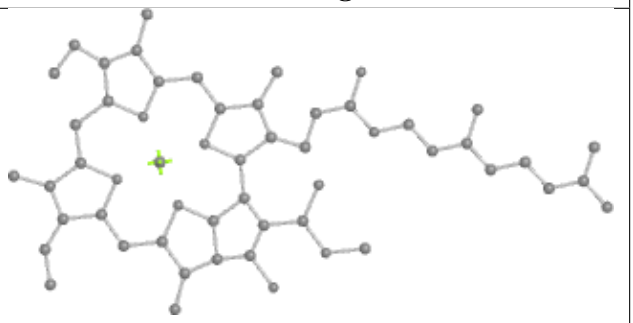
Bond lengths



Bond angles

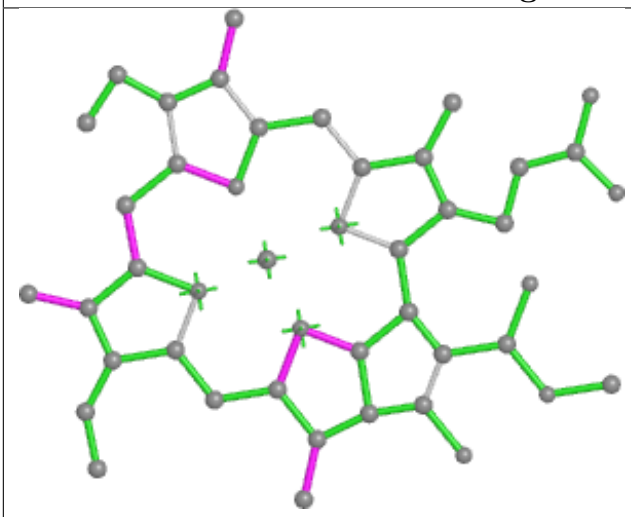


Torsions

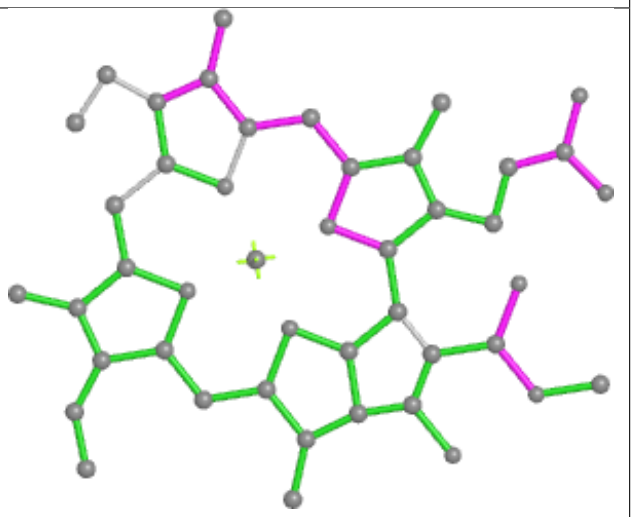


Rings

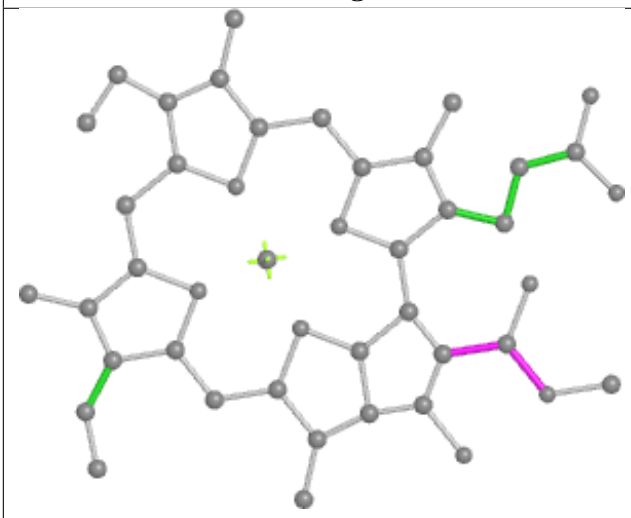
Ligand CLA a5 406



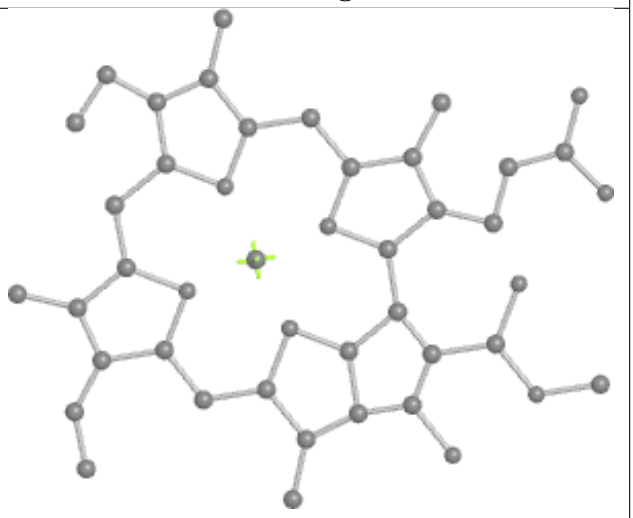
Bond lengths



Bond angles

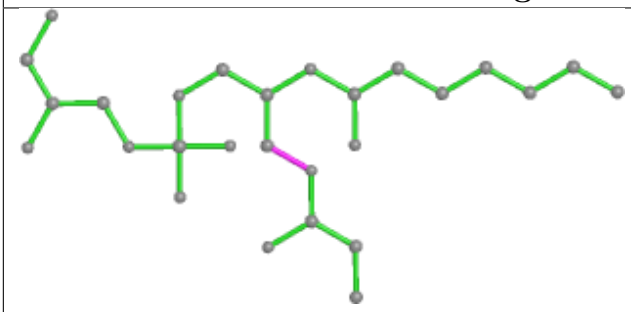


Torsions

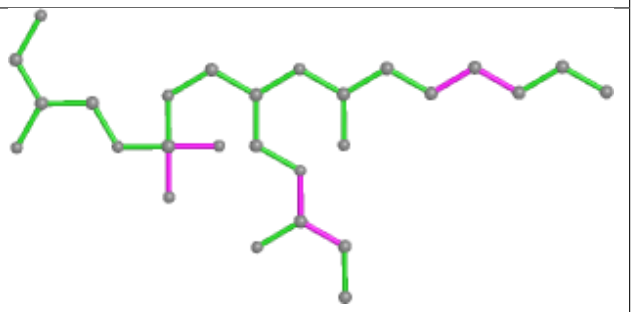


Rings

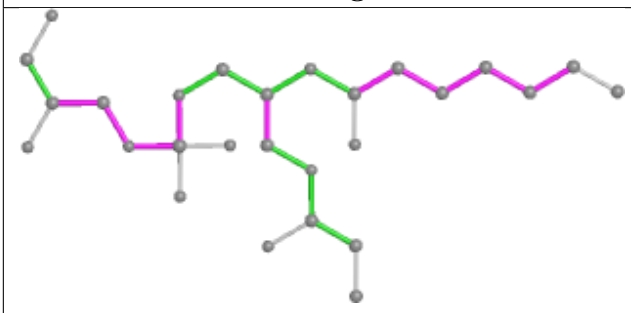
Ligand LHG cA 853



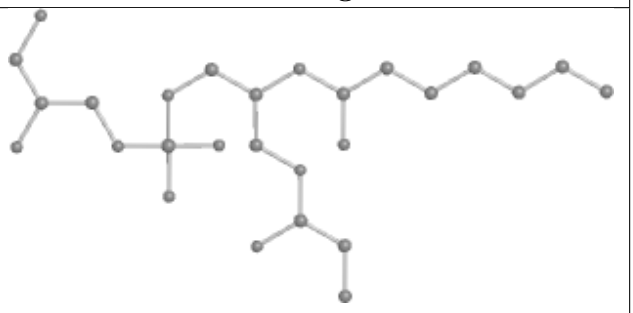
Bond lengths



Bond angles

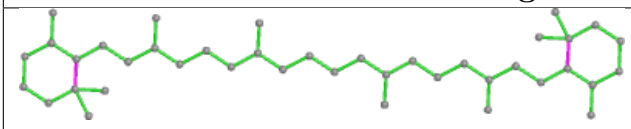


Torsions

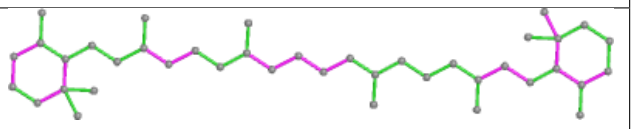


Rings

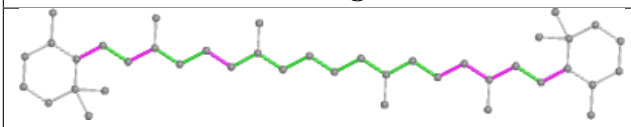
Ligand BCR c3 419



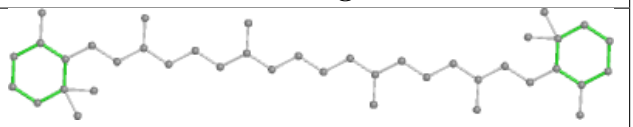
Bond lengths



Bond angles

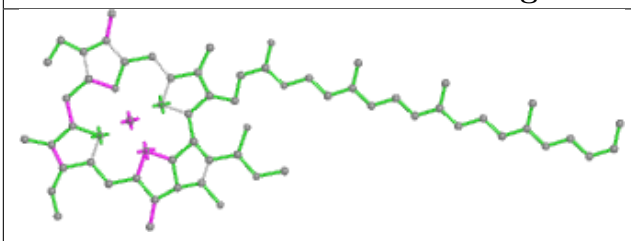


Torsions

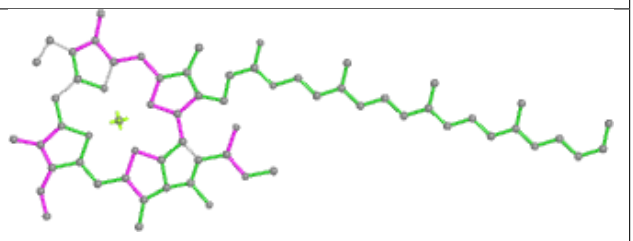


Rings

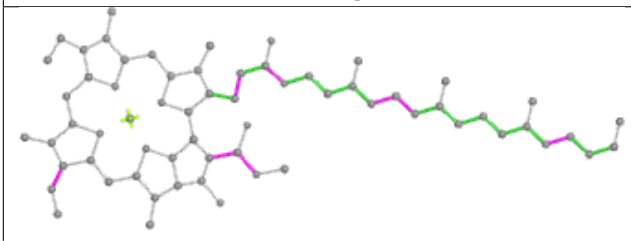
Ligand CLA c5 410



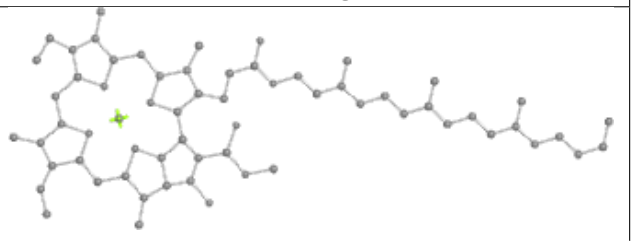
Bond lengths



Bond angles

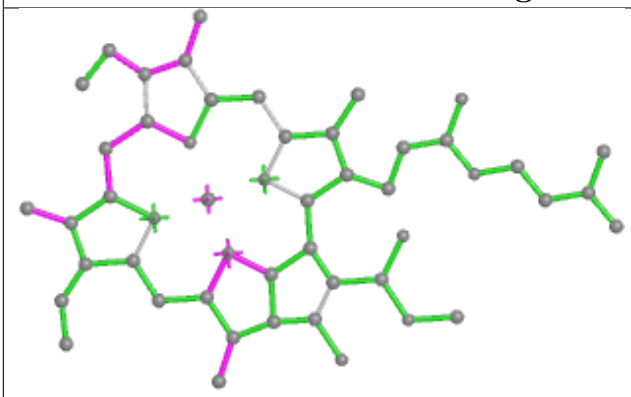


Torsions

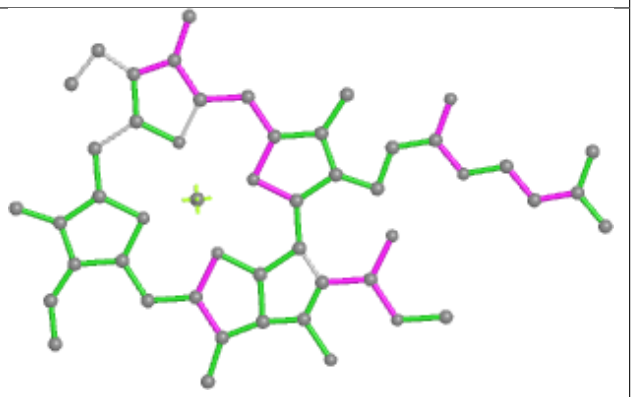


Rings

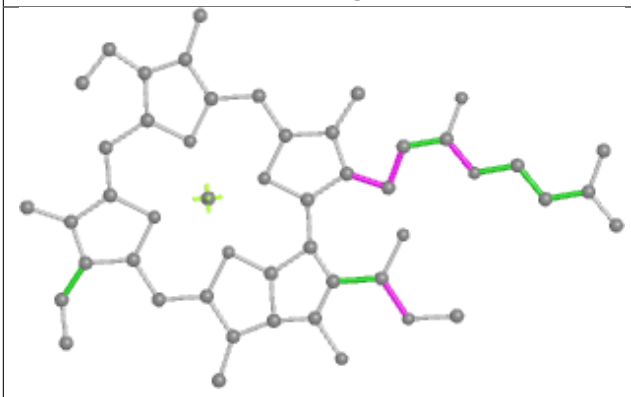
Ligand CLA aA 832



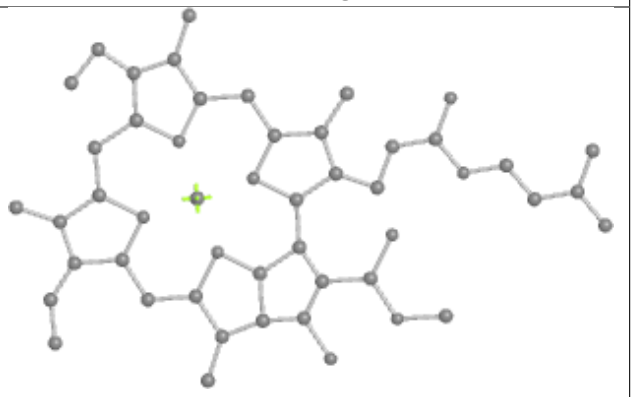
Bond lengths



Bond angles

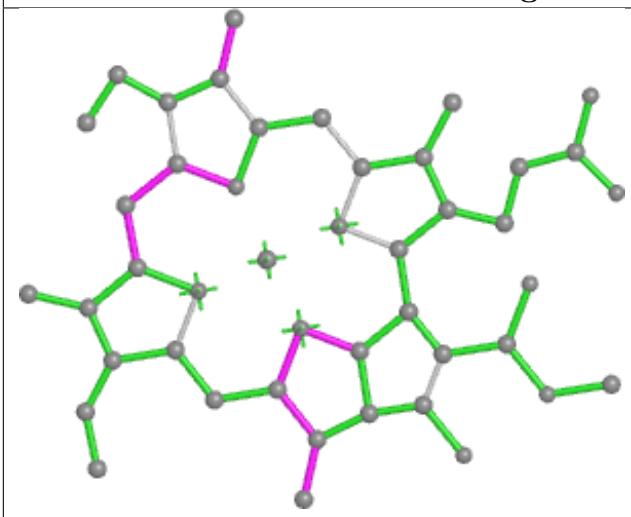


Torsions

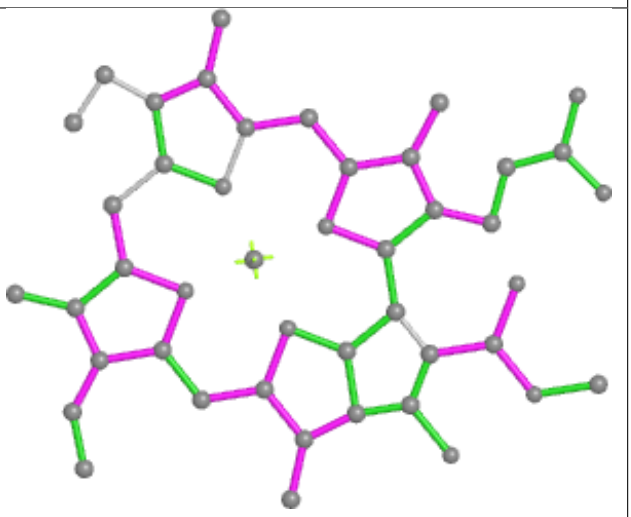


Rings

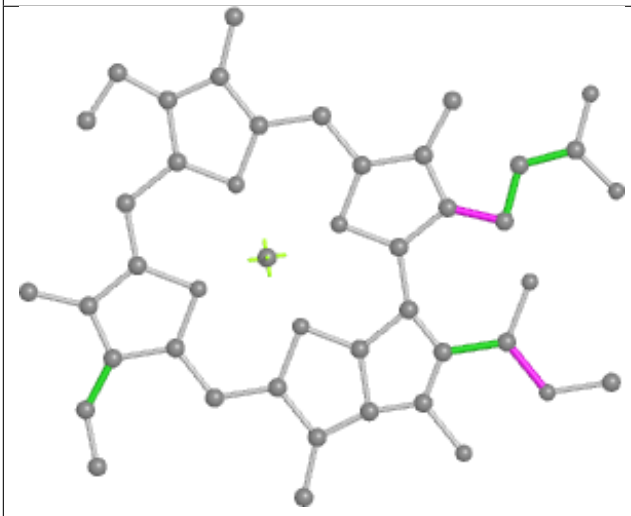
Ligand CLA c1 405



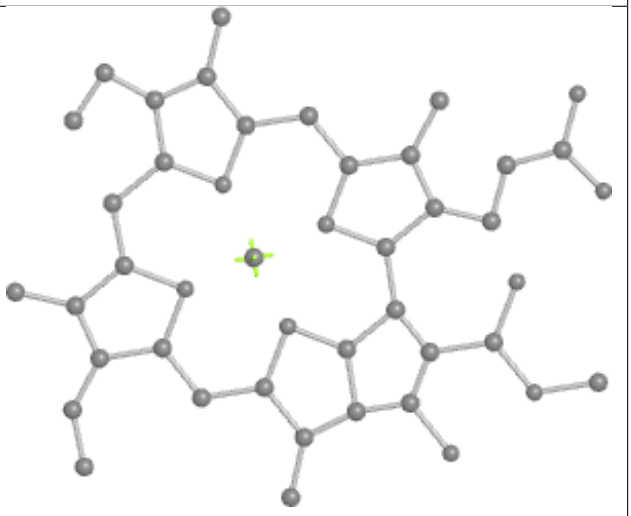
Bond lengths



Bond angles

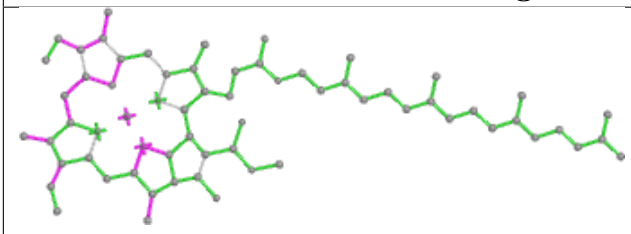


Torsions

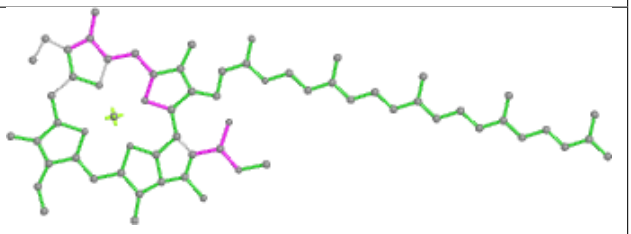


Rings

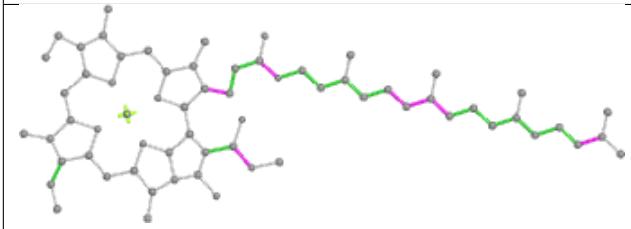
Ligand CLA aA 833



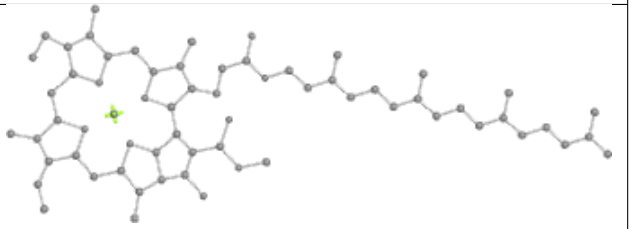
Bond lengths



Bond angles

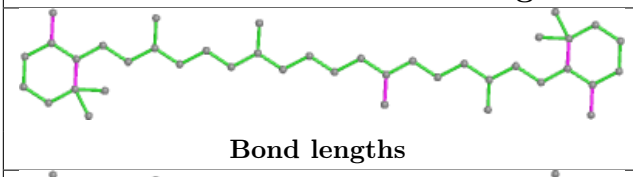


Torsions

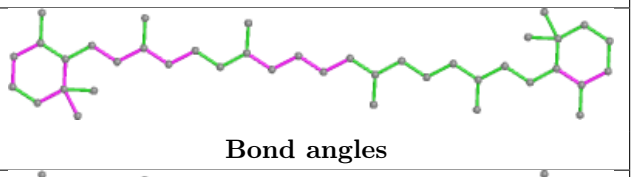


Rings

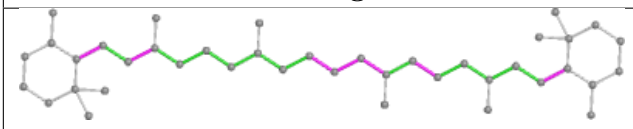
Ligand BCR cF 205



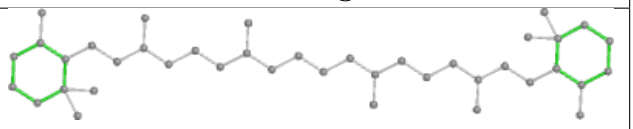
Bond lengths



Bond angles

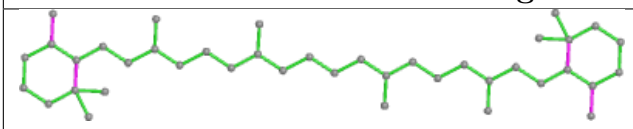


Torsions

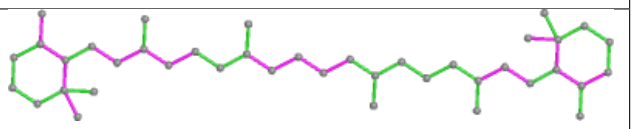


Rings

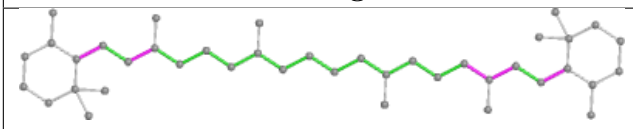
Ligand BCR cL 204



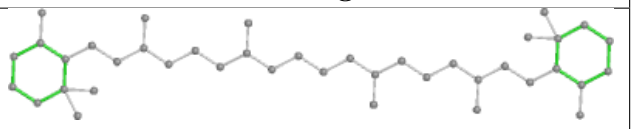
Bond lengths



Bond angles

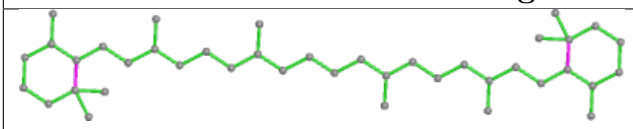


Torsions

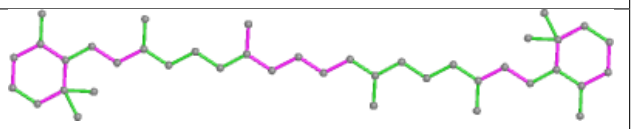


Rings

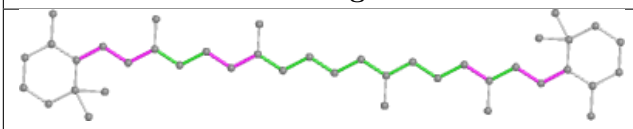
Ligand BCR a6 420



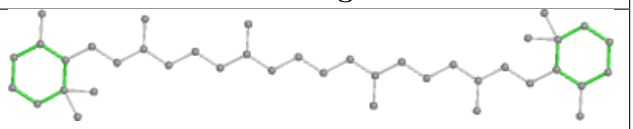
Bond lengths



Bond angles

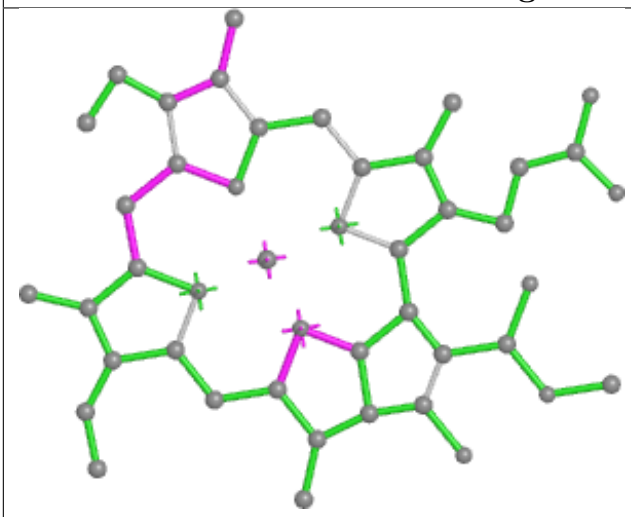


Torsions

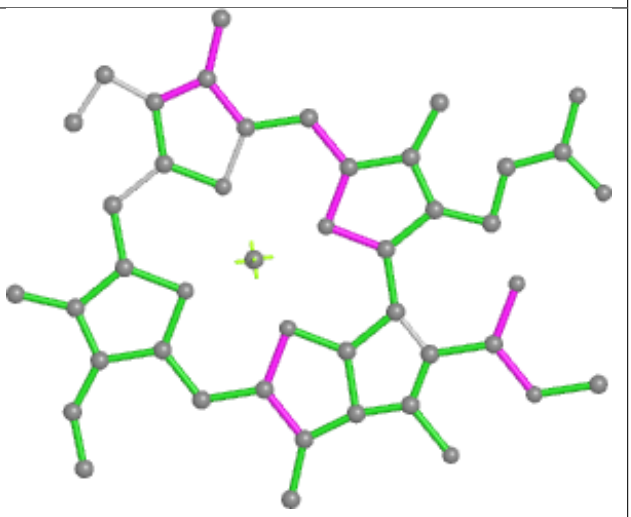


Rings

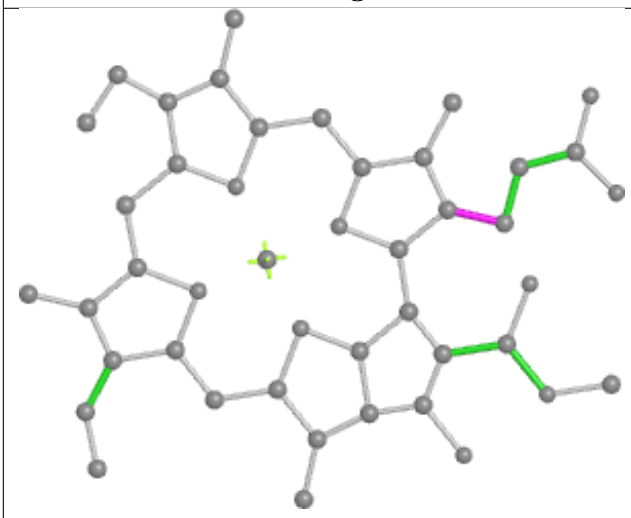
Ligand CLA b2 414



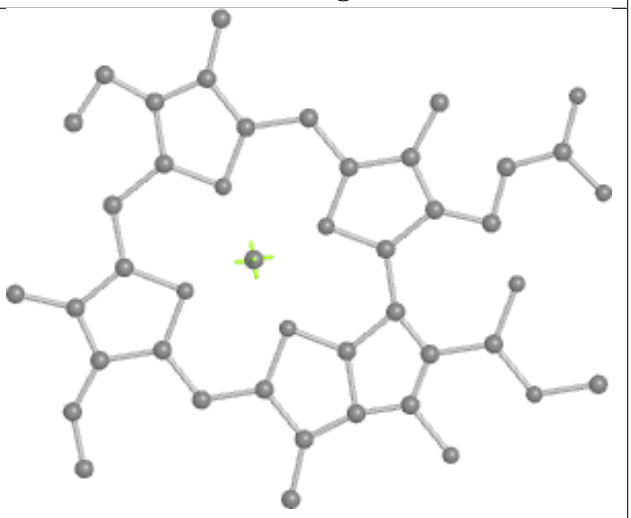
Bond lengths



Bond angles

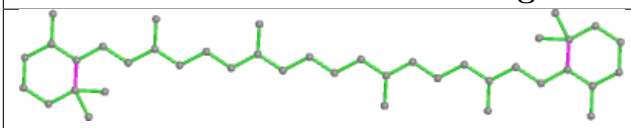


Torsions

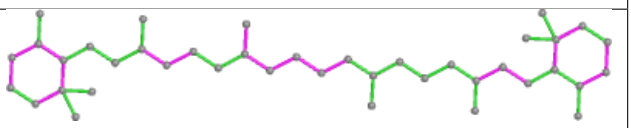


Rings

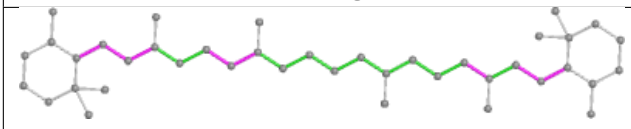
Ligand BCR a4 420



Bond lengths



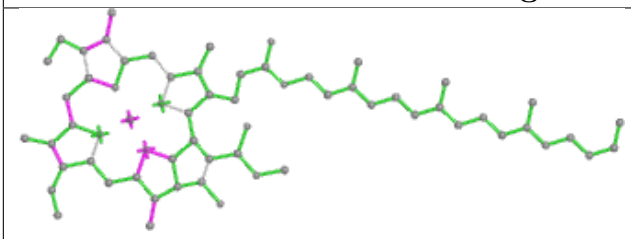
Bond angles



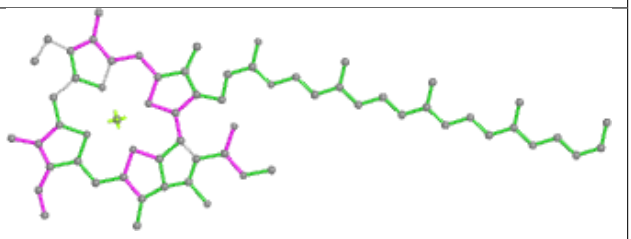
Torsions

Rings

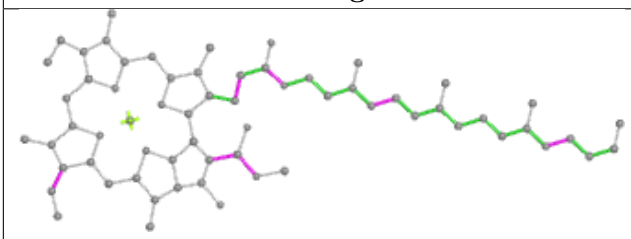
Ligand CLA c3 410



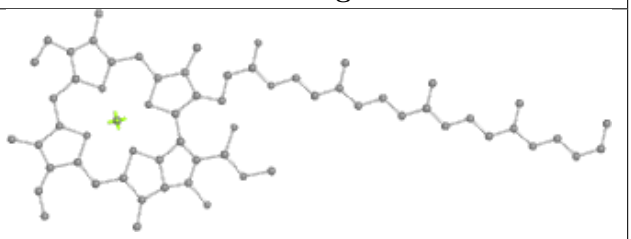
Bond lengths



Bond angles

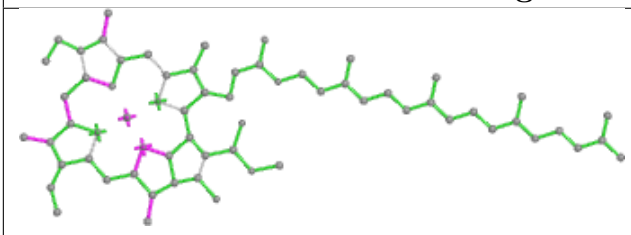


Torsions

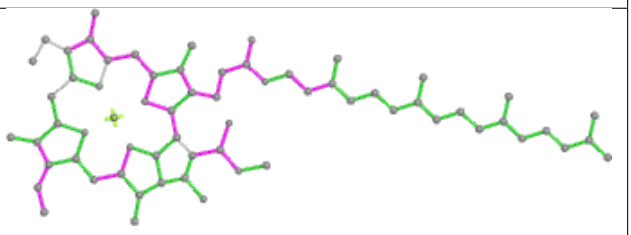


Rings

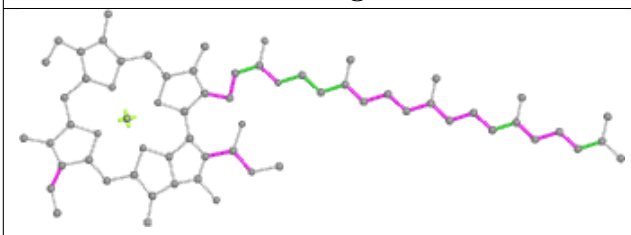
Ligand CLA aB 814



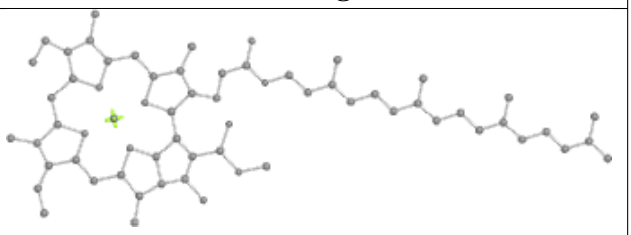
Bond lengths



Bond angles

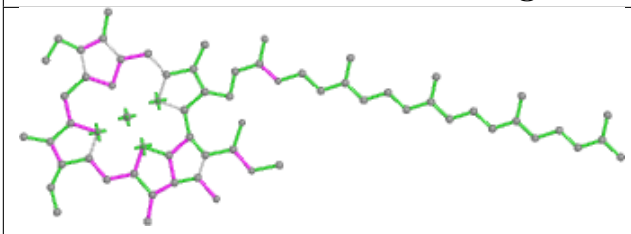


Torsions

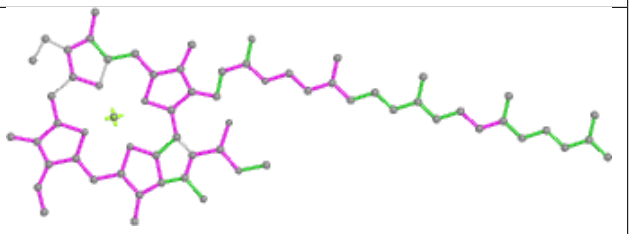


Rings

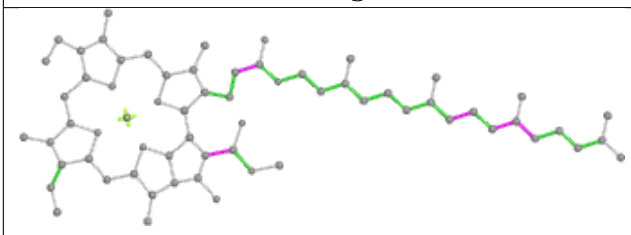
Ligand CL0 bA 801



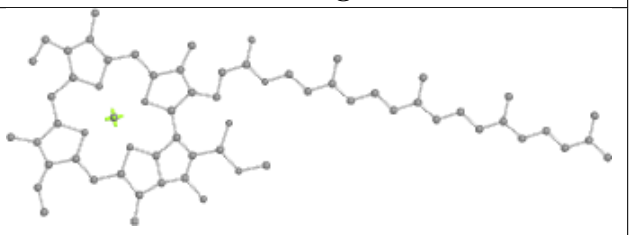
Bond lengths



Bond angles

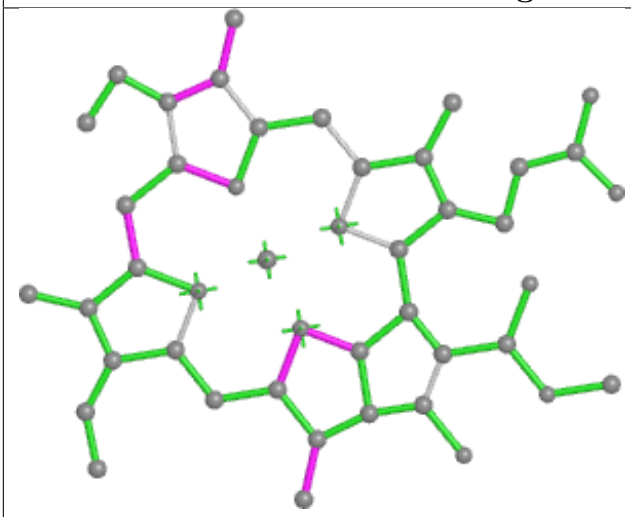


Torsions

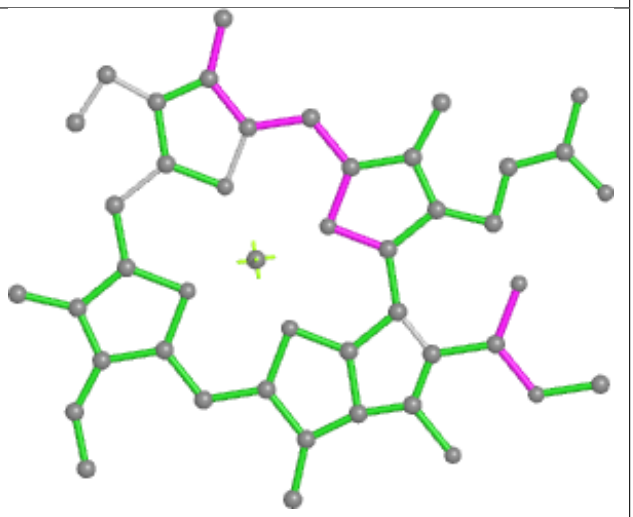


Rings

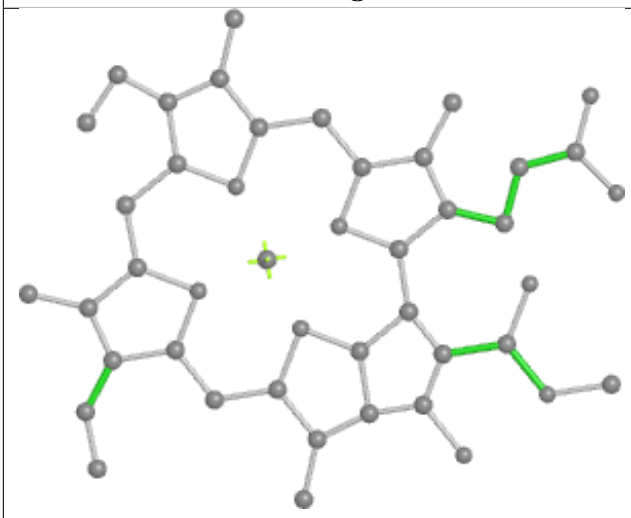
Ligand CLA cB 842



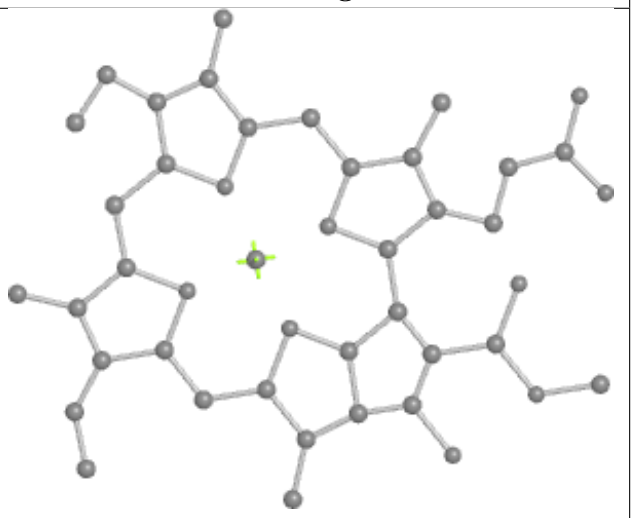
Bond lengths



Bond angles

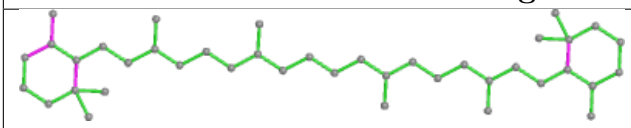


Torsions

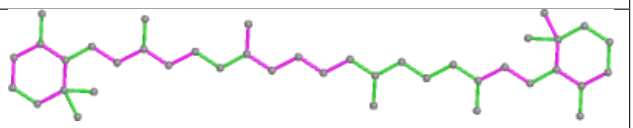


Rings

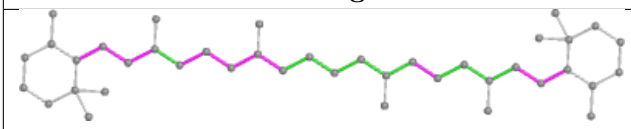
Ligand BCR c5 401



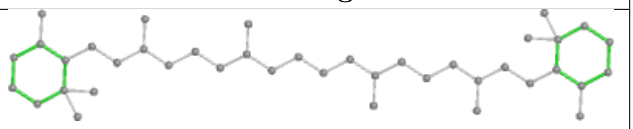
Bond lengths



Bond angles

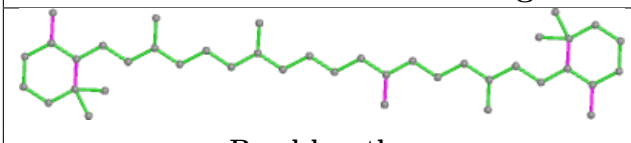


Torsions

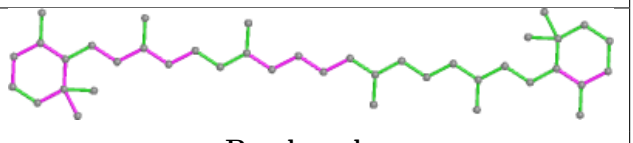


Rings

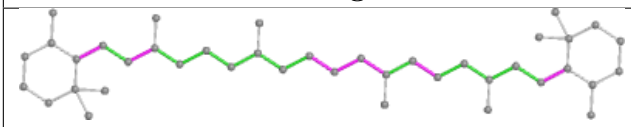
Ligand BCR bJ 105



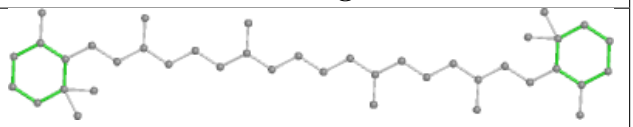
Bond lengths



Bond angles

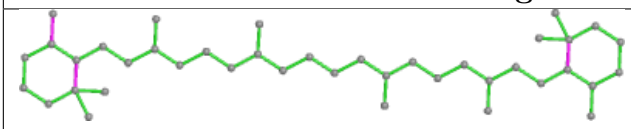


Torsions

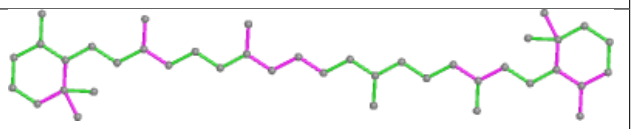


Rings

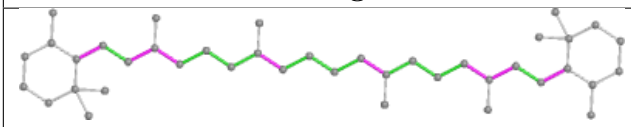
Ligand BCR aF 202



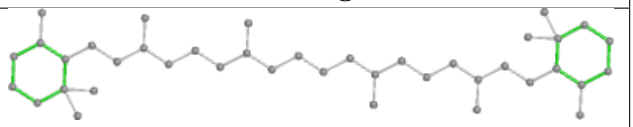
Bond lengths



Bond angles

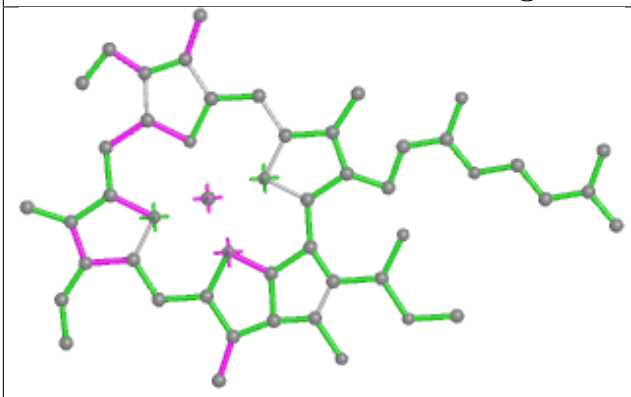


Torsions

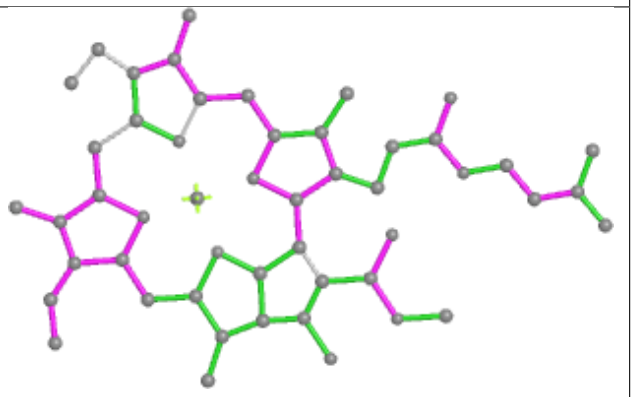


Rings

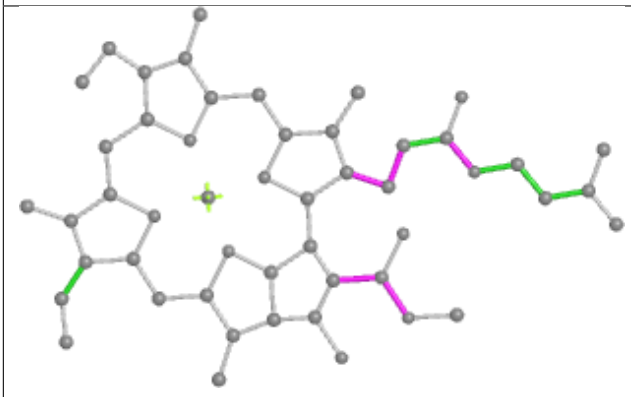
Ligand CLA b3 416



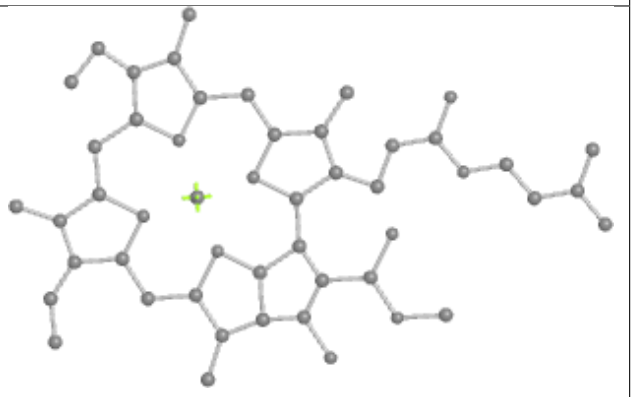
Bond lengths



Bond angles

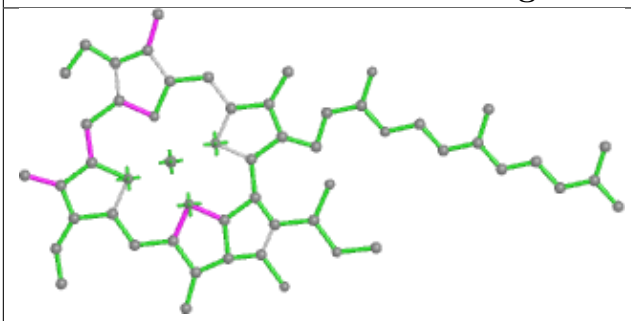


Torsions

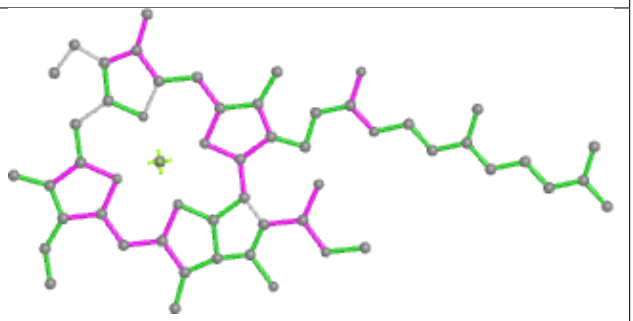


Rings

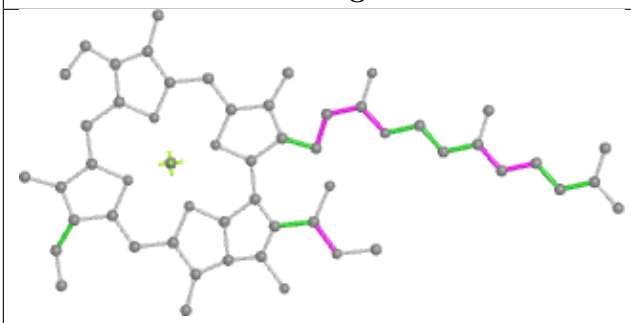
Ligand CLA b3 417



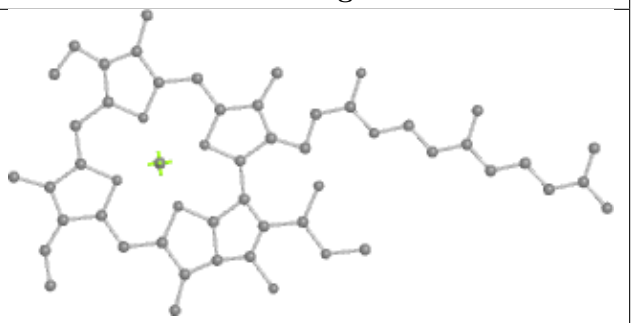
Bond lengths



Bond angles

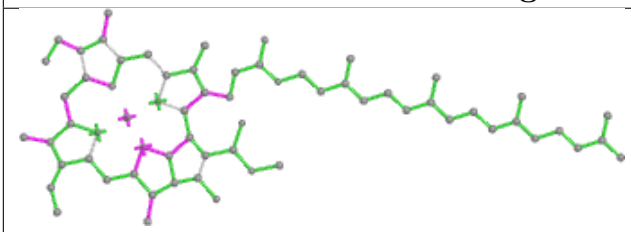


Torsions

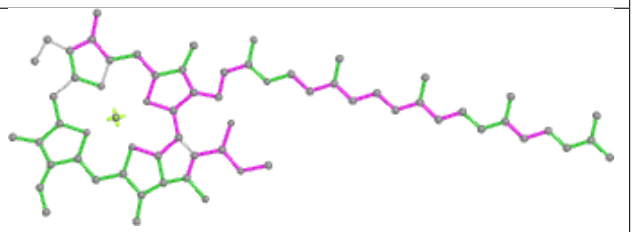


Rings

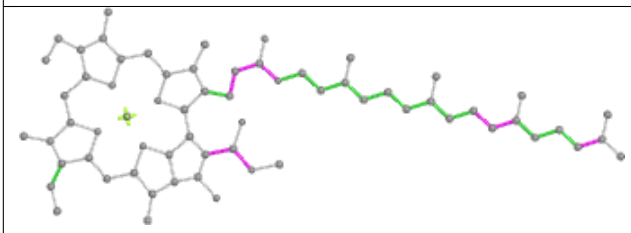
Ligand CLA a1 422



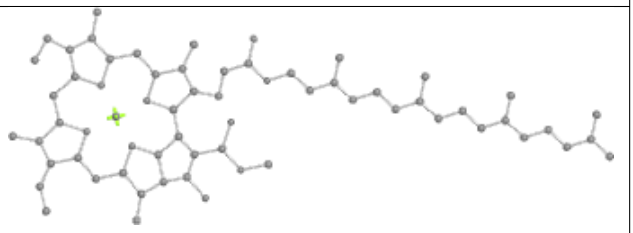
Bond lengths



Bond angles



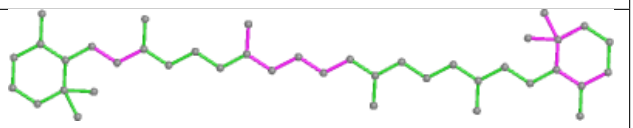
Torsions



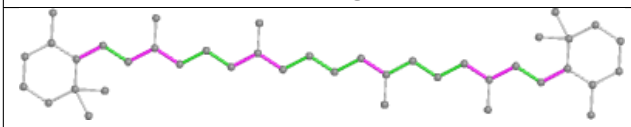
Rings

Ligand BCR bB 846

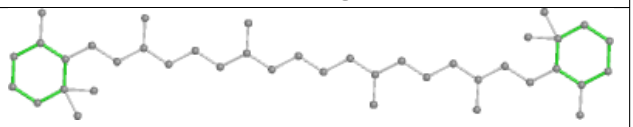
Bond lengths



Bond angles

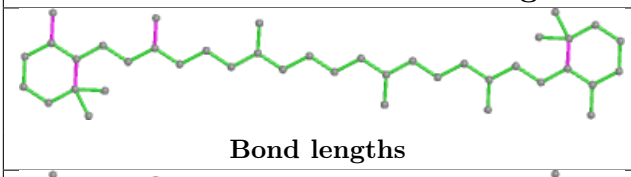


Torsions

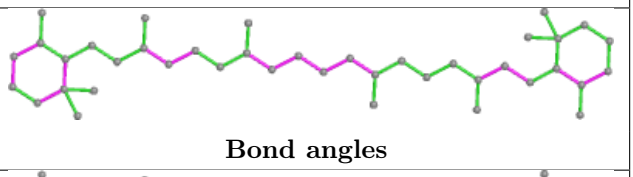


Rings

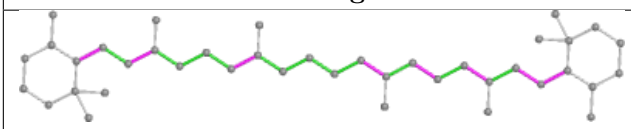
Ligand BCR aI 102



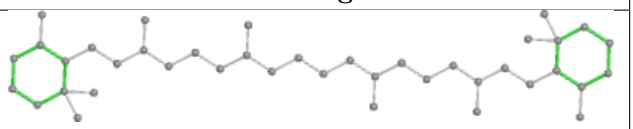
Bond lengths



Bond angles

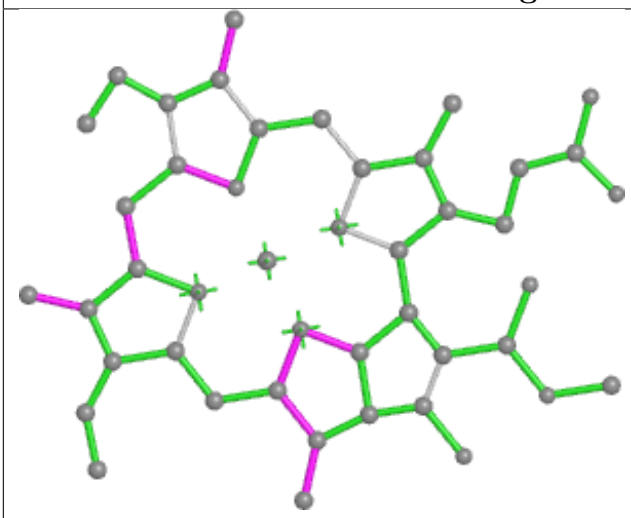


Torsions

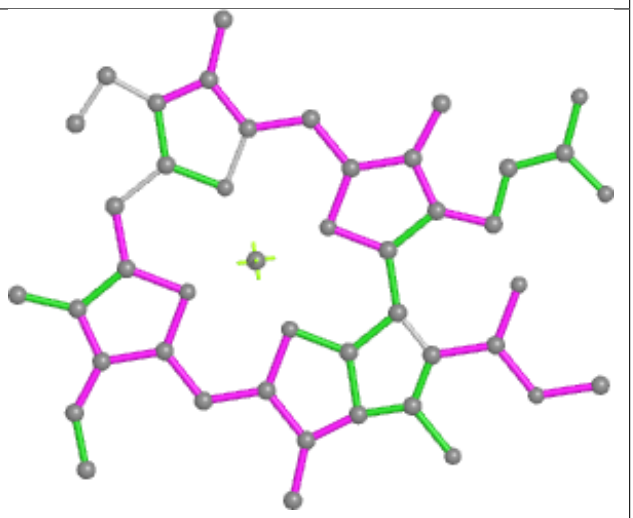


Rings

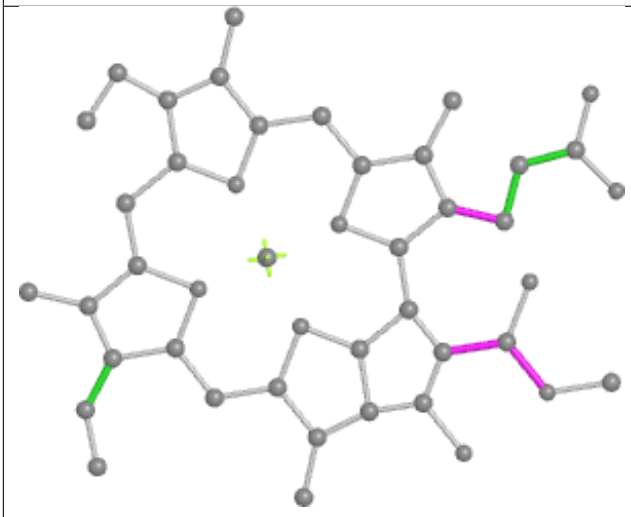
Ligand CLA a5 405



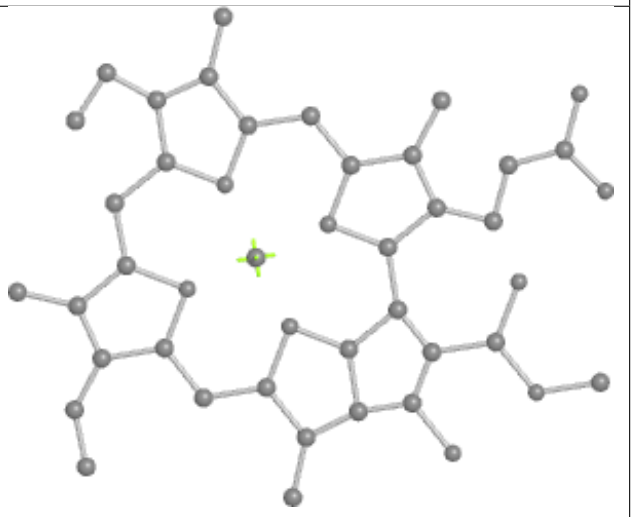
Bond lengths



Bond angles

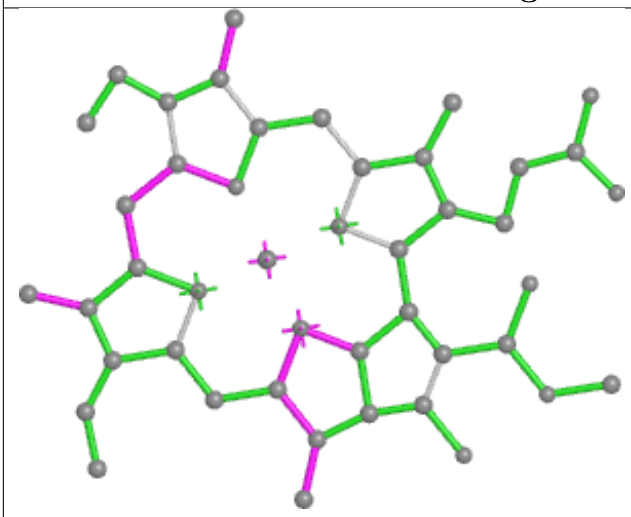


Torsions

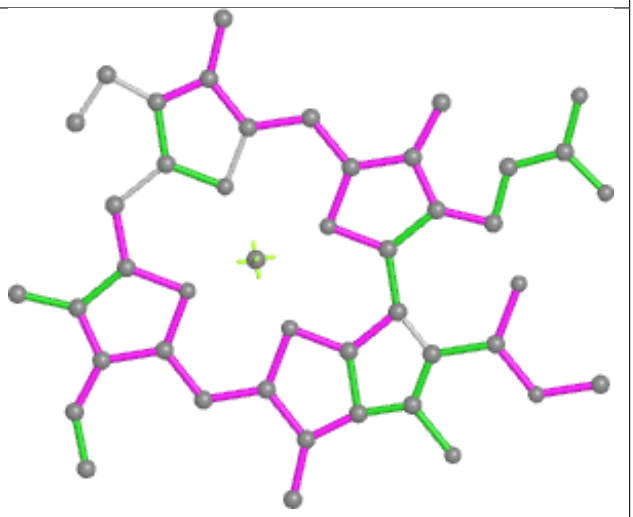


Rings

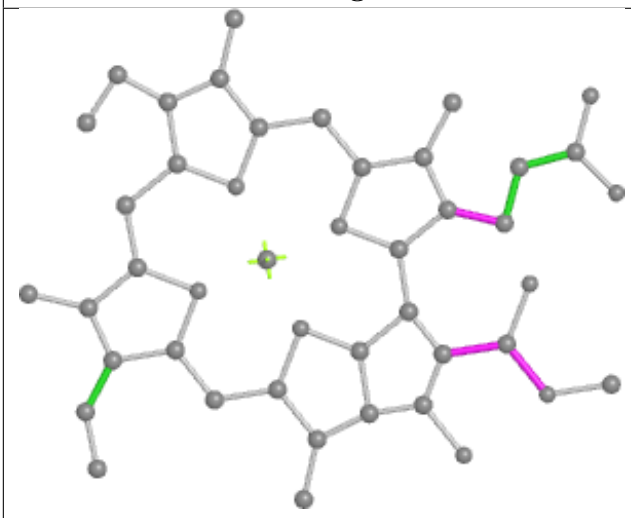
Ligand CLA c4 405



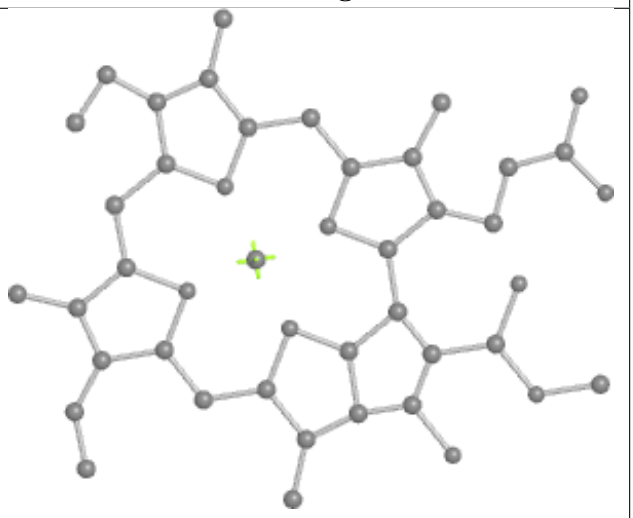
Bond lengths



Bond angles

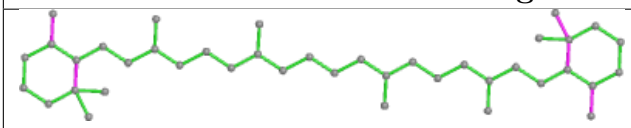


Torsions

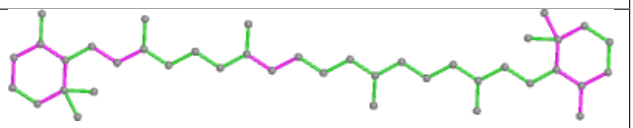


Rings

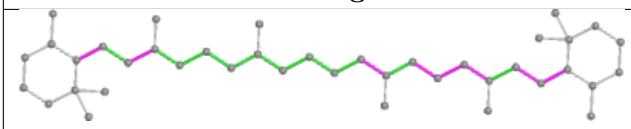
Ligand BCR b5 418



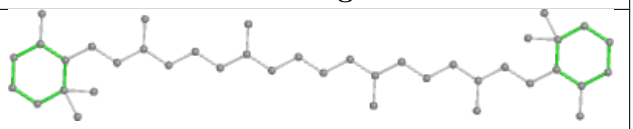
Bond lengths



Bond angles

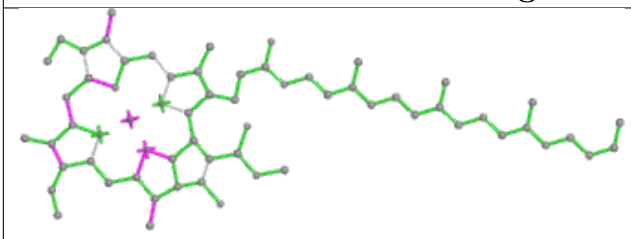


Torsions

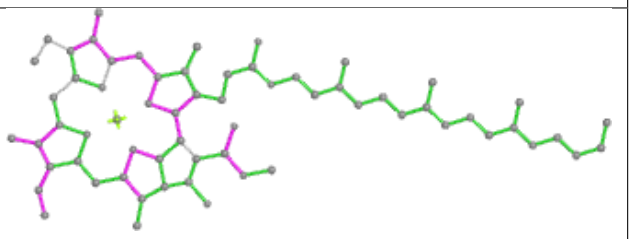


Rings

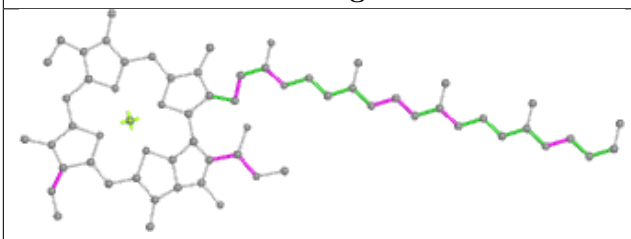
Ligand CLA b6 411



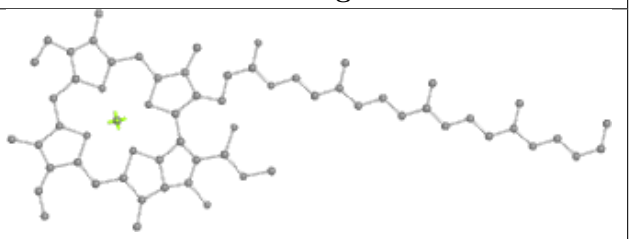
Bond lengths



Bond angles

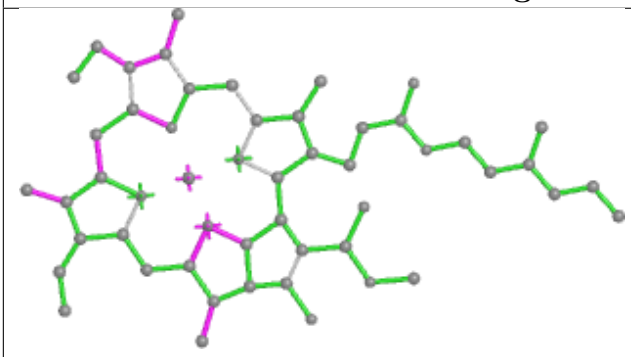


Torsions

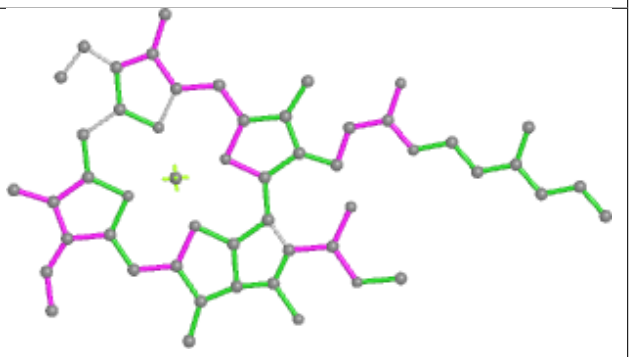


Rings

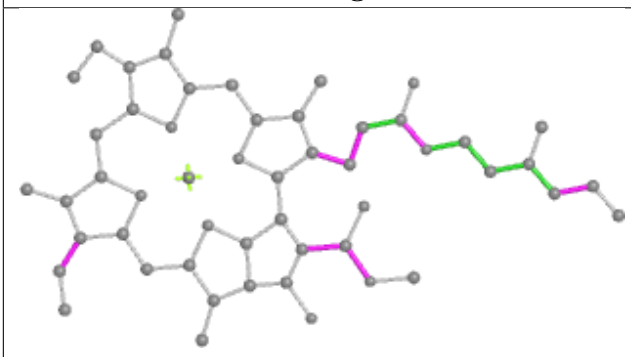
Ligand CLA bA 845



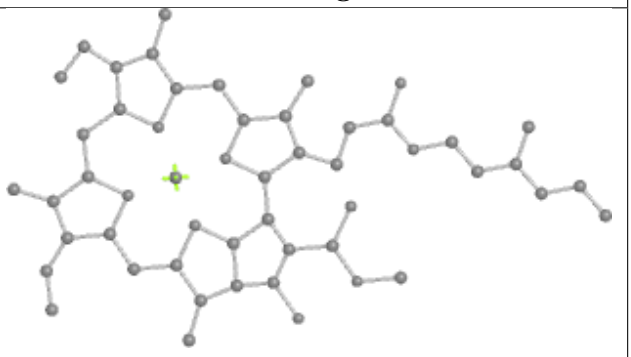
Bond lengths



Bond angles

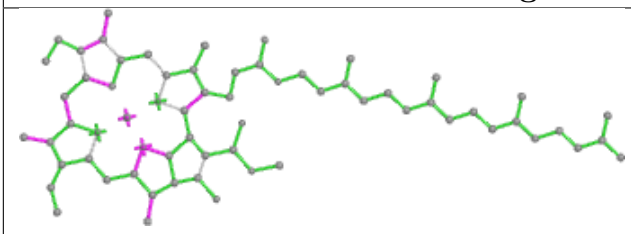


Torsions

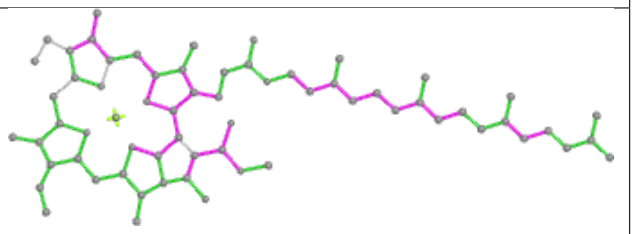


Rings

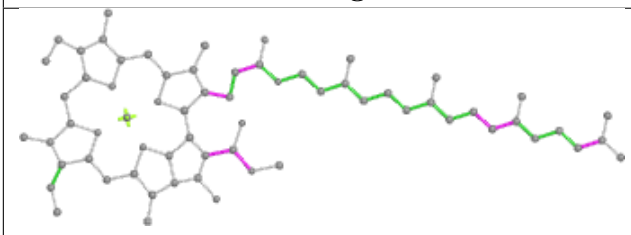
Ligand CLA a5 420



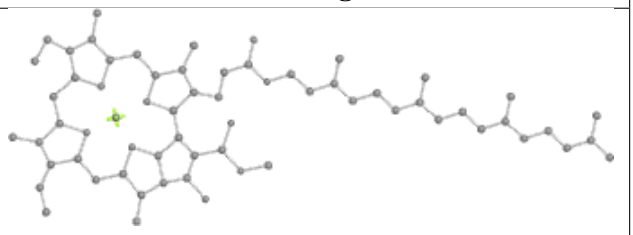
Bond lengths



Bond angles

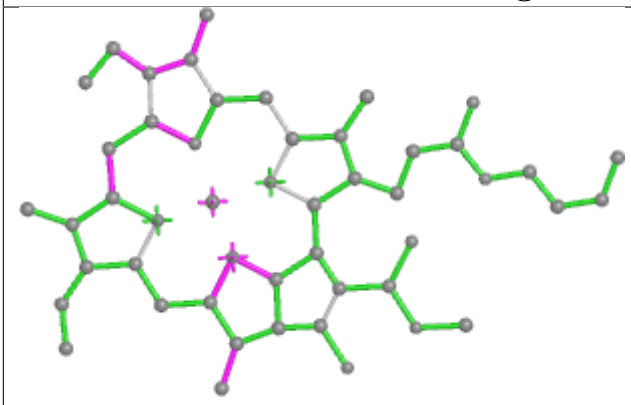


Torsions

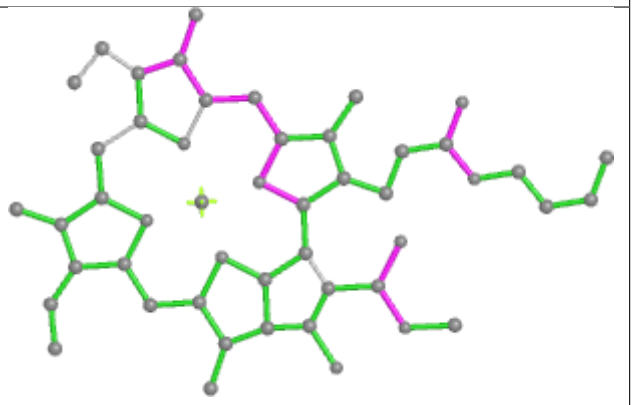


Rings

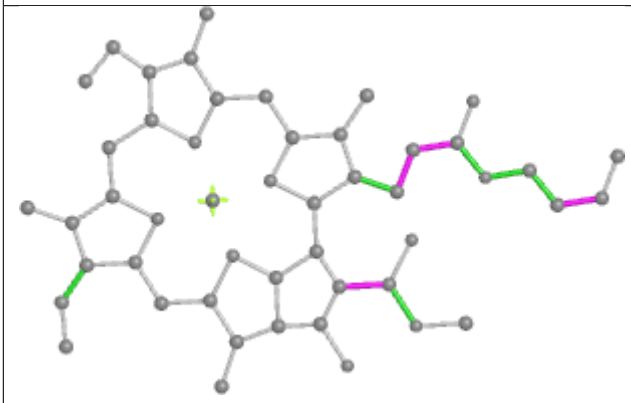
Ligand CLA cA 823



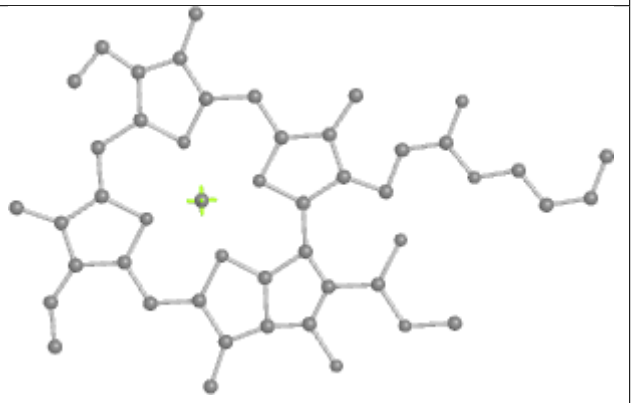
Bond lengths



Bond angles

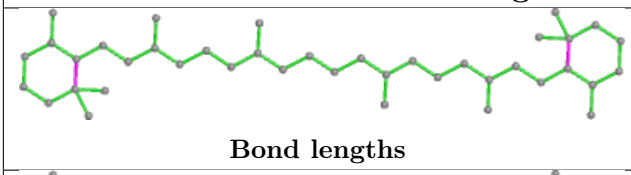


Torsions

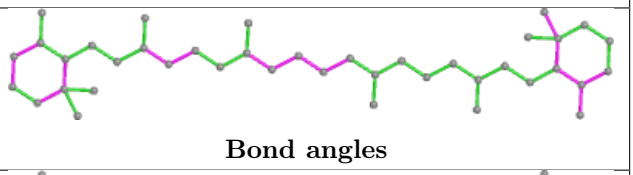


Rings

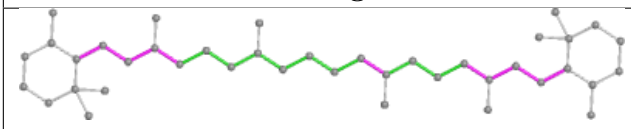
Ligand BCR bA 850



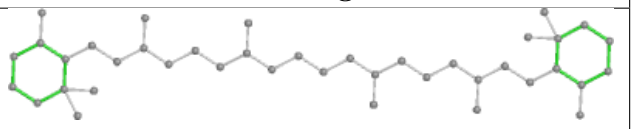
Bond lengths



Bond angles

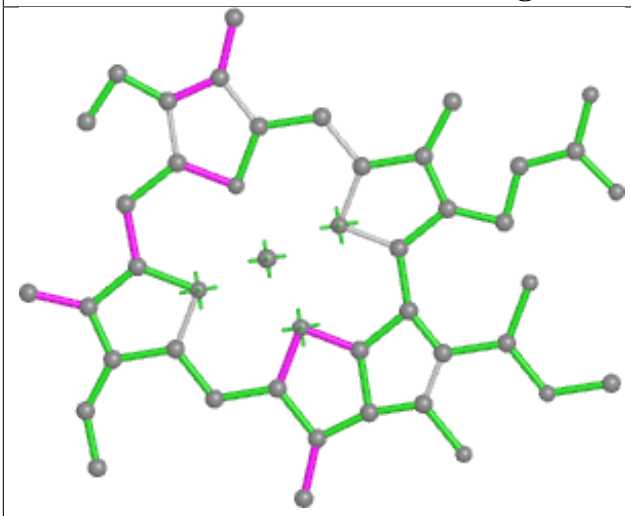


Torsions

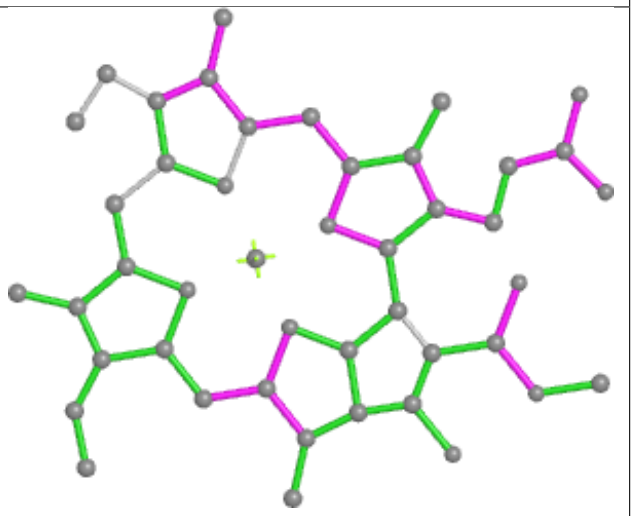


Rings

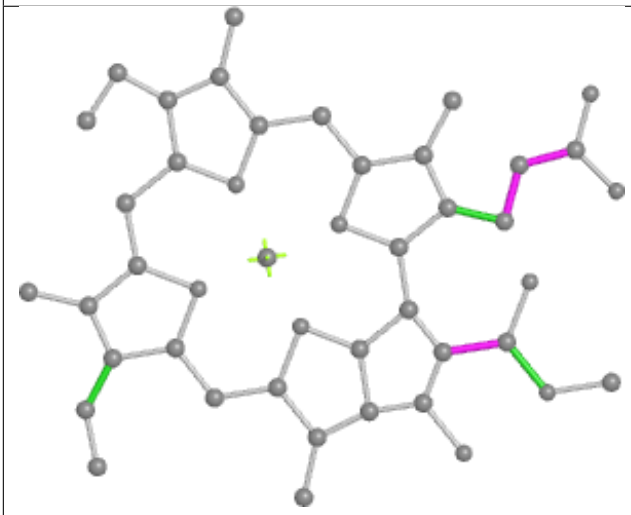
Ligand CLA cB 824



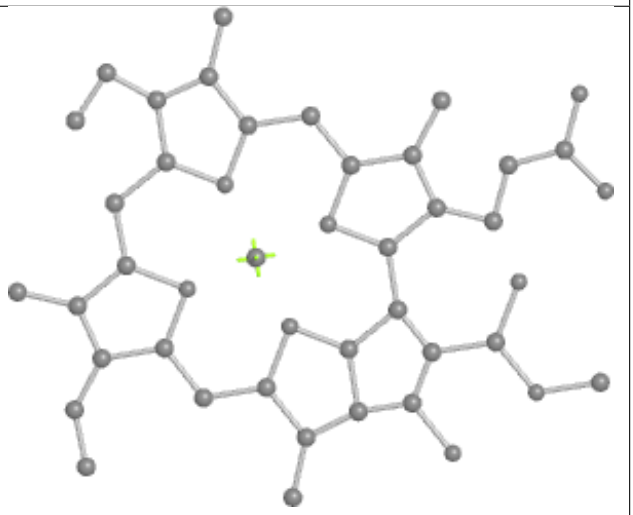
Bond lengths



Bond angles

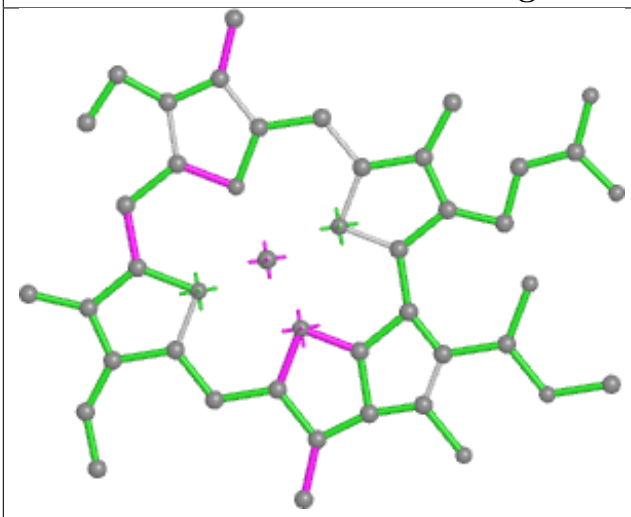


Torsions

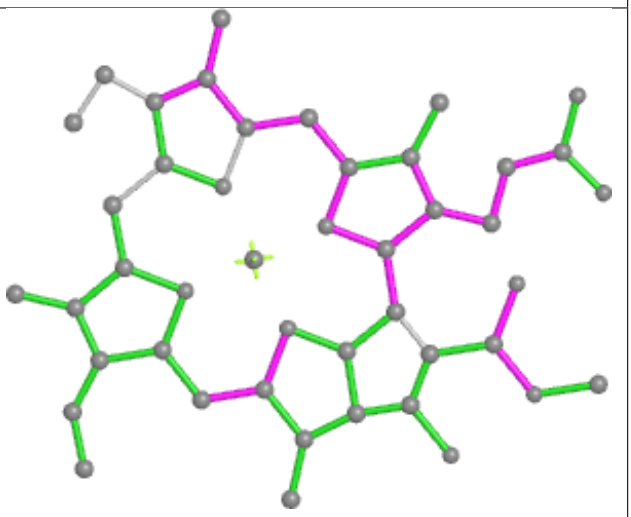


Rings

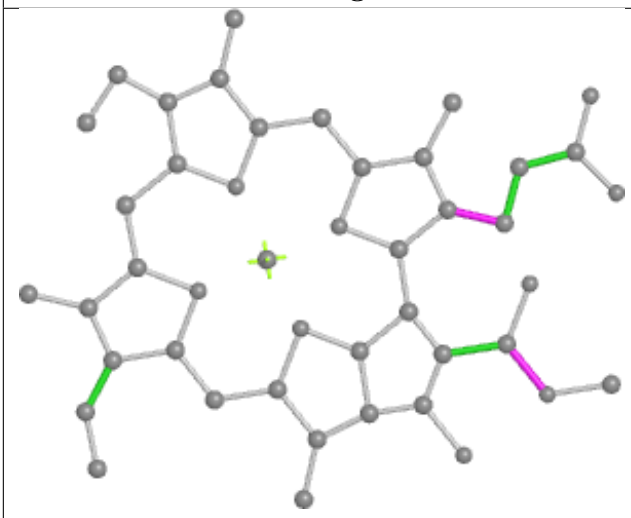
Ligand CLA b6 412



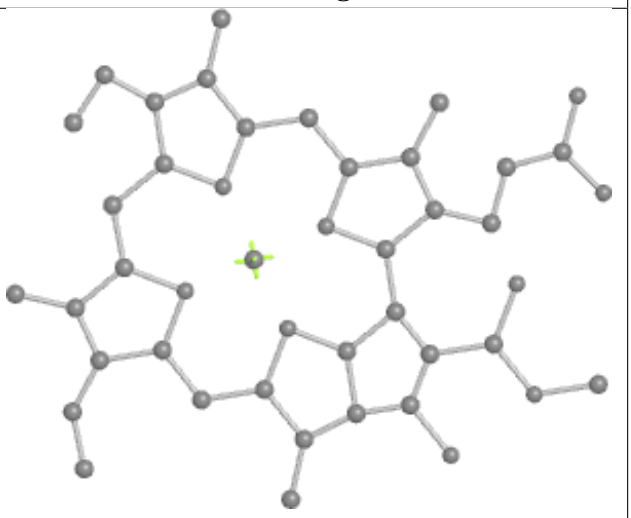
Bond lengths



Bond angles

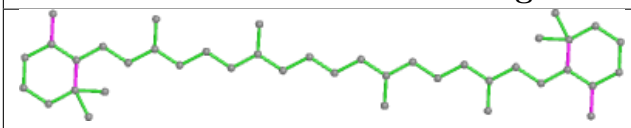


Torsions

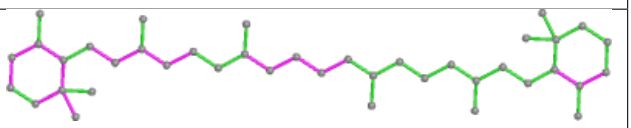


Rings

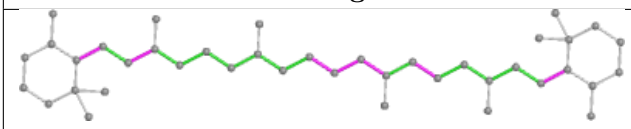
Ligand BCR aF 203



Bond lengths



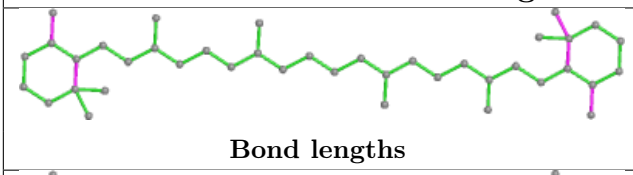
Bond angles

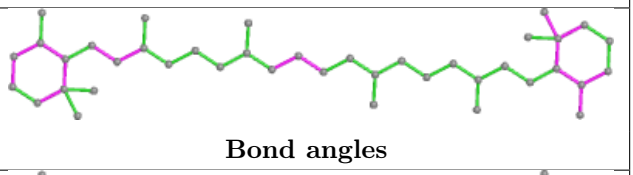


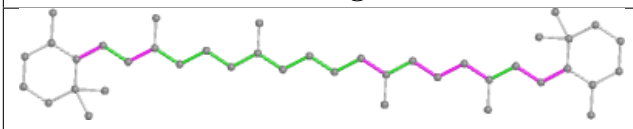
Torsions

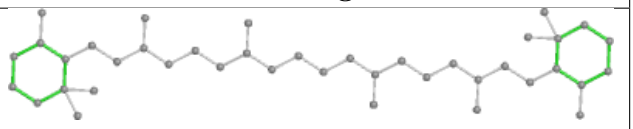
Rings

Ligand BCR a3 418

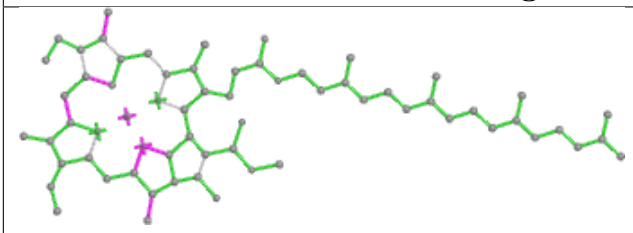

Bond lengths

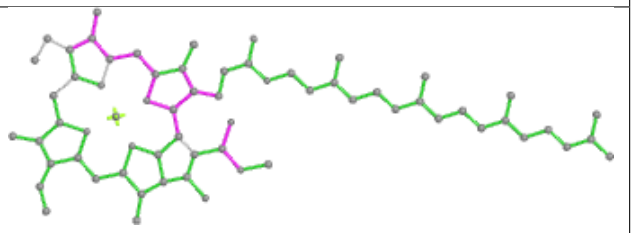

Bond angles

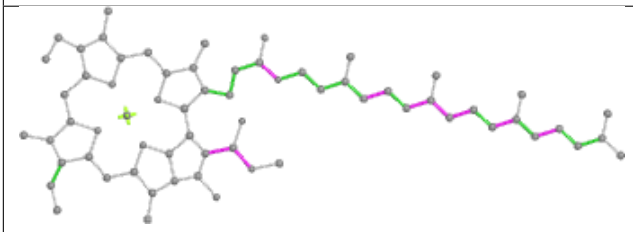

Torsions

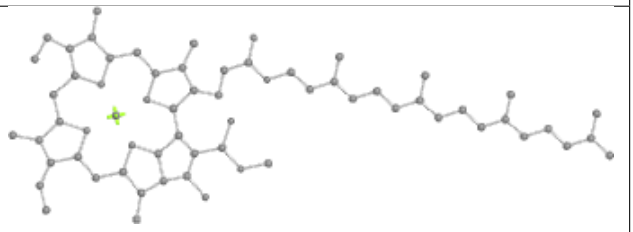

Rings

Ligand CLA c2 403

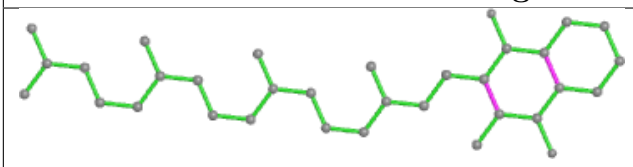

Bond lengths

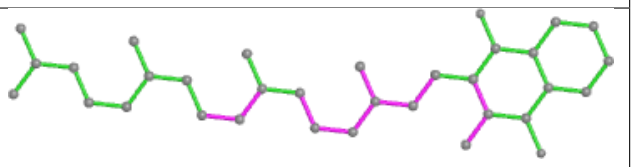

Bond angles

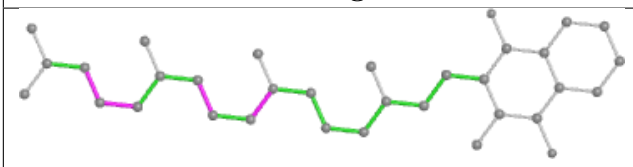

Torsions

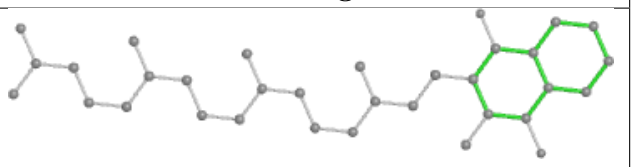

Rings

Ligand PQN aA 846

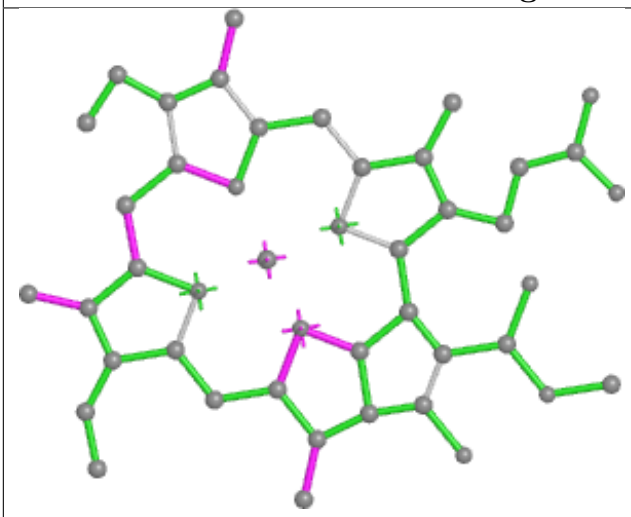

Bond lengths


Bond angles

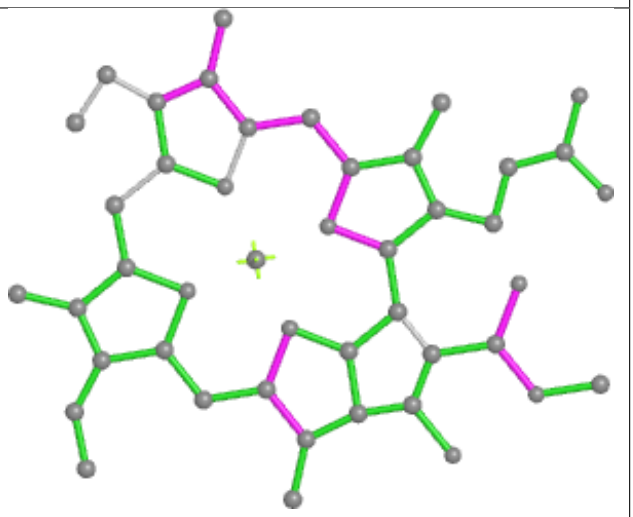

Torsions


Rings

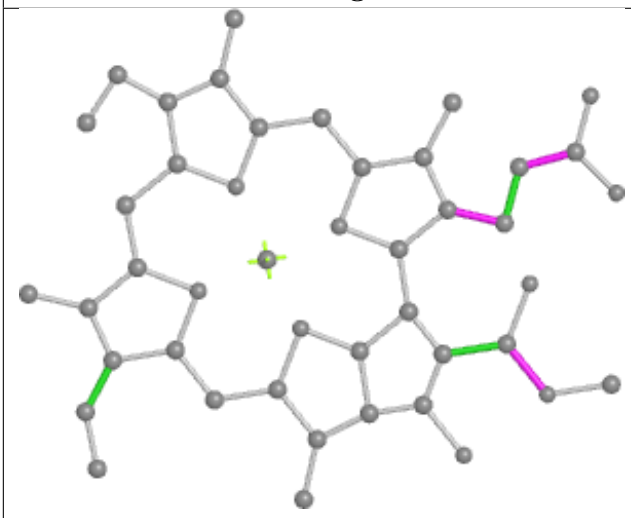
Ligand CLA a6 409



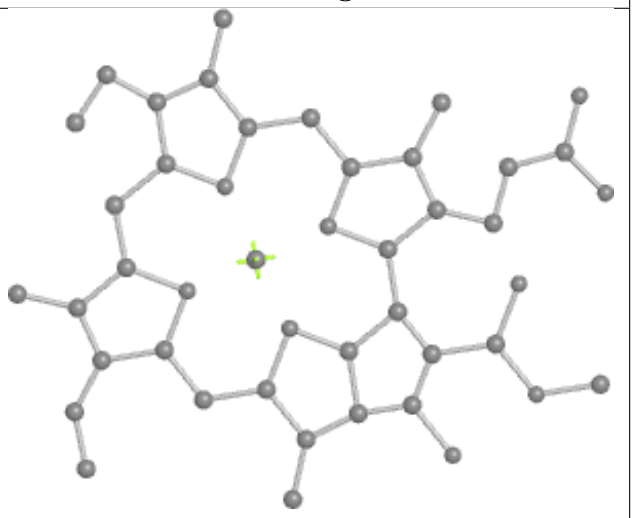
Bond lengths



Bond angles

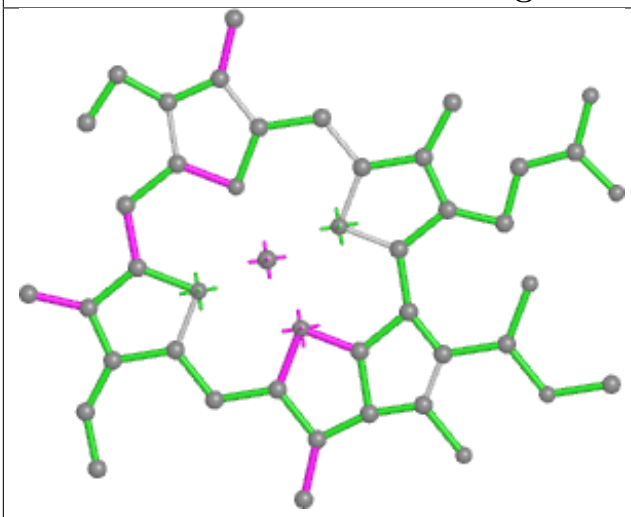


Torsions

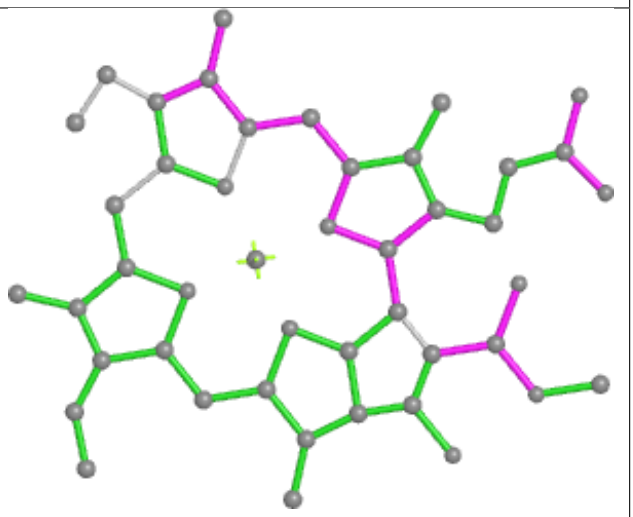


Rings

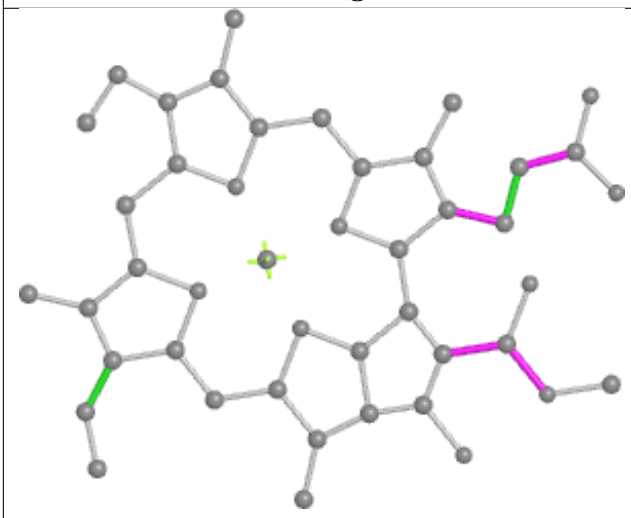
Ligand CLA cK 102



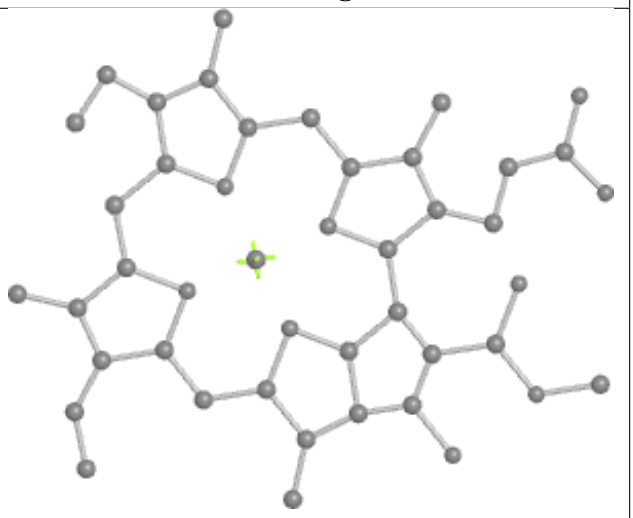
Bond lengths



Bond angles

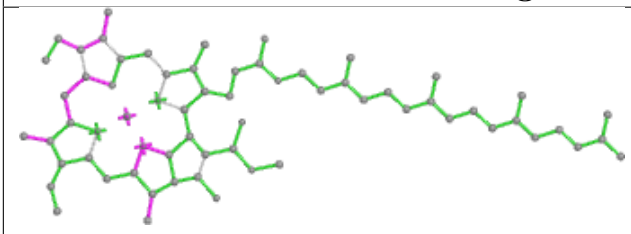


Torsions

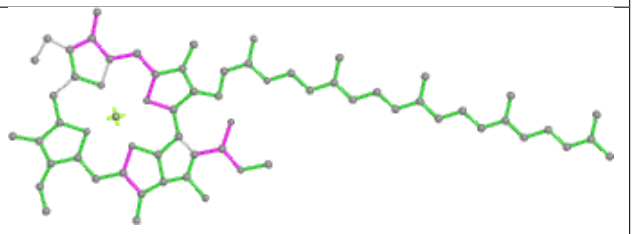


Rings

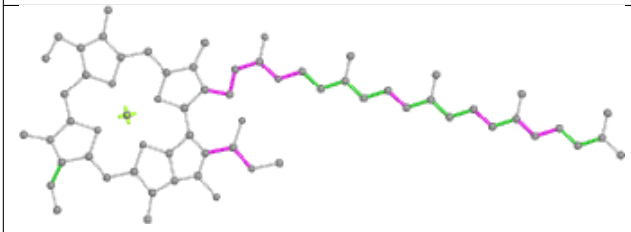
Ligand CLA cB 829



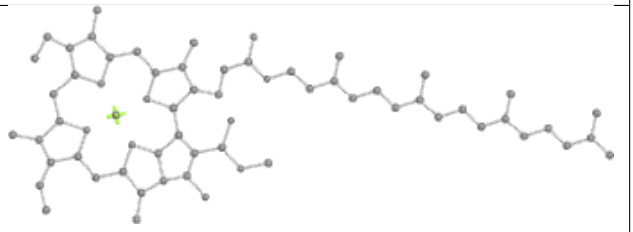
Bond lengths



Bond angles

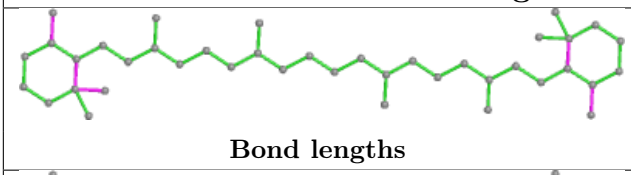


Torsions

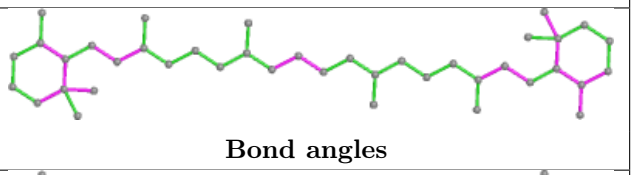


Rings

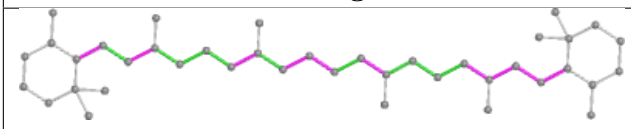
Ligand BCR bB 849



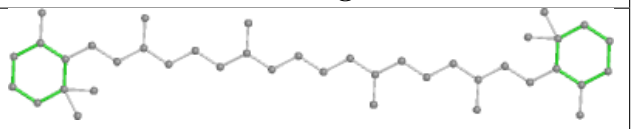
Bond lengths



Bond angles

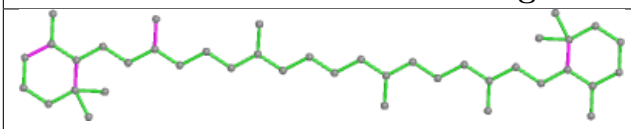


Torsions

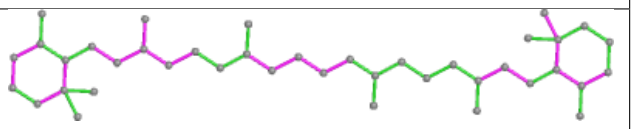


Rings

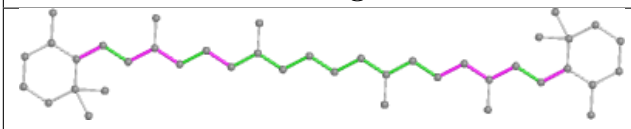
Ligand BCR c6 401



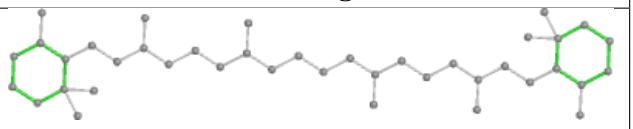
Bond lengths



Bond angles

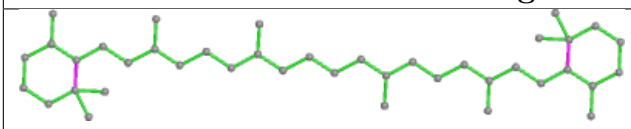


Torsions

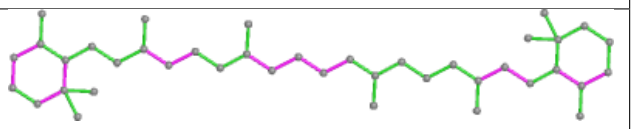


Rings

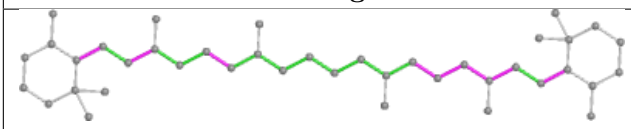
Ligand BCR a4 419



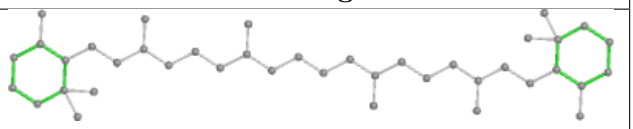
Bond lengths



Bond angles

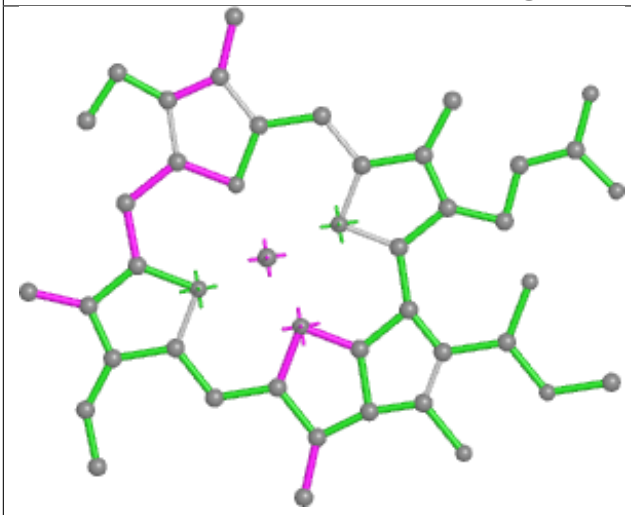


Torsions

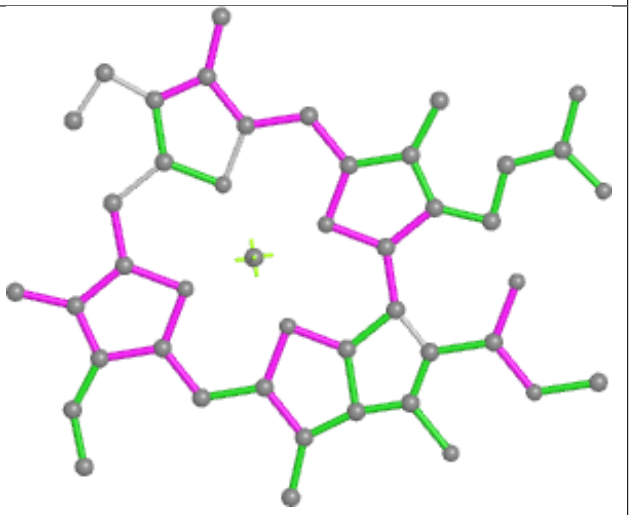


Rings

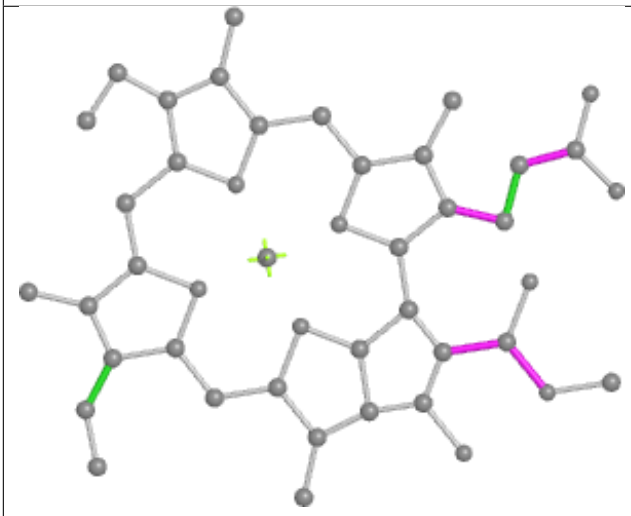
Ligand CLA c2 413



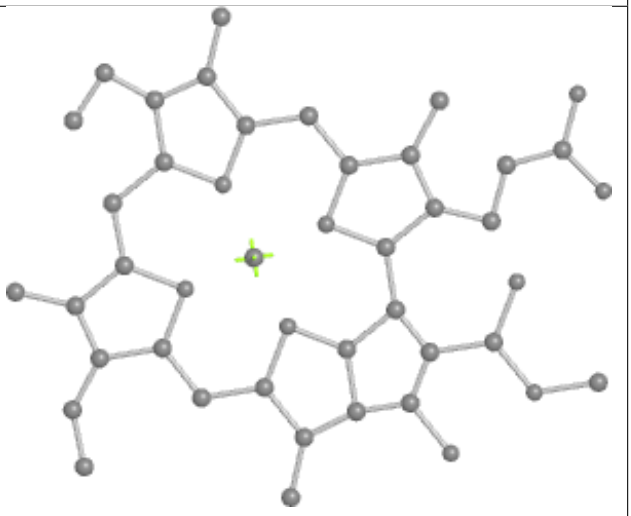
Bond lengths



Bond angles

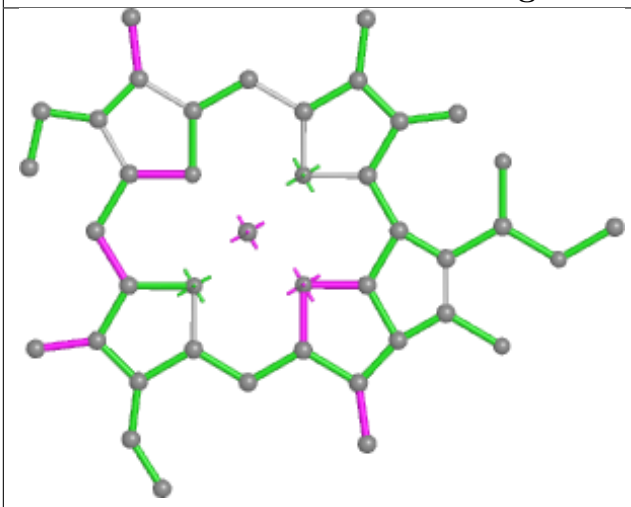


Torsions

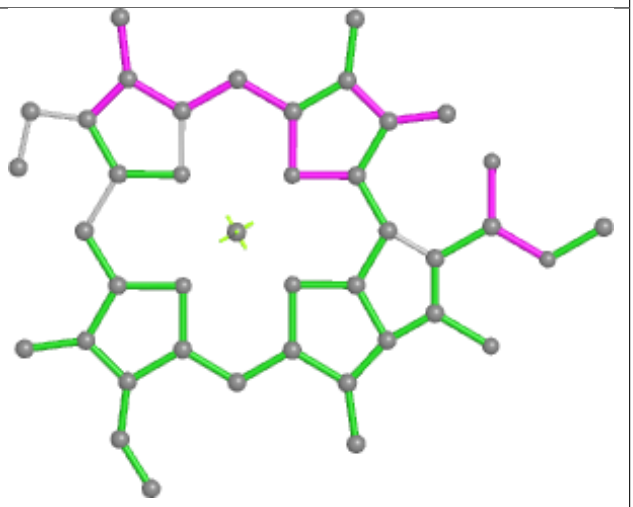


Rings

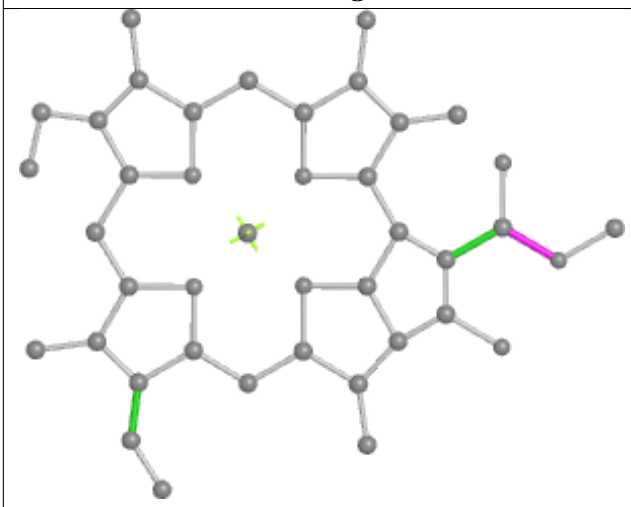
Ligand CLA b3 414



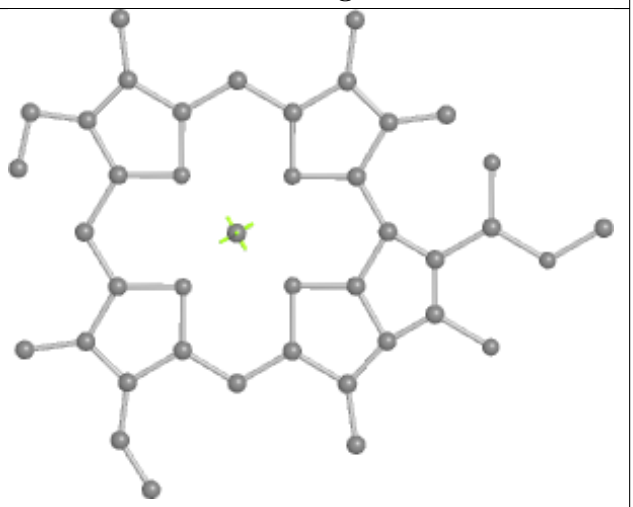
Bond lengths



Bond angles

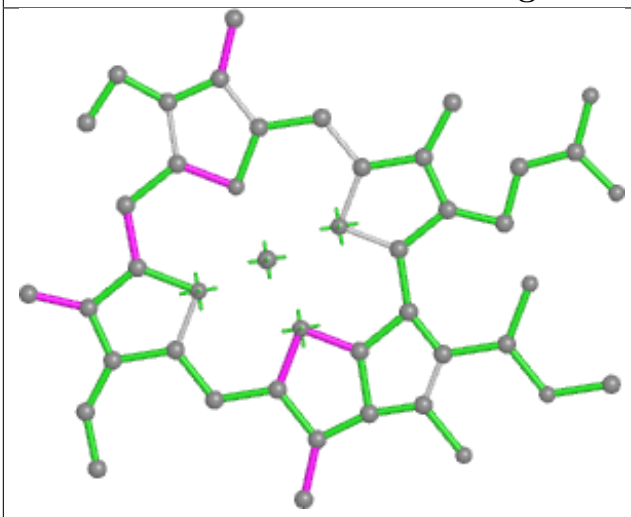


Torsions

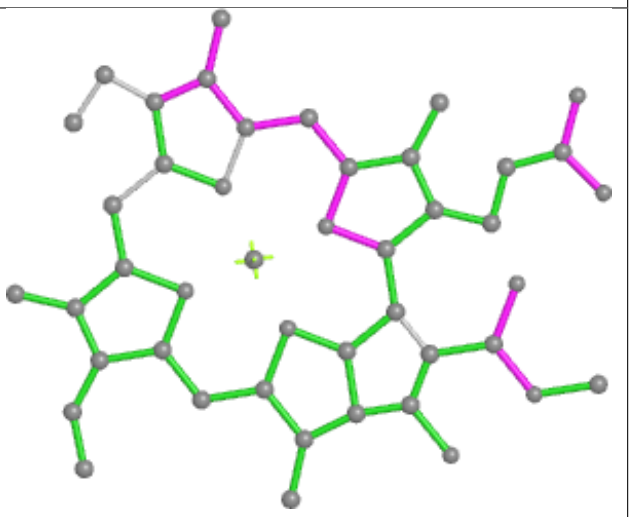


Rings

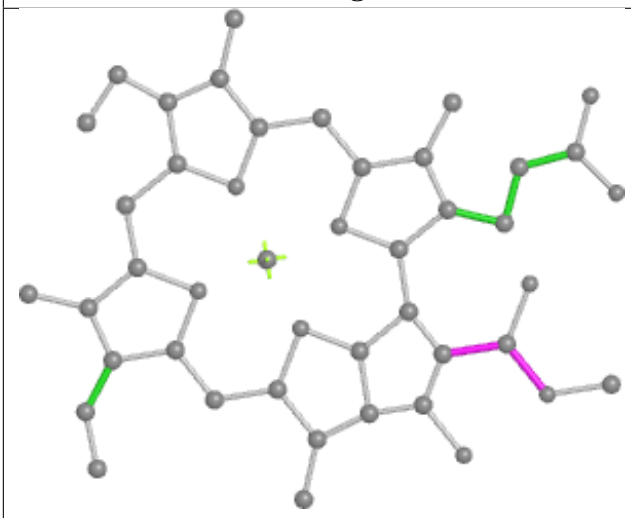
Ligand CLA b6 407



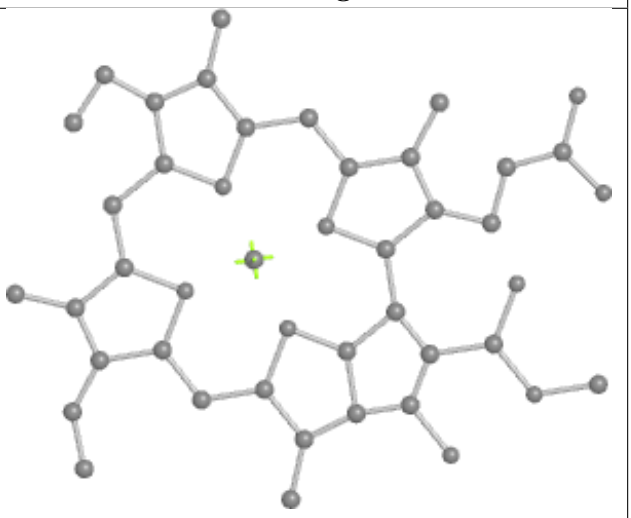
Bond lengths



Bond angles

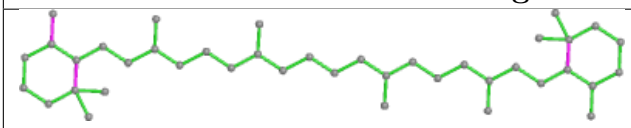


Torsions

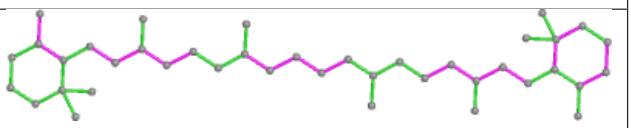


Rings

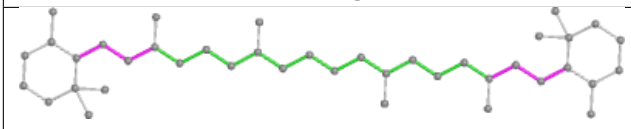
Ligand BCR bA 848



Bond lengths



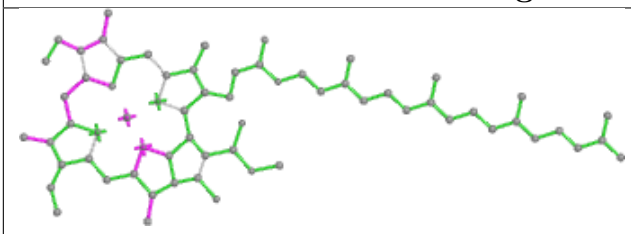
Bond angles



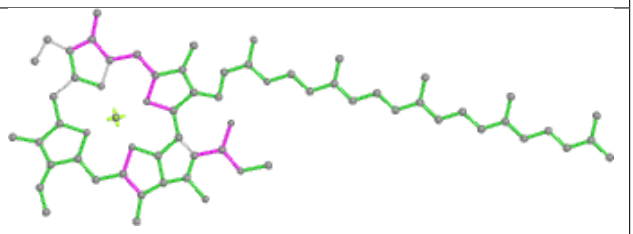
Torsions

Rings

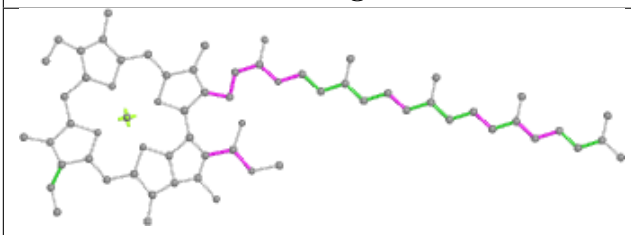
Ligand CLA aB 829



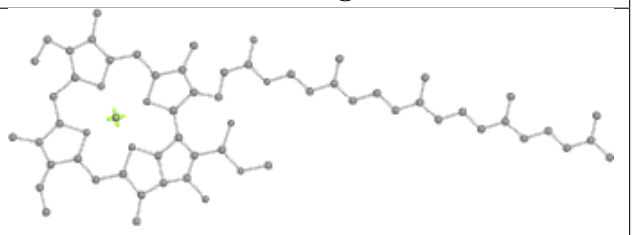
Bond lengths



Bond angles

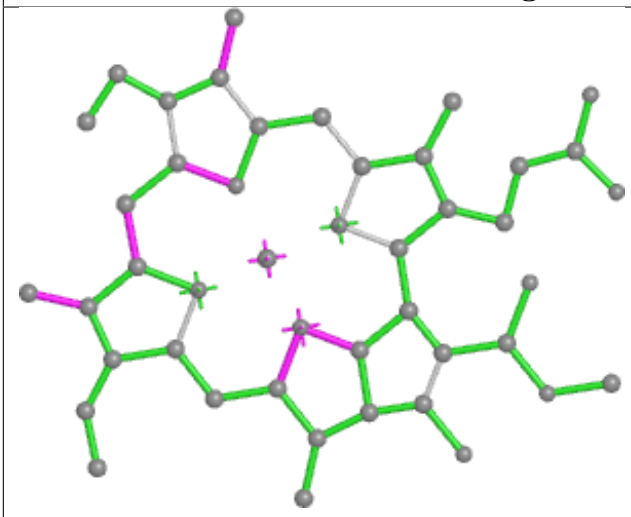


Torsions

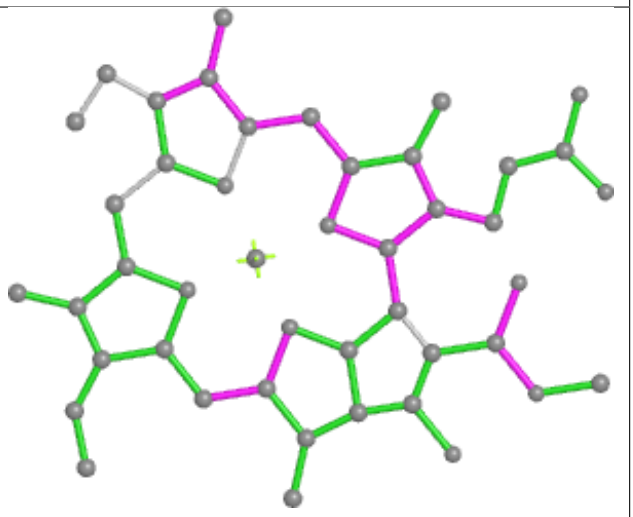


Rings

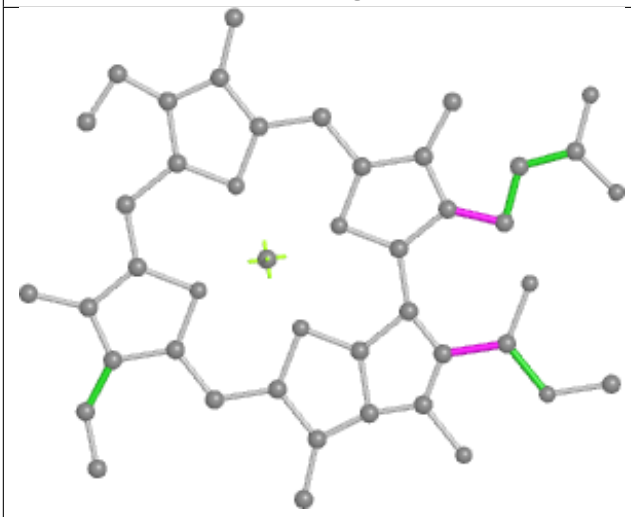
Ligand CLA c5 411



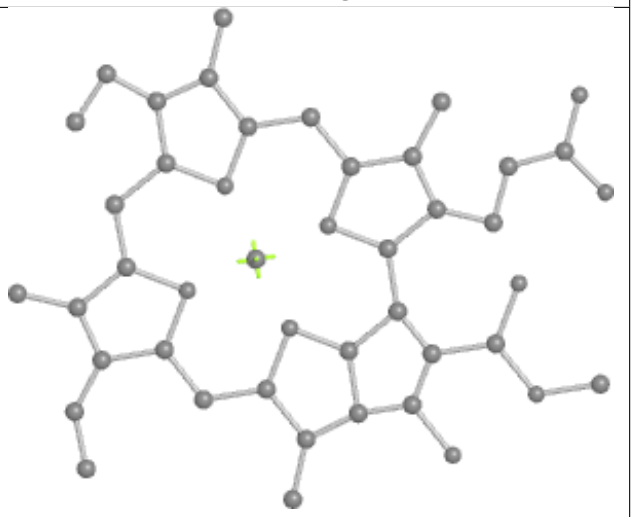
Bond lengths



Bond angles

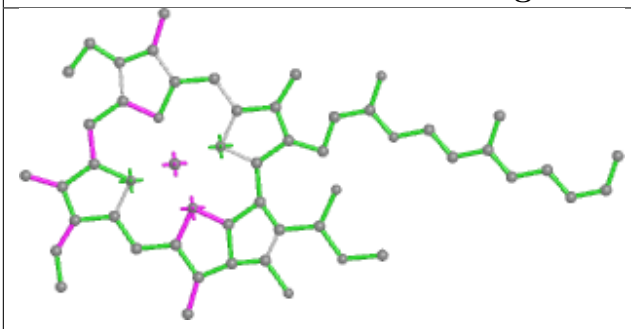


Torsions

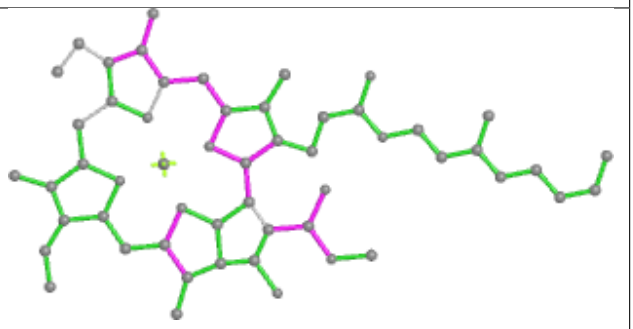


Rings

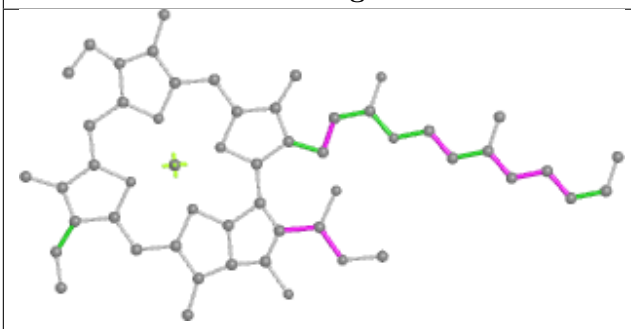
Ligand CLA bB 825



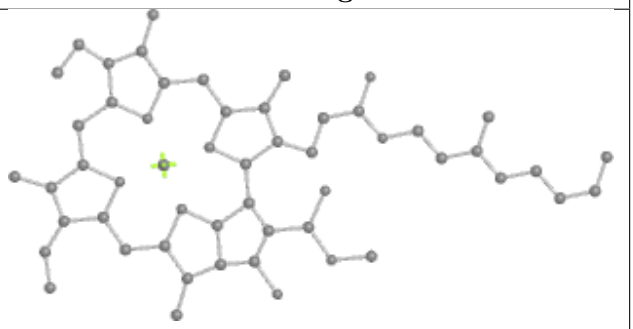
Bond lengths



Bond angles

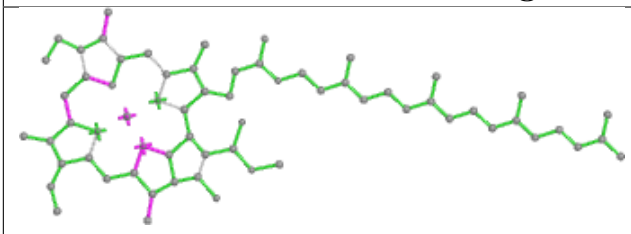


Torsions

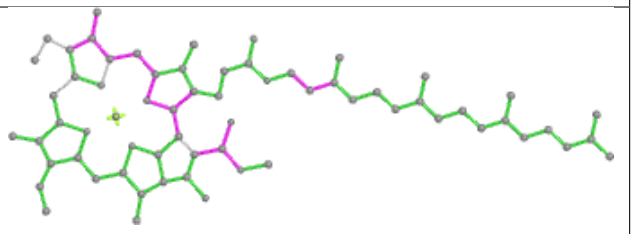


Rings

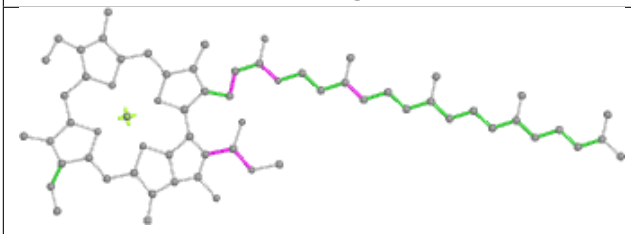
Ligand CLA b5 404



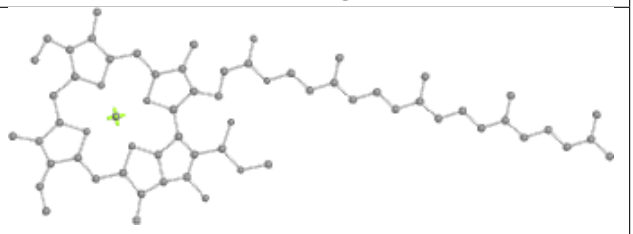
Bond lengths



Bond angles

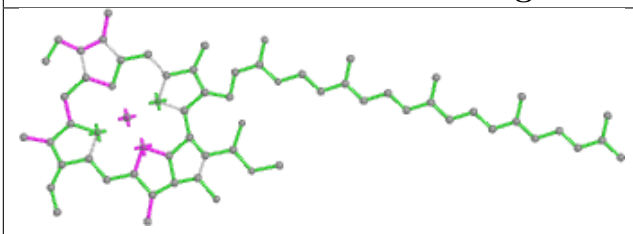


Torsions

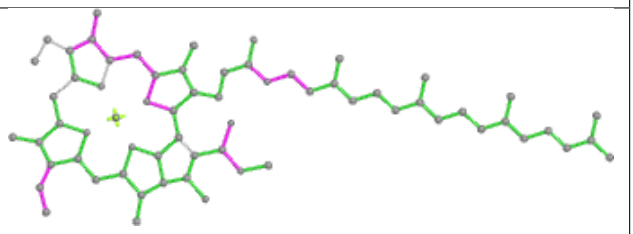


Rings

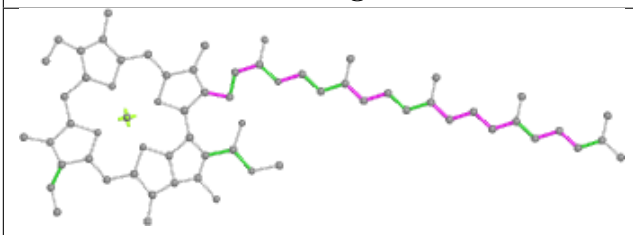
Ligand CLA aA 843



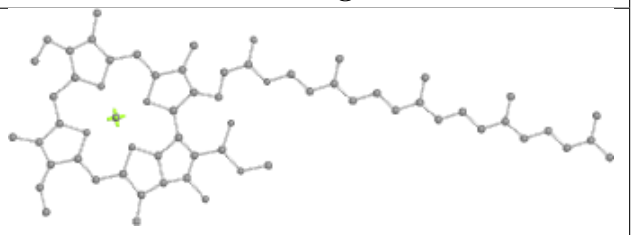
Bond lengths



Bond angles

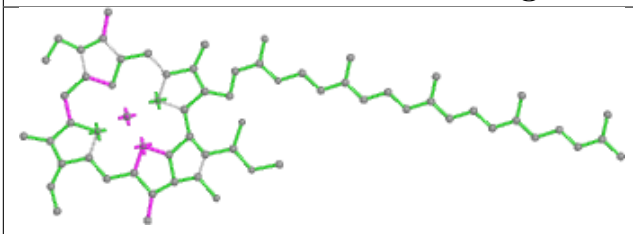


Torsions

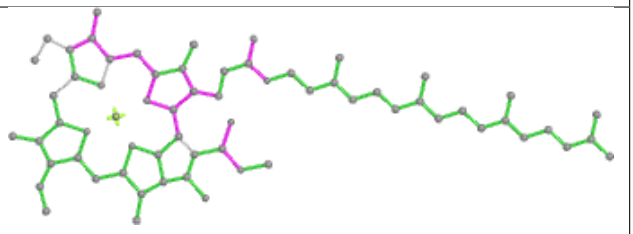


Rings

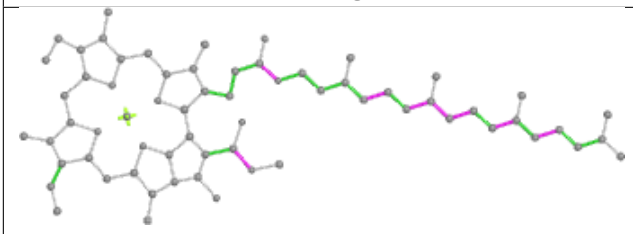
Ligand CLA c3 403



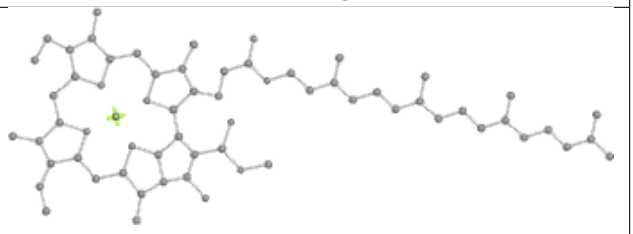
Bond lengths



Bond angles

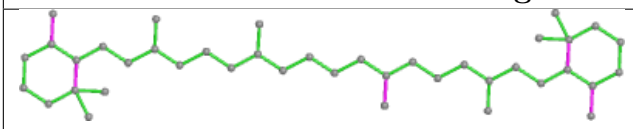


Torsions

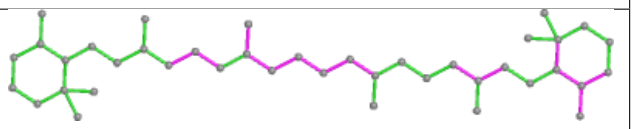


Rings

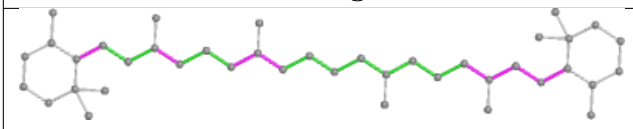
Ligand BCR aB 849



Bond lengths



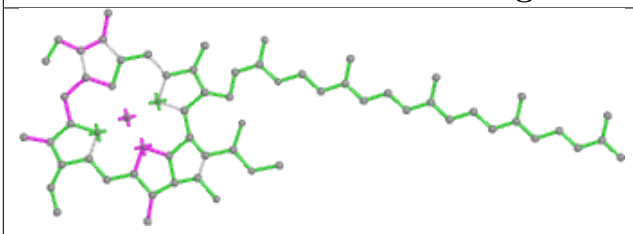
Bond angles



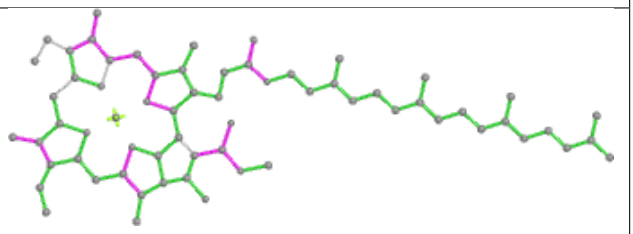
Torsions

Rings

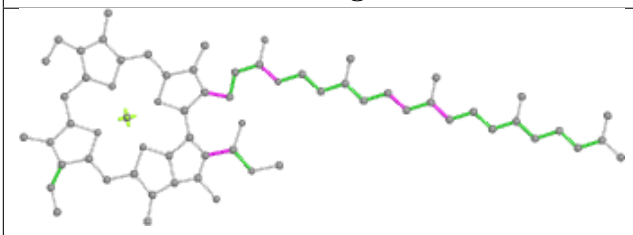
Ligand CLA cA 831



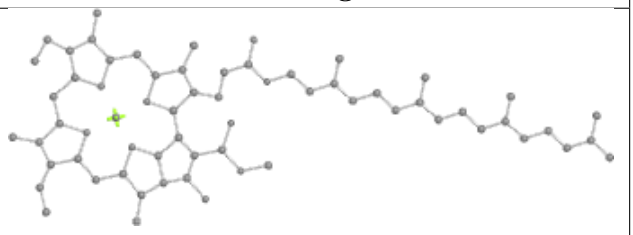
Bond lengths



Bond angles

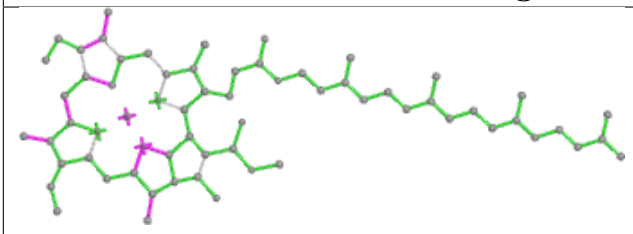


Torsions

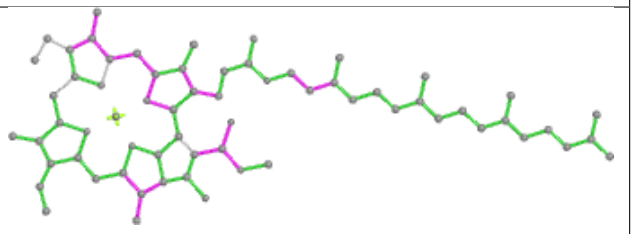


Rings

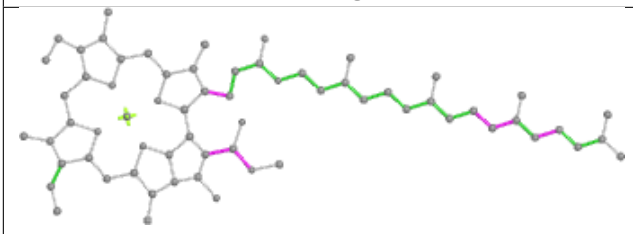
Ligand CLA aA 804



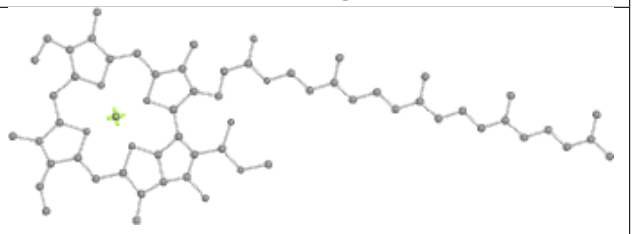
Bond lengths



Bond angles

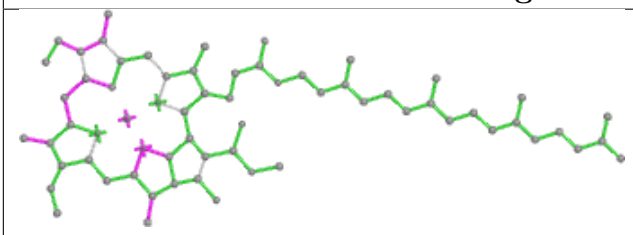


Torsions

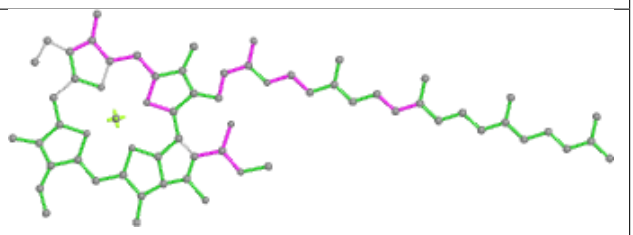


Rings

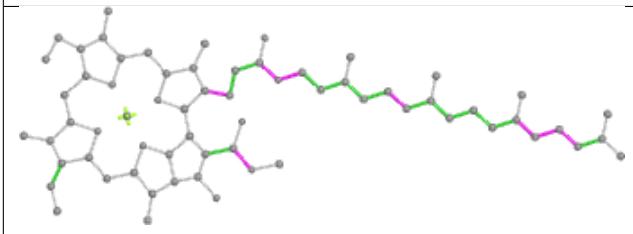
Ligand CLA aA 812



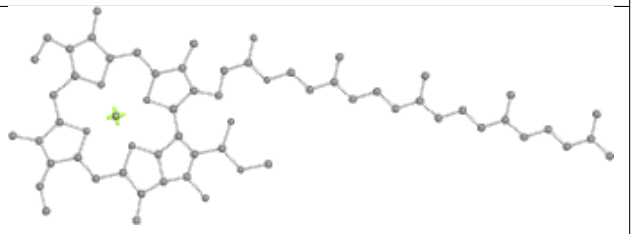
Bond lengths



Bond angles

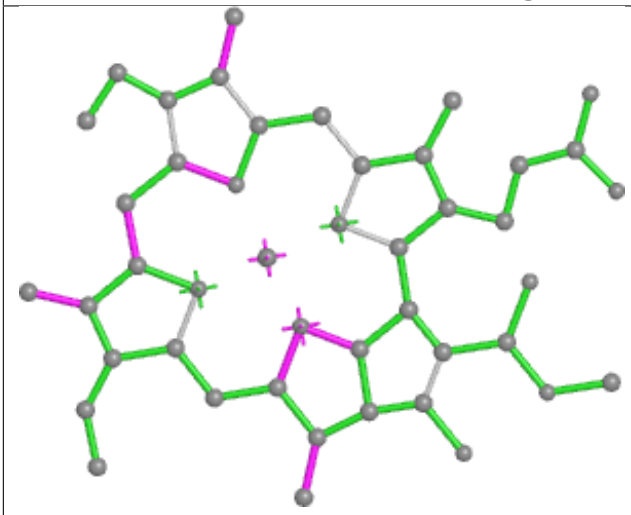


Torsions

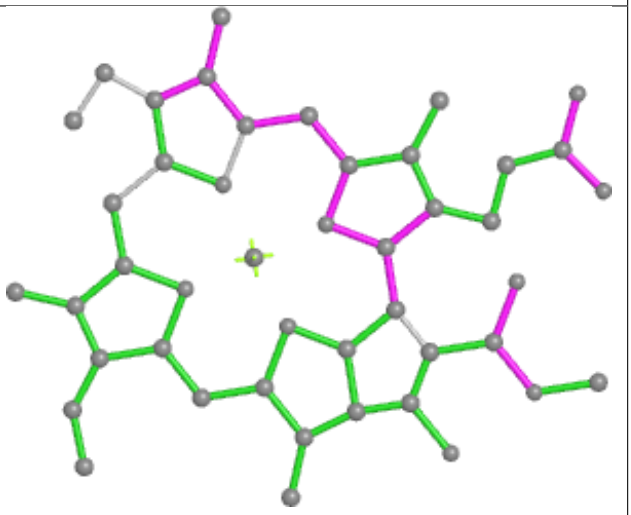


Rings

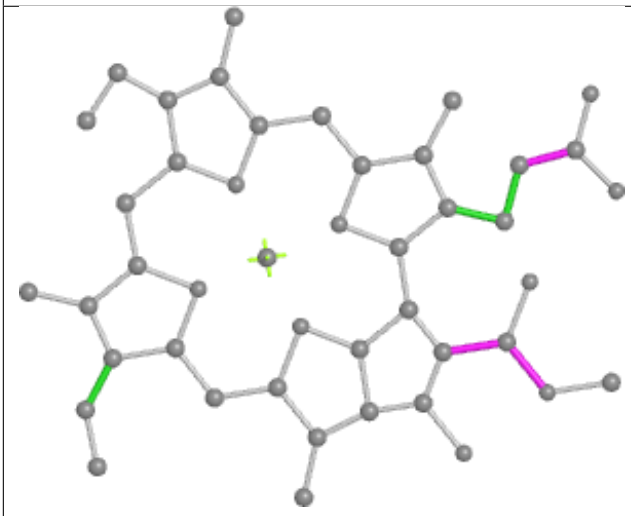
Ligand CLA a2 408



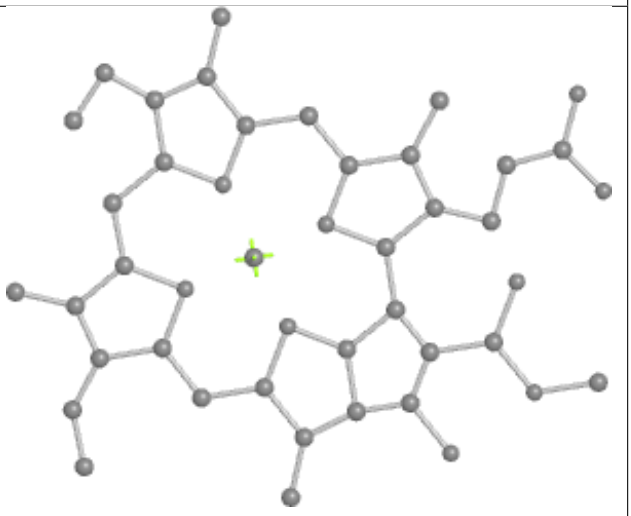
Bond lengths



Bond angles

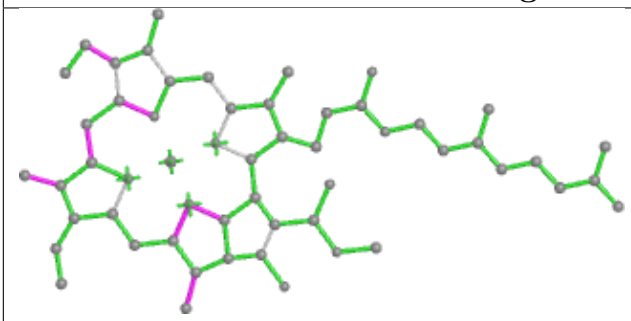


Torsions

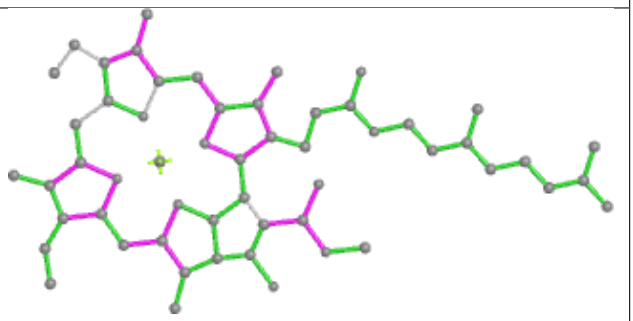


Rings

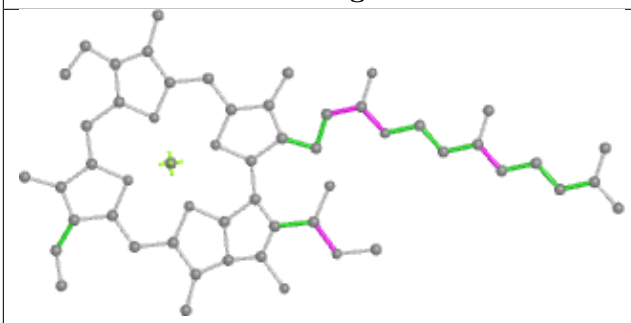
Ligand CLA a4 417



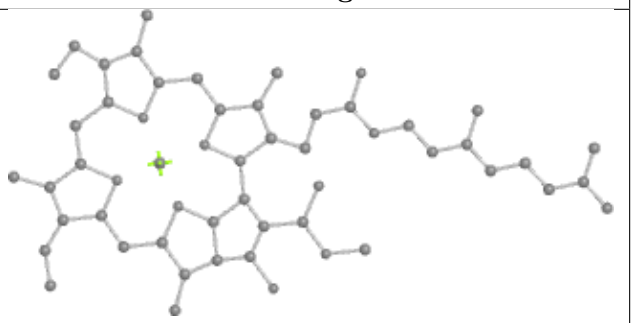
Bond lengths



Bond angles

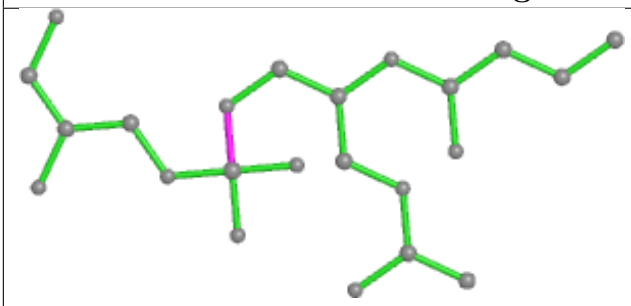


Torsions

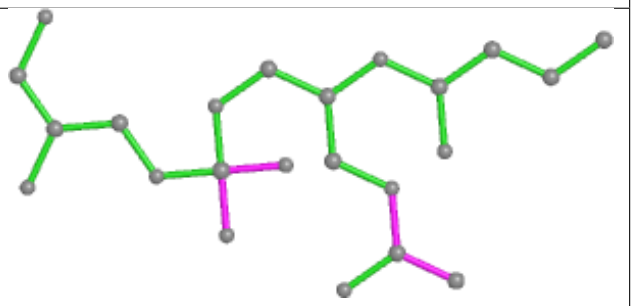


Rings

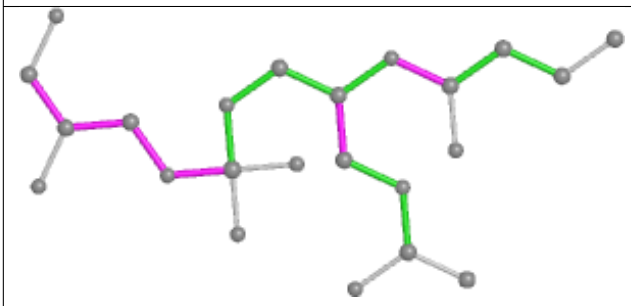
Ligand LHG aX 101



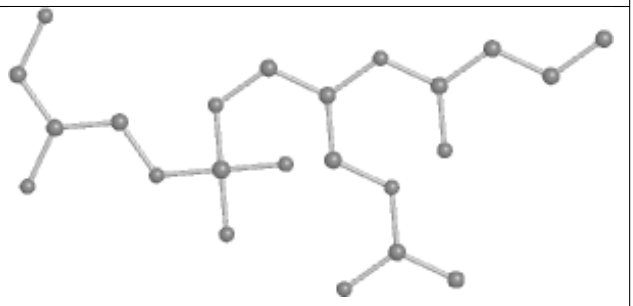
Bond lengths



Bond angles

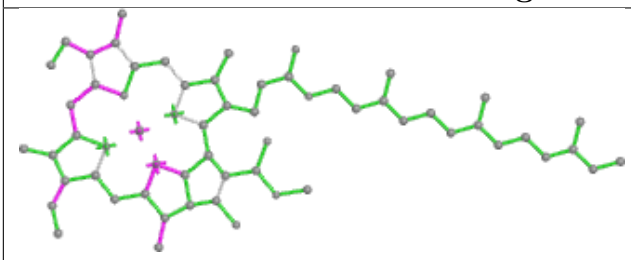


Torsions

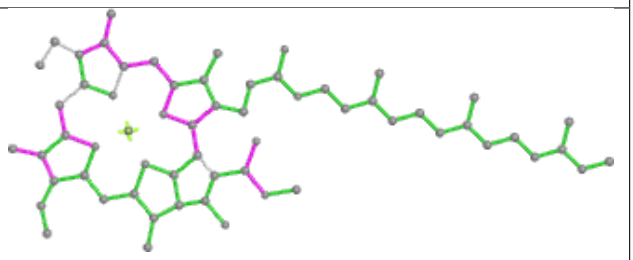


Rings

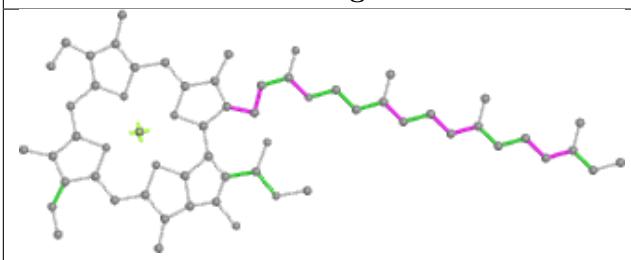
Ligand CLA cA 821



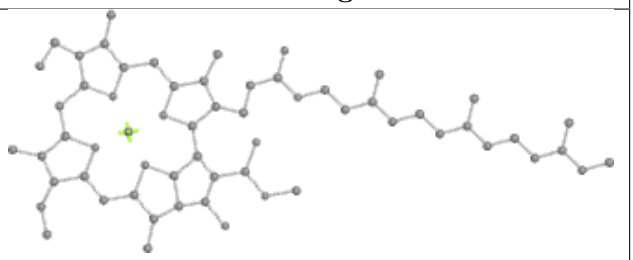
Bond lengths



Bond angles

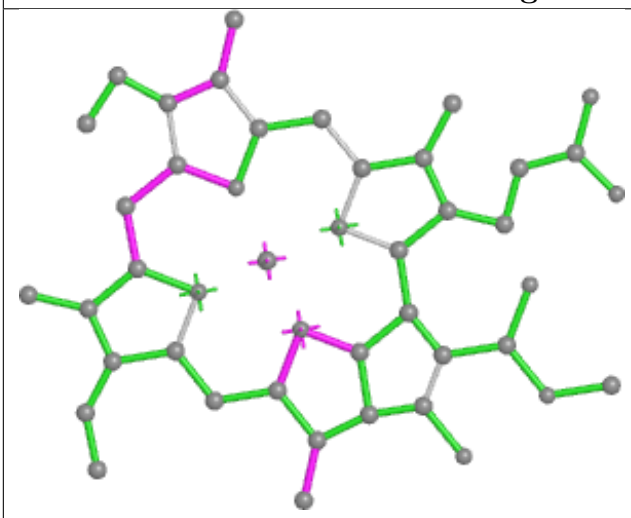


Torsions

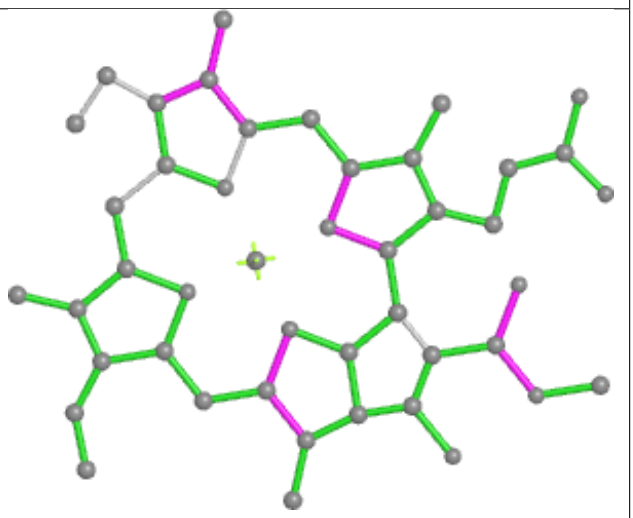


Rings

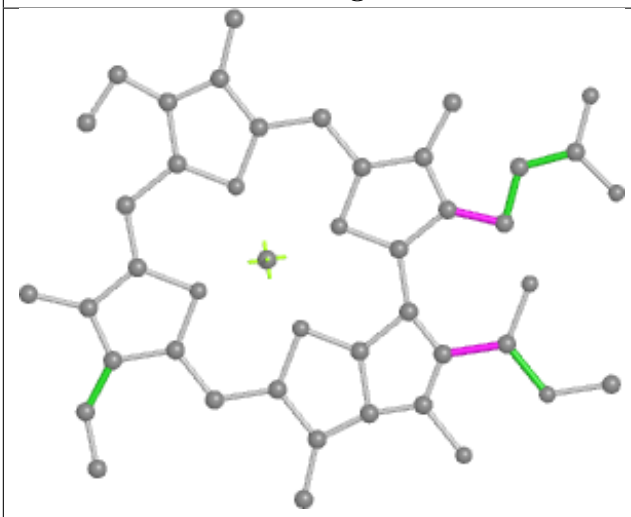
Ligand CLA c3 413



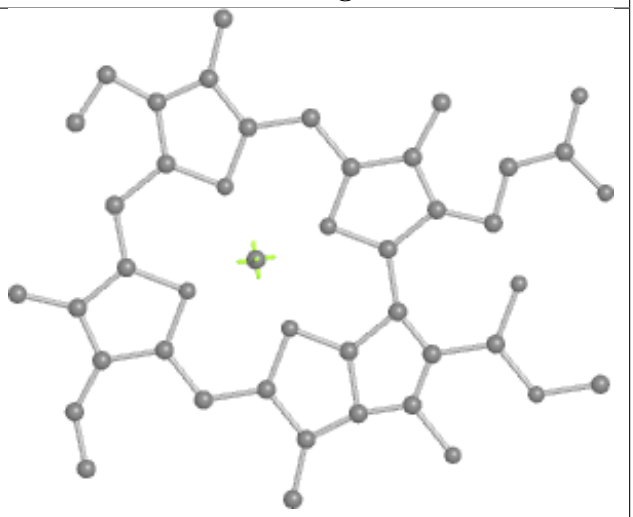
Bond lengths



Bond angles

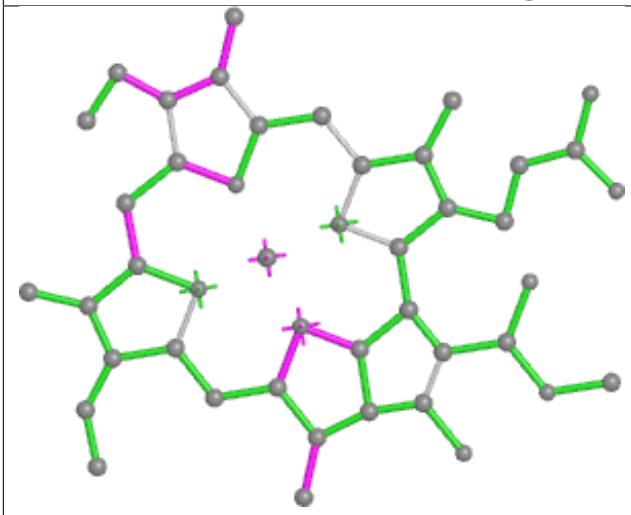


Torsions

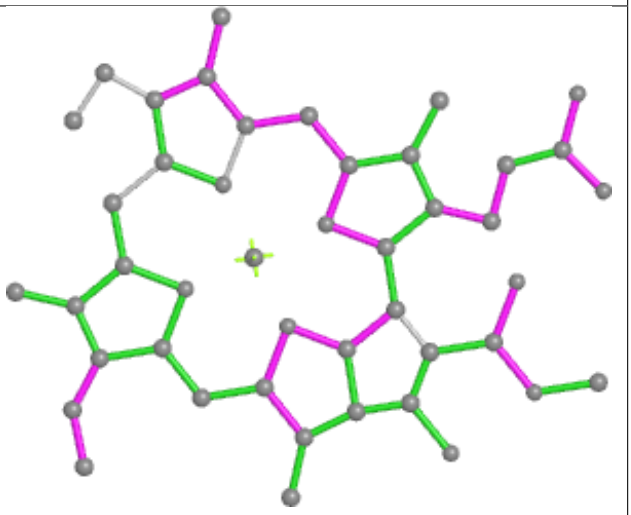


Rings

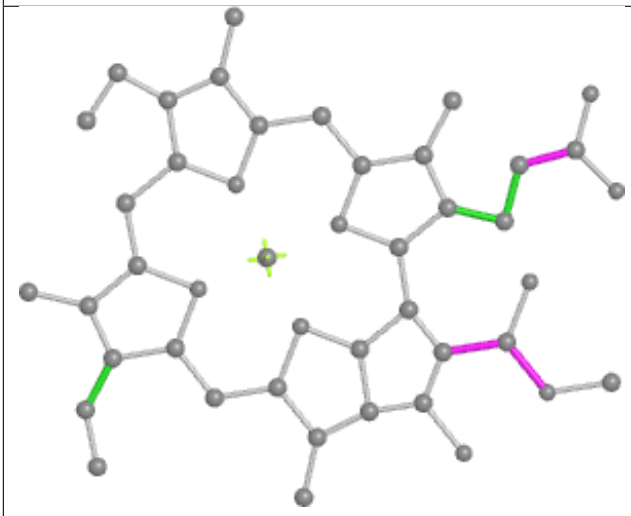
Ligand CLA c4 415



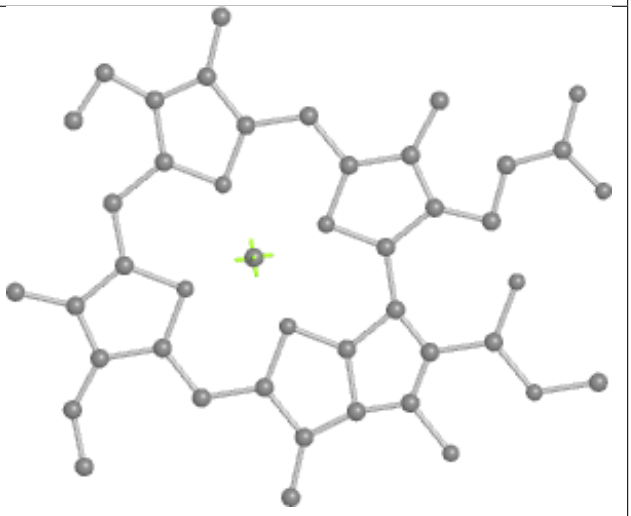
Bond lengths



Bond angles

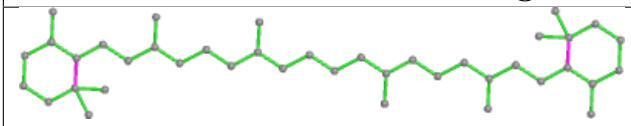


Torsions

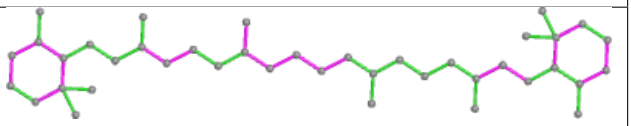


Rings

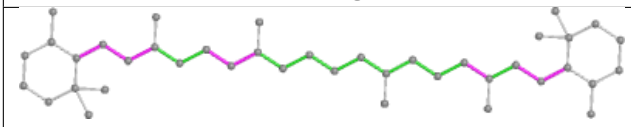
Ligand BCR b5 419



Bond lengths



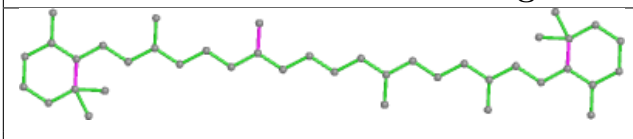
Bond angles



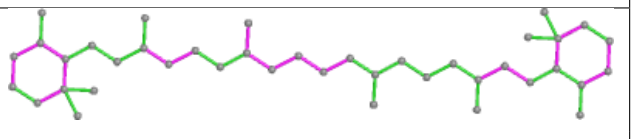
Torsions

Rings

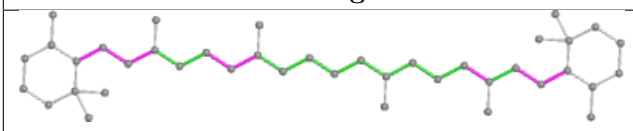
Ligand BCR a1 419



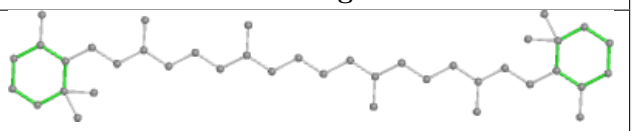
Bond lengths



Bond angles

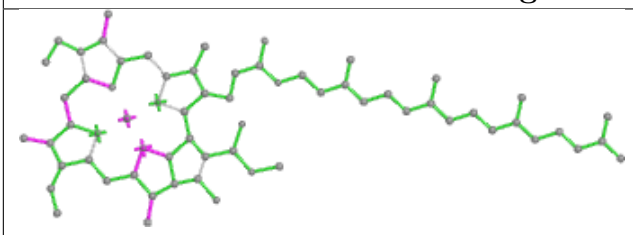


Torsions

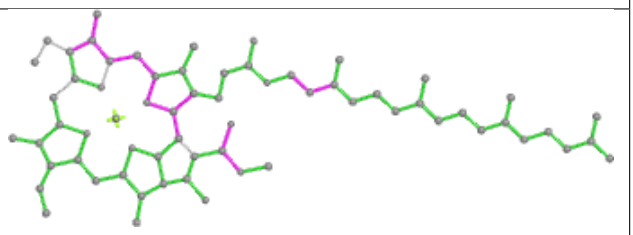


Rings

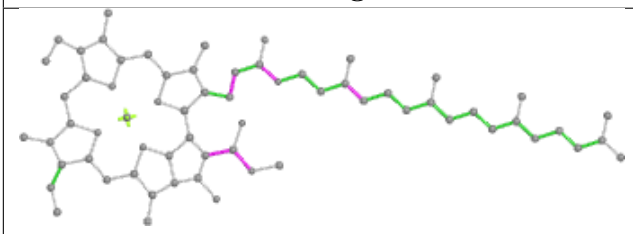
Ligand CLA a6 405



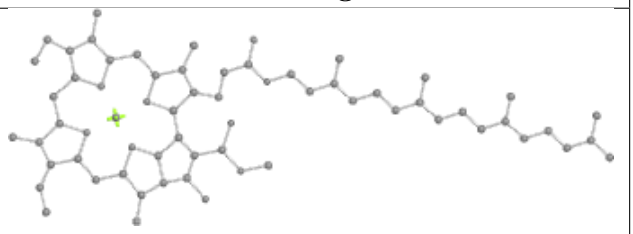
Bond lengths



Bond angles

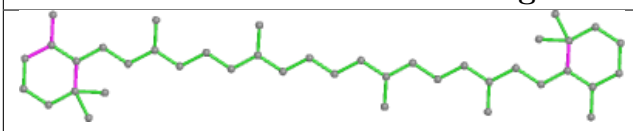


Torsions

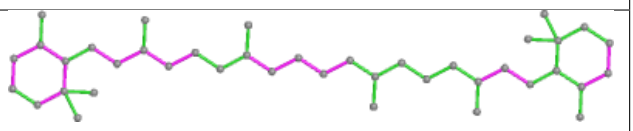


Rings

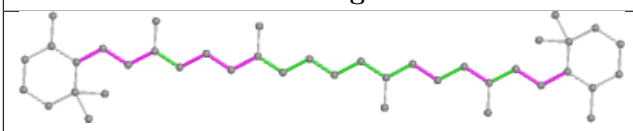
Ligand BCR c6 402



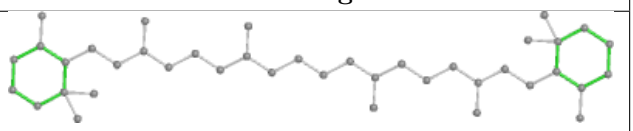
Bond lengths



Bond angles

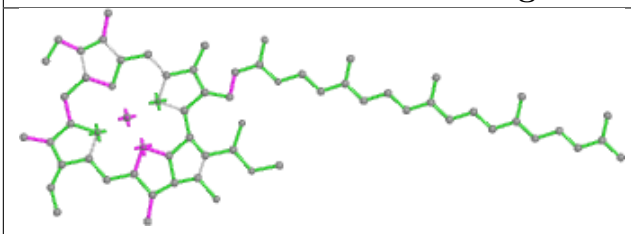


Torsions

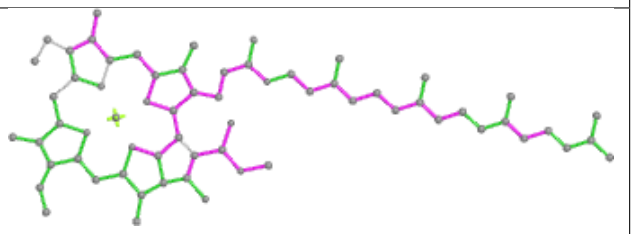


Rings

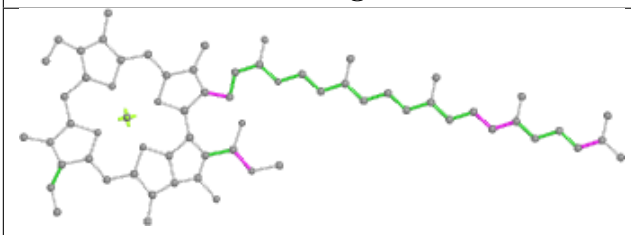
Ligand CLA b2 406



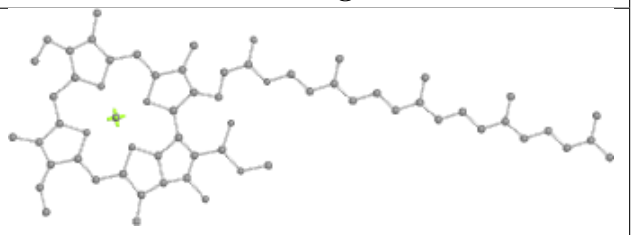
Bond lengths



Bond angles

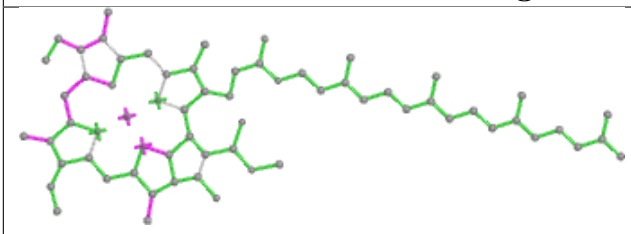


Torsions

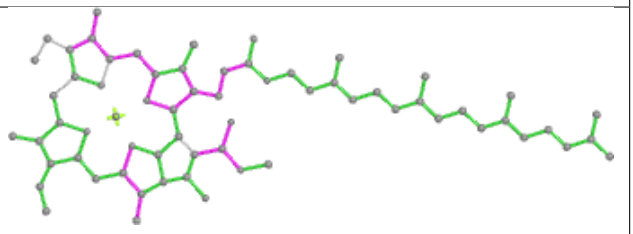


Rings

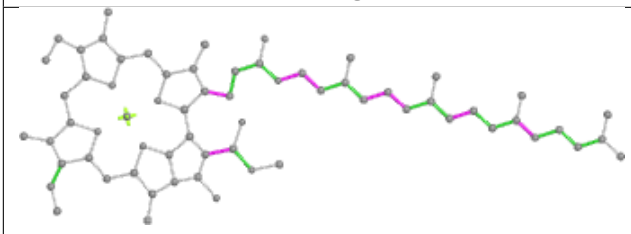
Ligand CLA cA 827



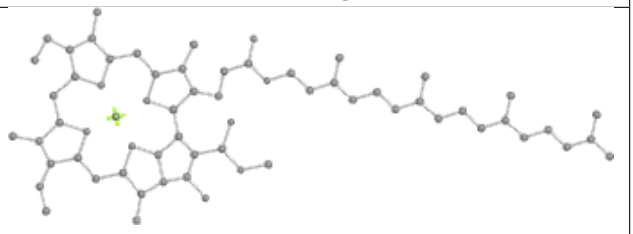
Bond lengths



Bond angles

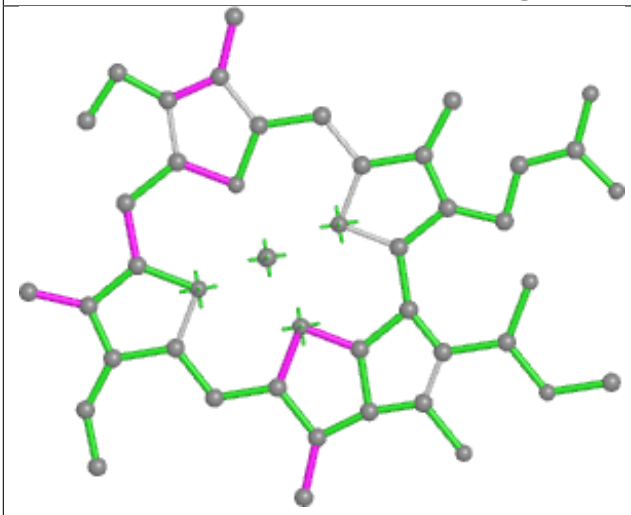


Torsions

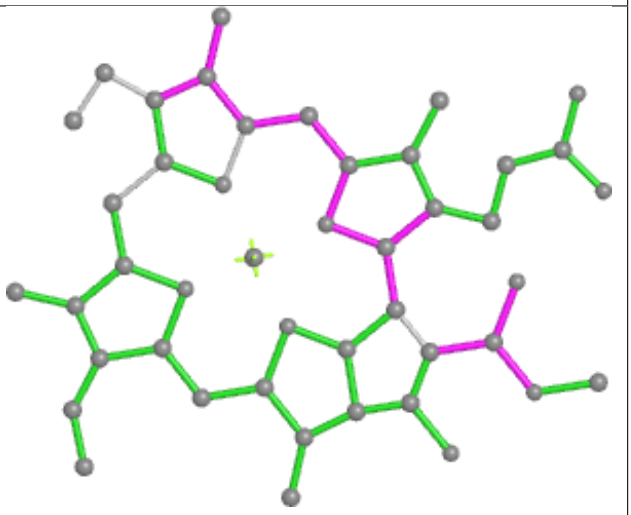


Rings

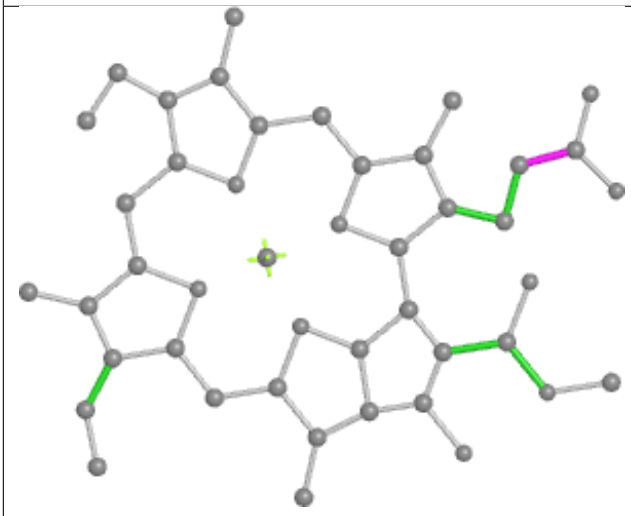
Ligand CLA aB 841



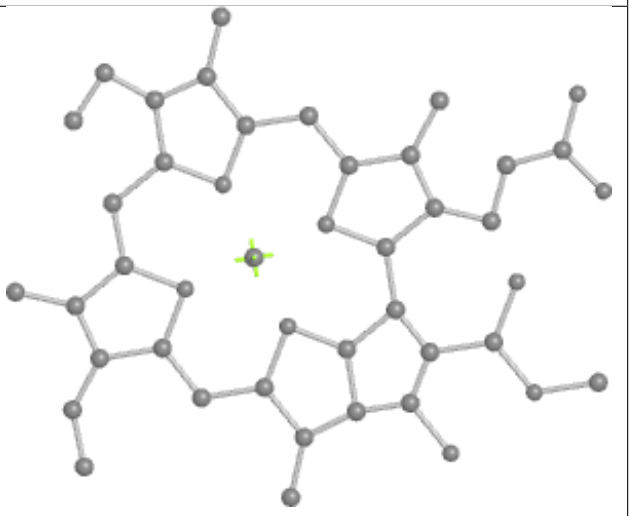
Bond lengths



Bond angles

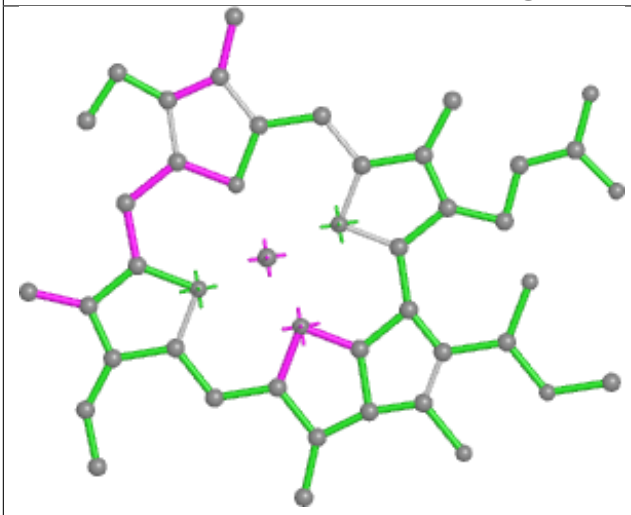


Torsions

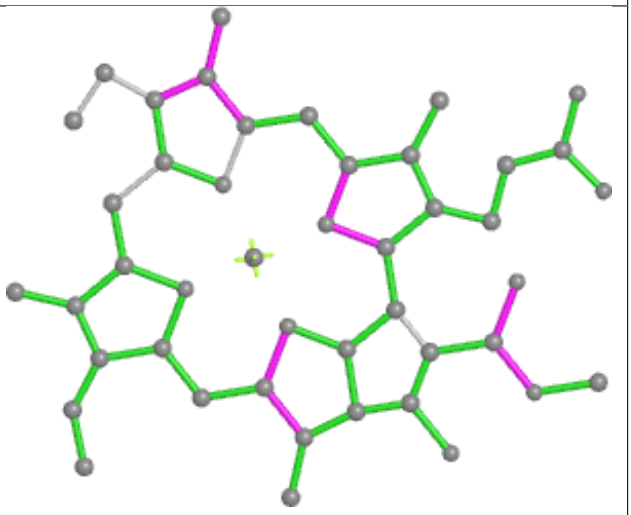


Rings

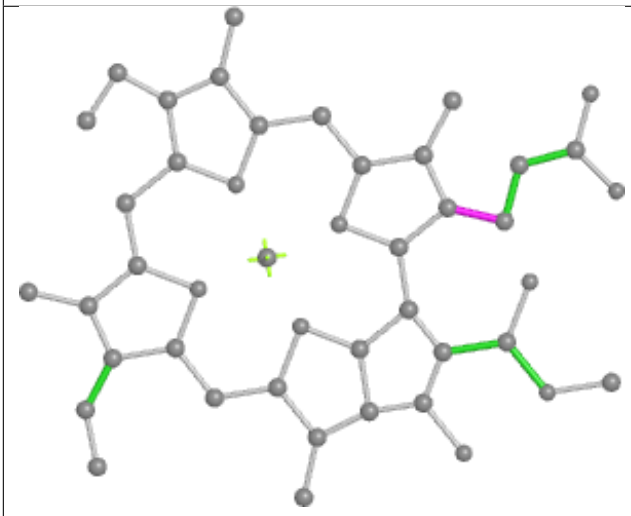
Ligand CLA a5 413



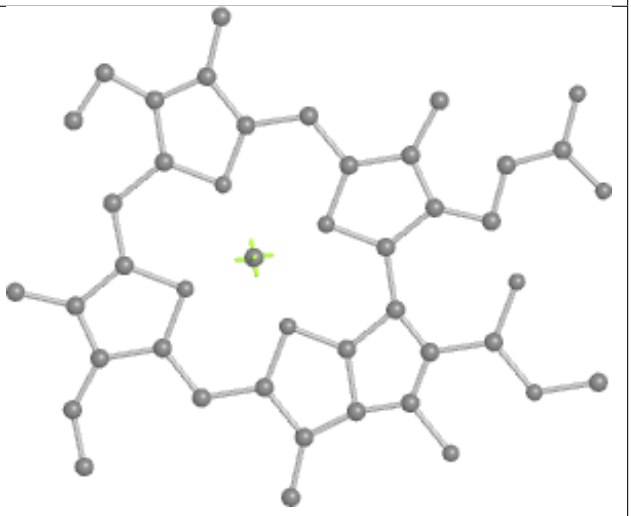
Bond lengths



Bond angles

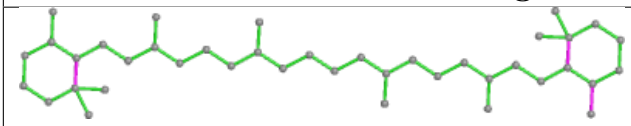


Torsions

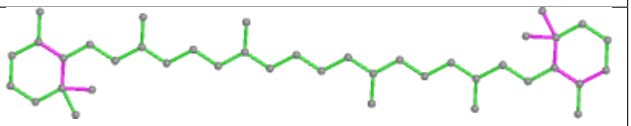


Rings

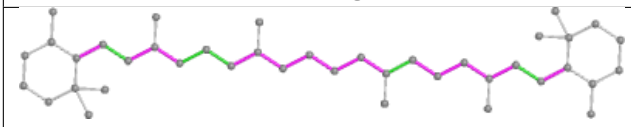
Ligand BCR cA 851



Bond lengths



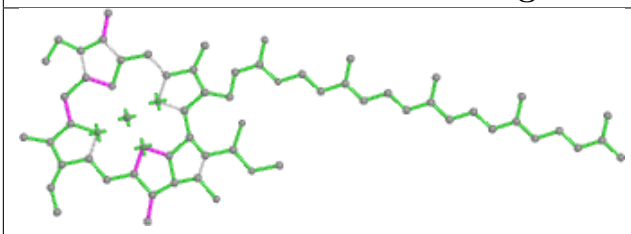
Bond angles



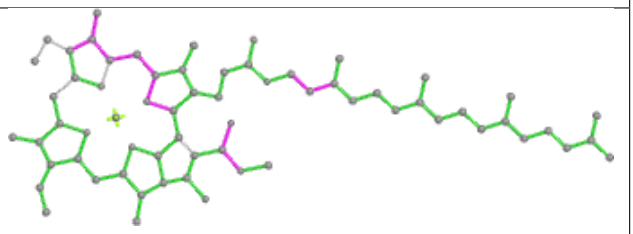
Torsions

Rings

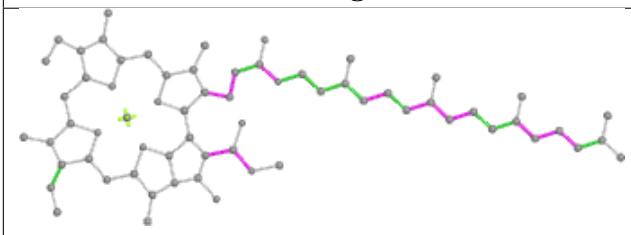
Ligand CLA b3 402



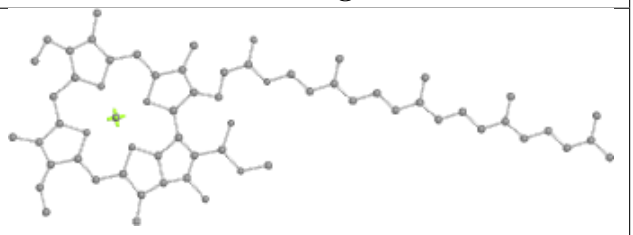
Bond lengths



Bond angles

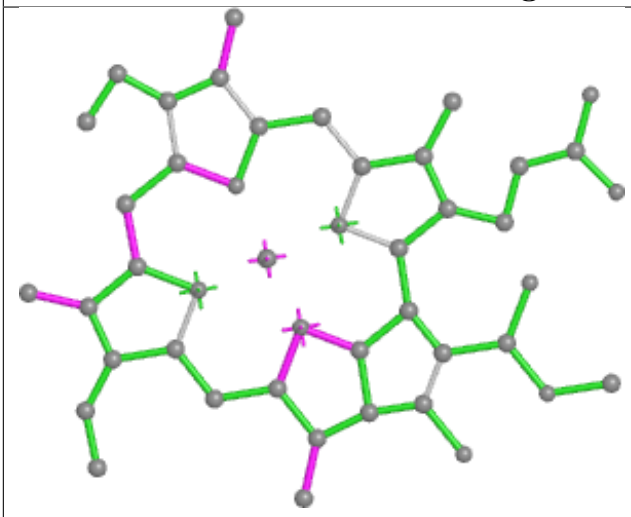


Torsions

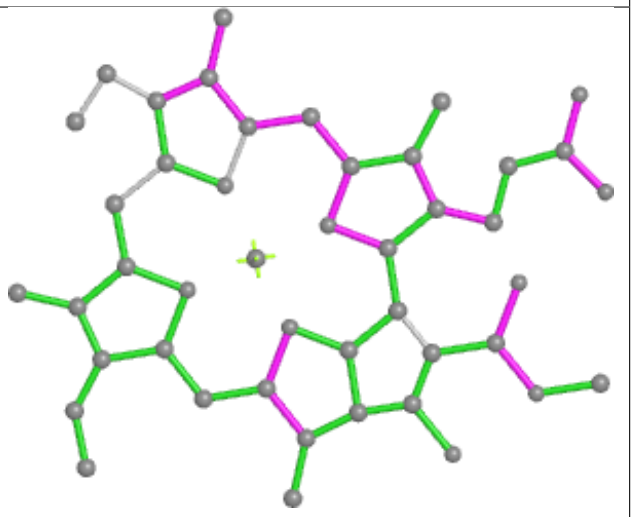


Rings

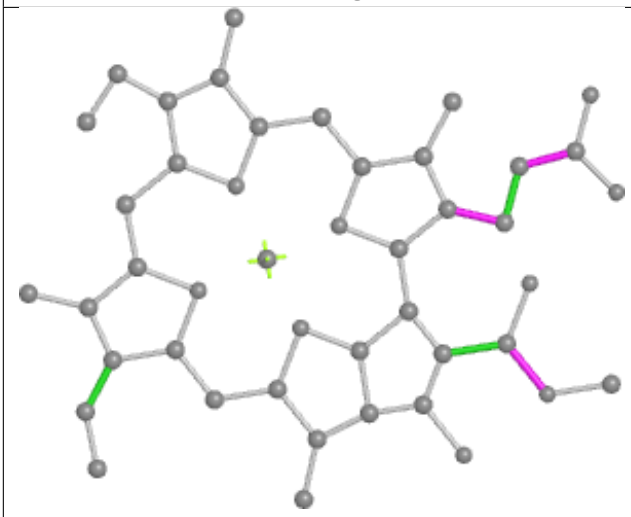
Ligand CLA c3 408



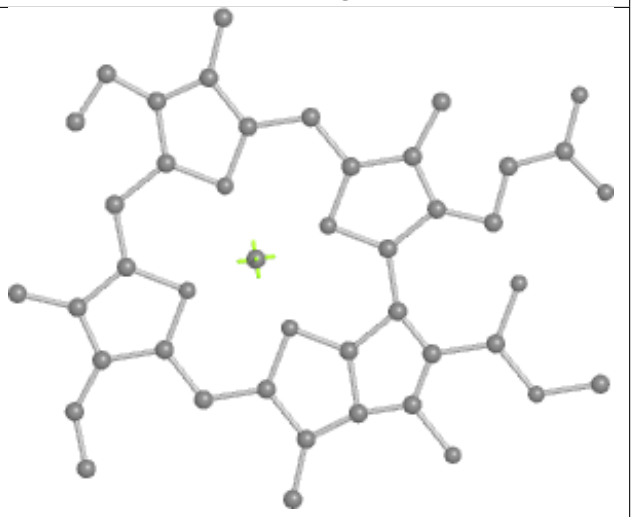
Bond lengths



Bond angles

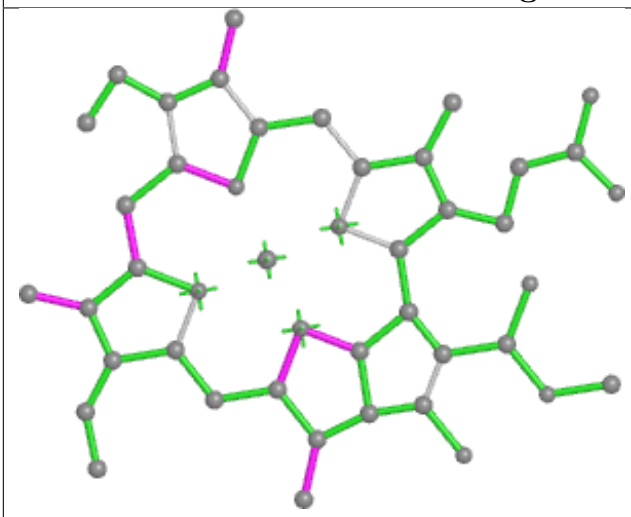


Torsions

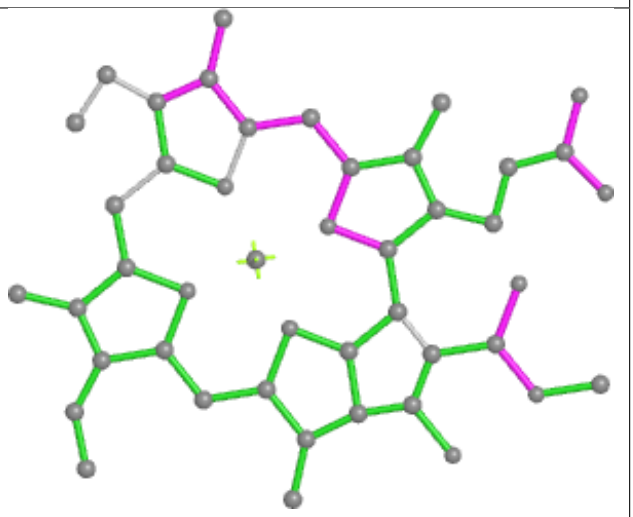


Rings

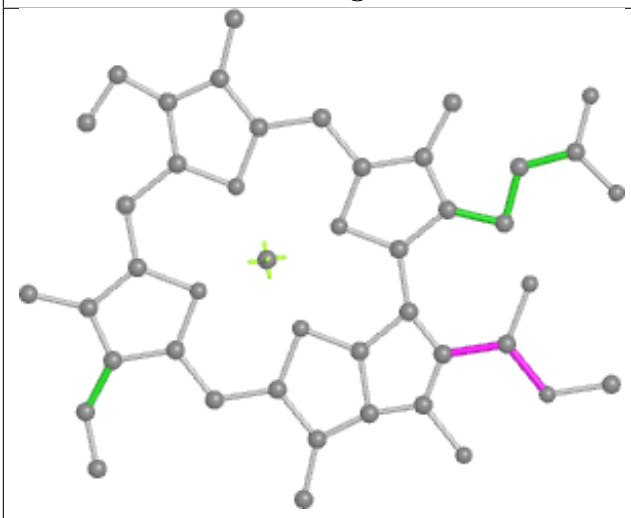
Ligand CLA a6 407



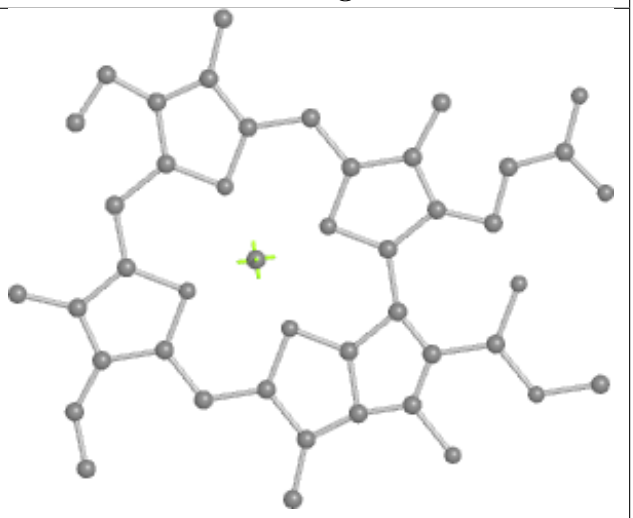
Bond lengths



Bond angles

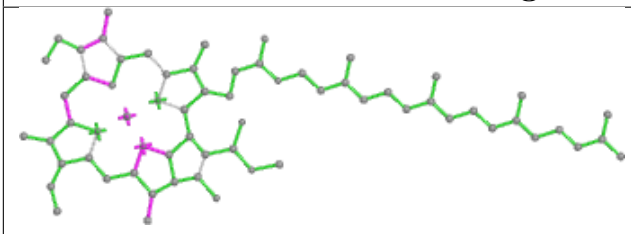


Torsions

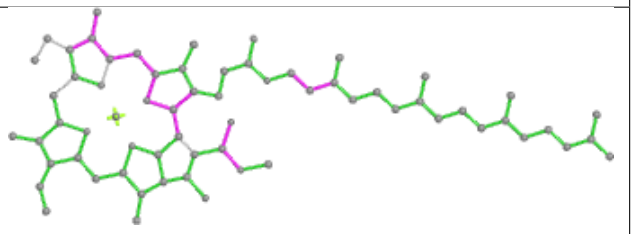


Rings

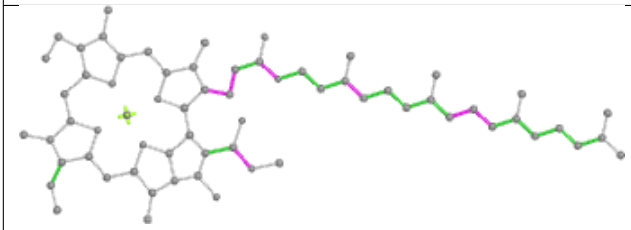
Ligand CLA c3 404



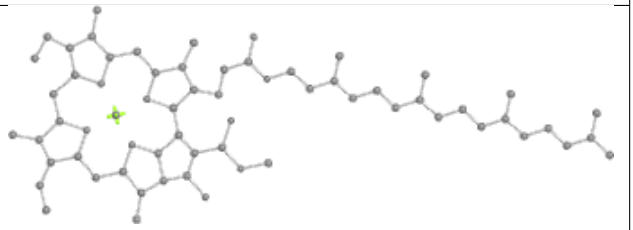
Bond lengths



Bond angles

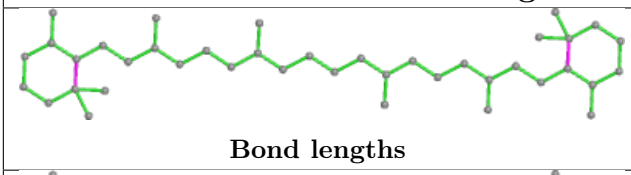


Torsions

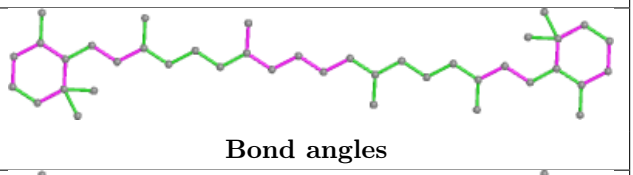


Rings

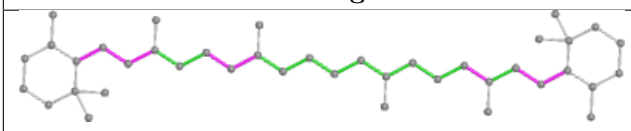
Ligand BCR c6 420



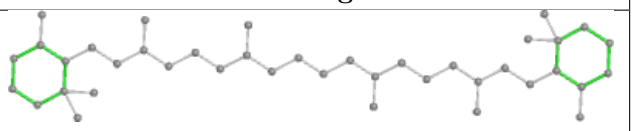
Bond lengths



Bond angles

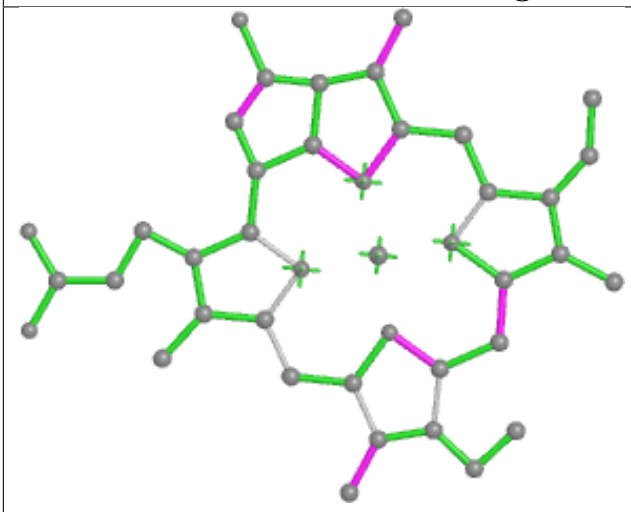


Torsions

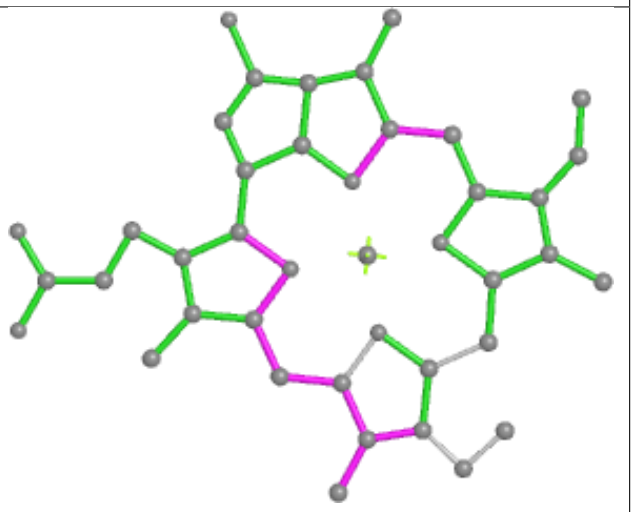


Rings

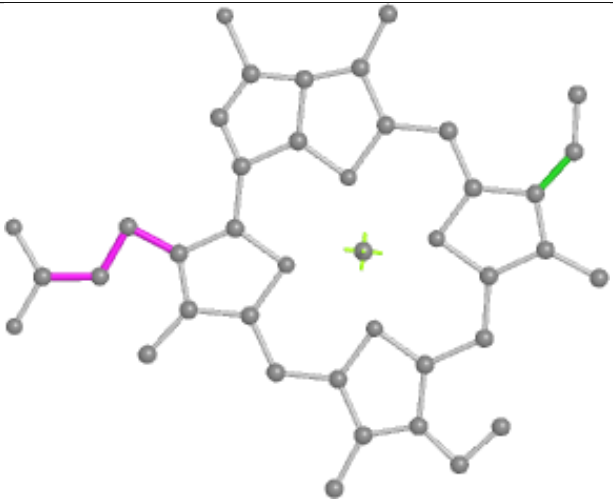
Ligand CLA bA 844



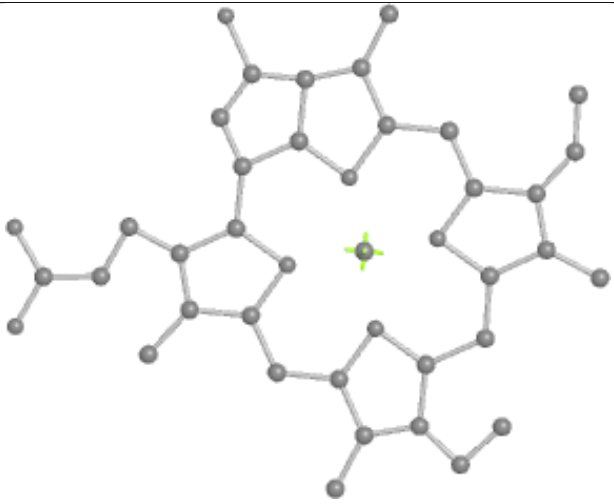
Bond lengths



Bond angles

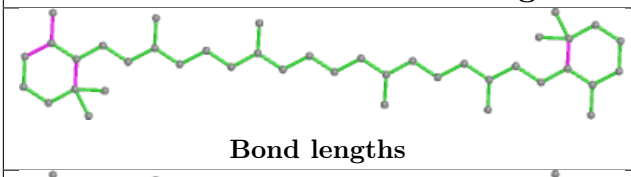


Torsions

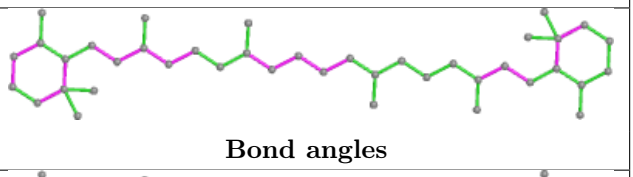


Rings

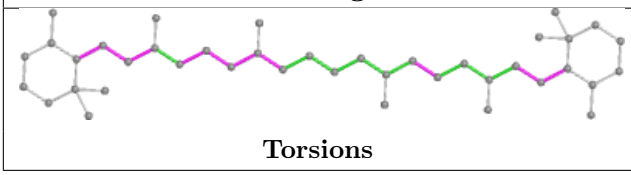
Ligand BCR c3 401



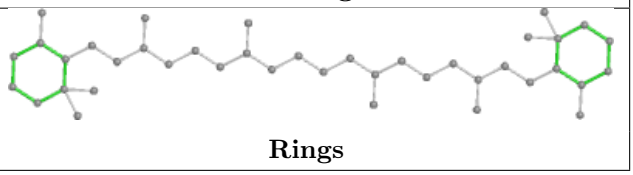
Bond lengths



Bond angles

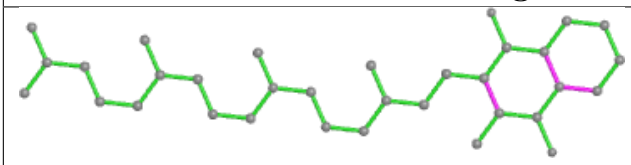


Torsions

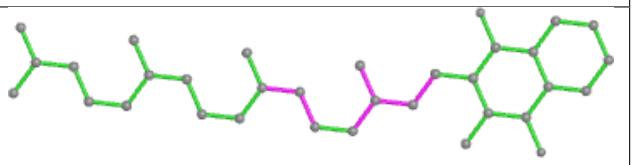


Rings

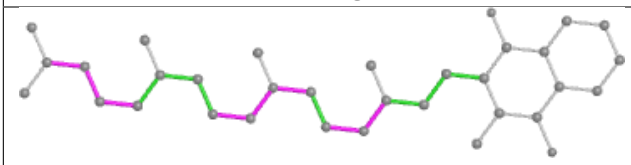
Ligand PQN bB 843



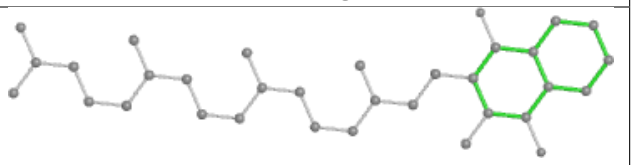
Bond lengths



Bond angles

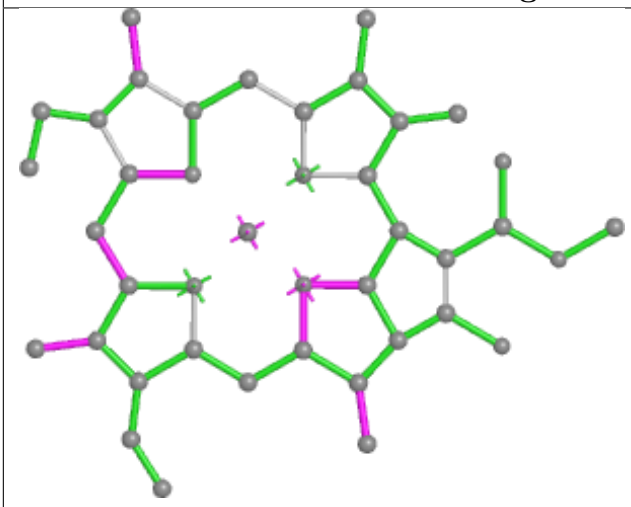


Torsions

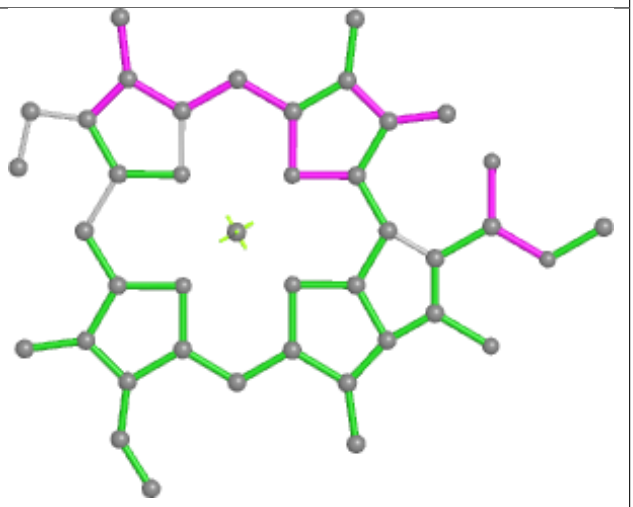


Rings

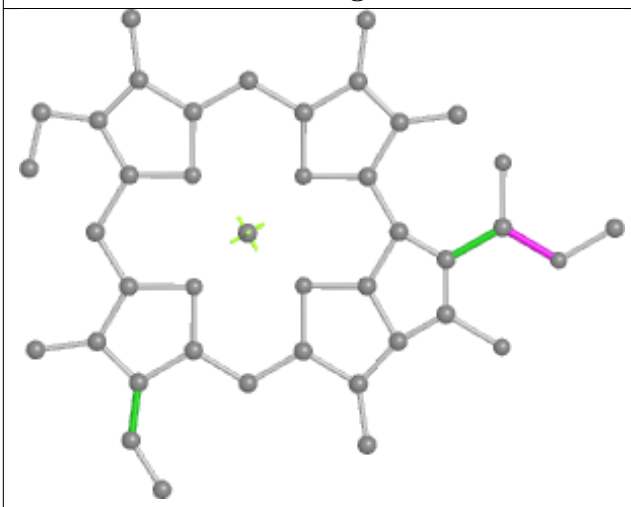
Ligand CLA a4 414



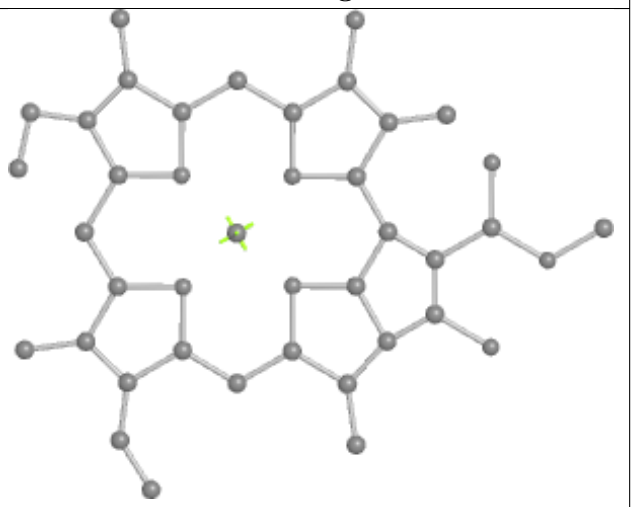
Bond lengths



Bond angles

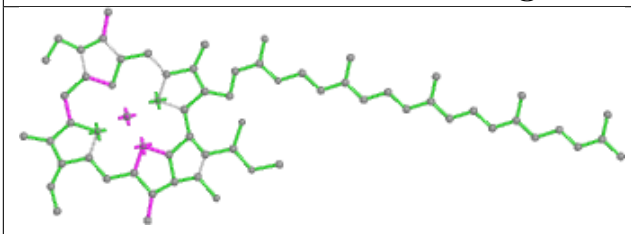


Torsions

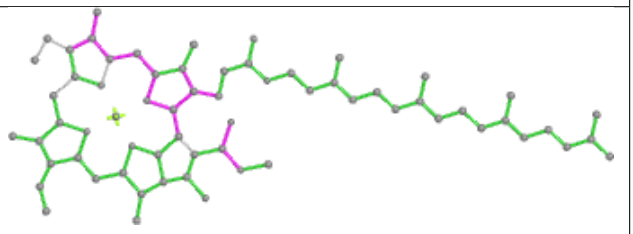


Rings

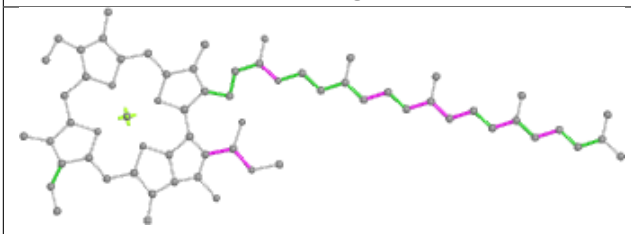
Ligand CLA b1 403



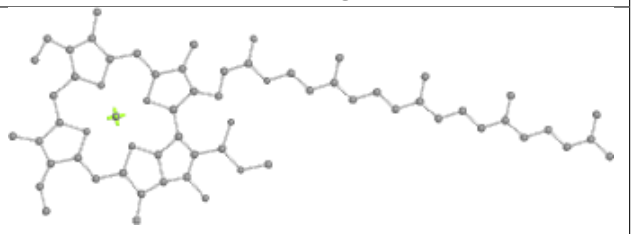
Bond lengths



Bond angles

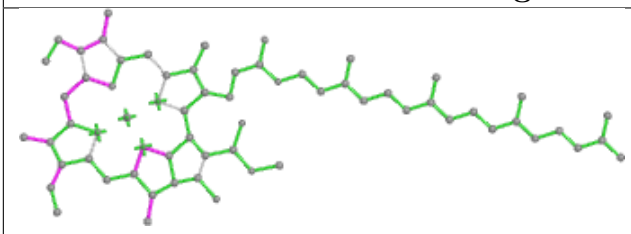


Torsions

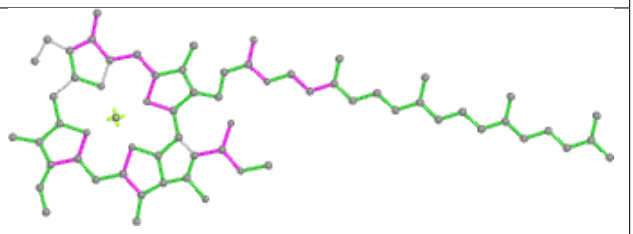


Rings

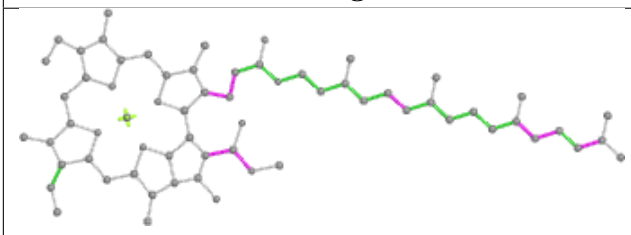
Ligand CLA bA 835



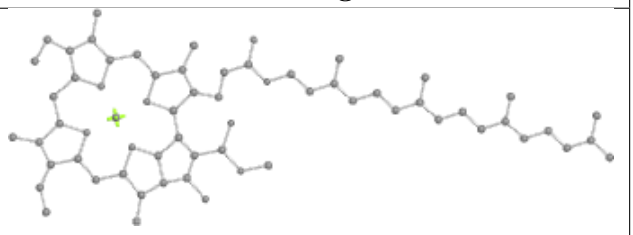
Bond lengths



Bond angles

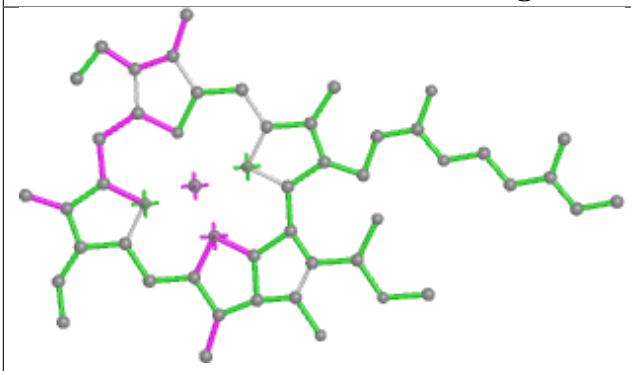


Torsions

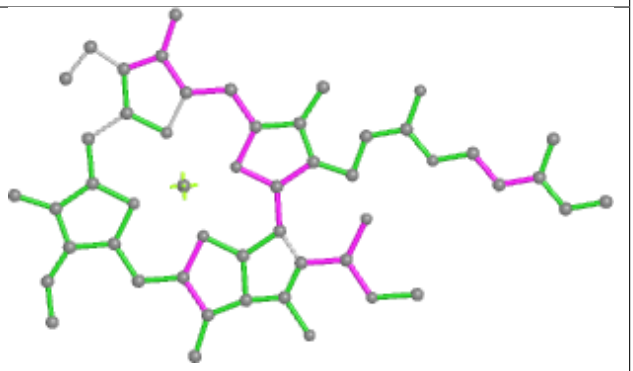


Rings

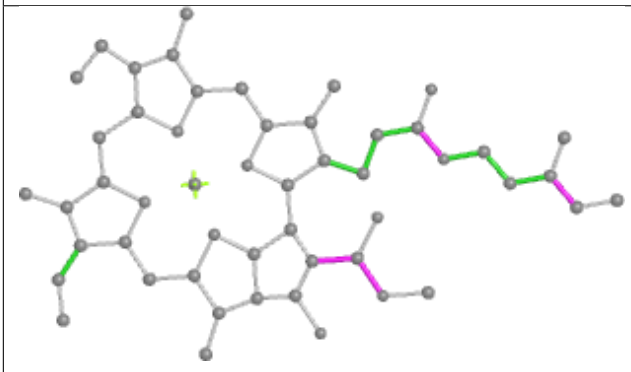
Ligand CLA cA 838



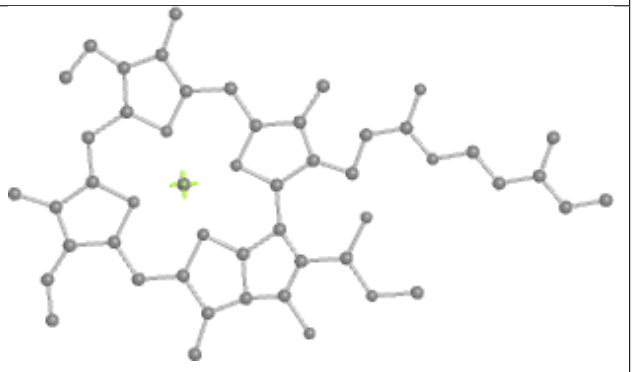
Bond lengths



Bond angles

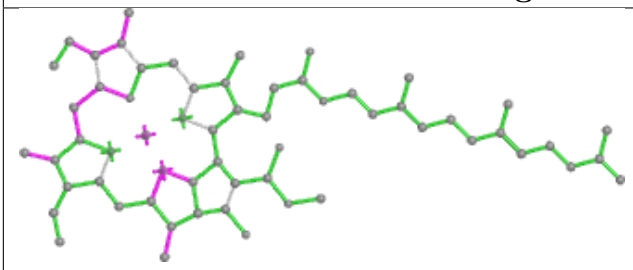


Torsions

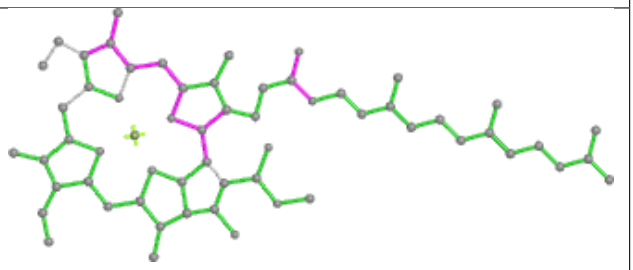


Rings

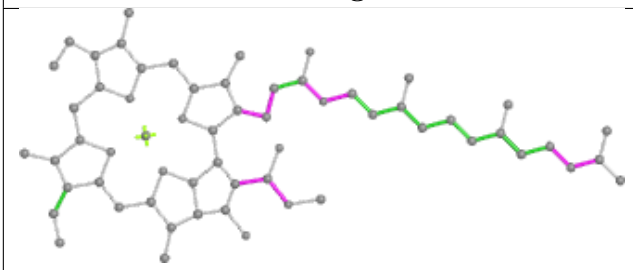
Ligand CLA aA 814



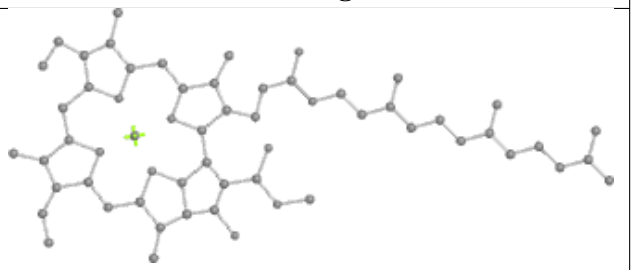
Bond lengths



Bond angles

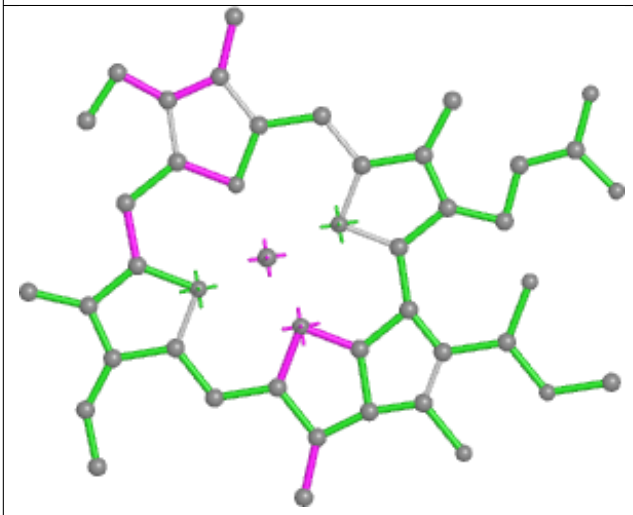


Torsions

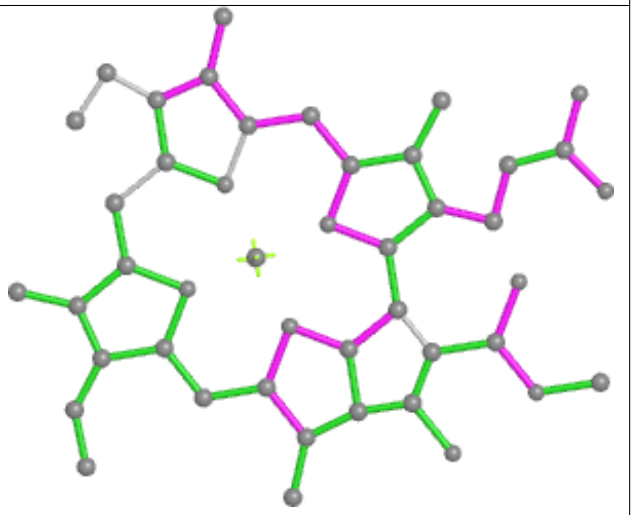


Rings

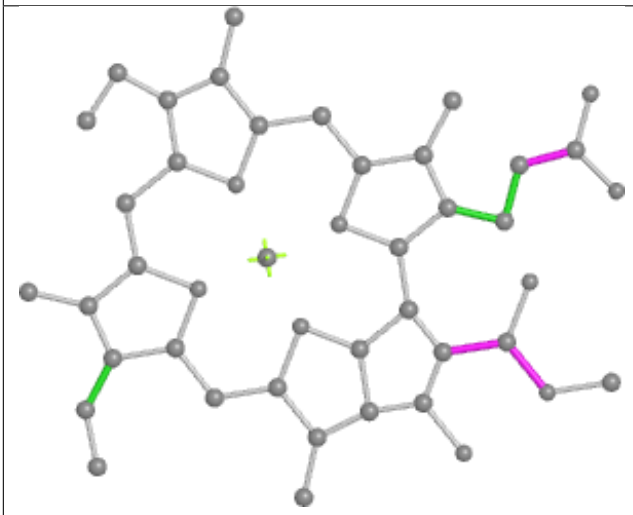
Ligand CLA c6 416



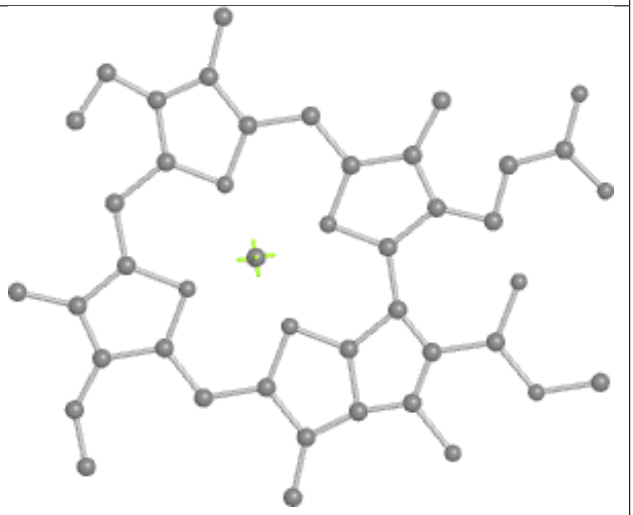
Bond lengths



Bond angles

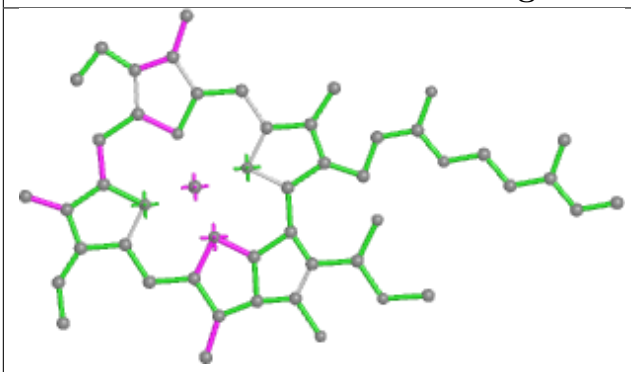


Torsions

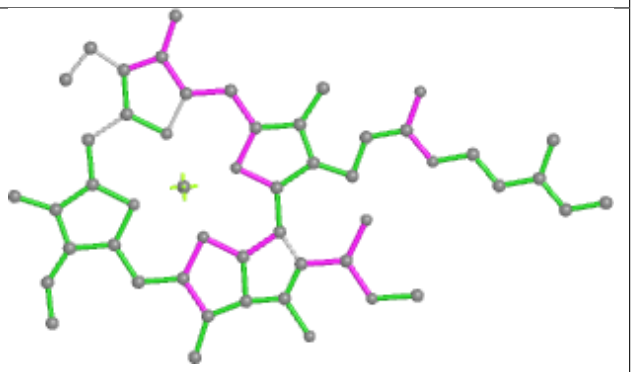


Rings

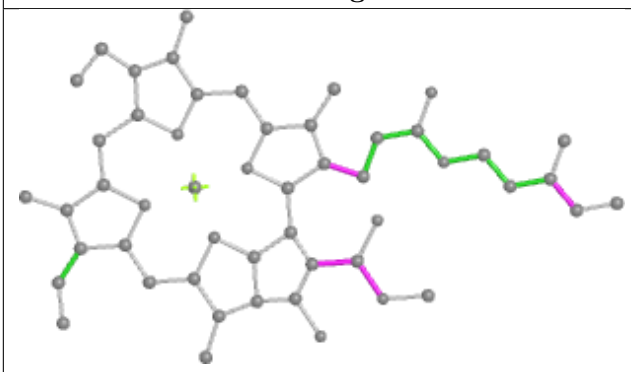
Ligand CLA cF 201



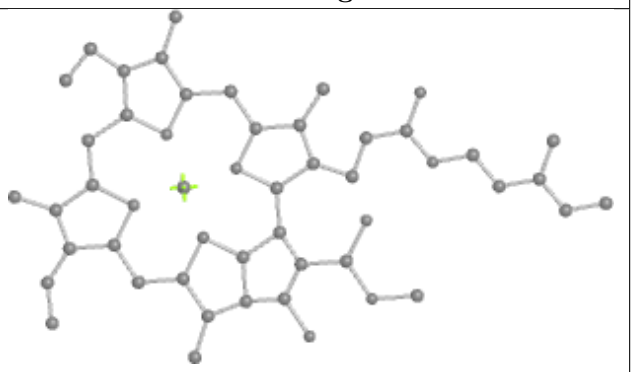
Bond lengths



Bond angles

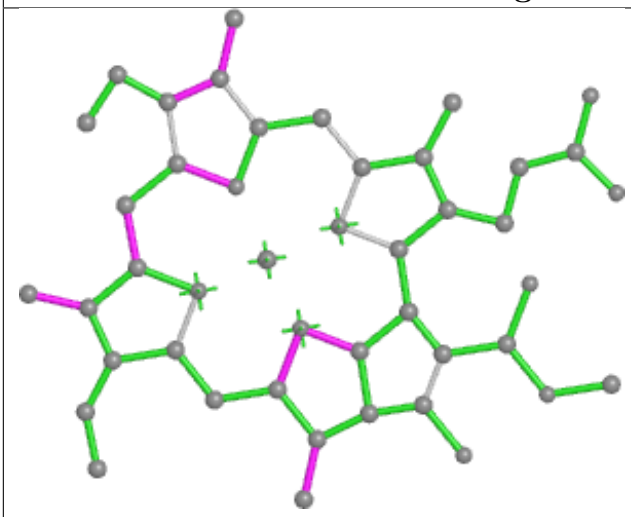


Torsions

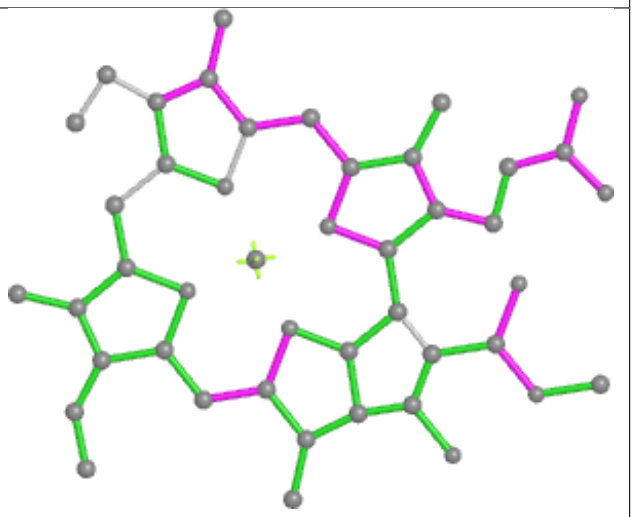


Rings

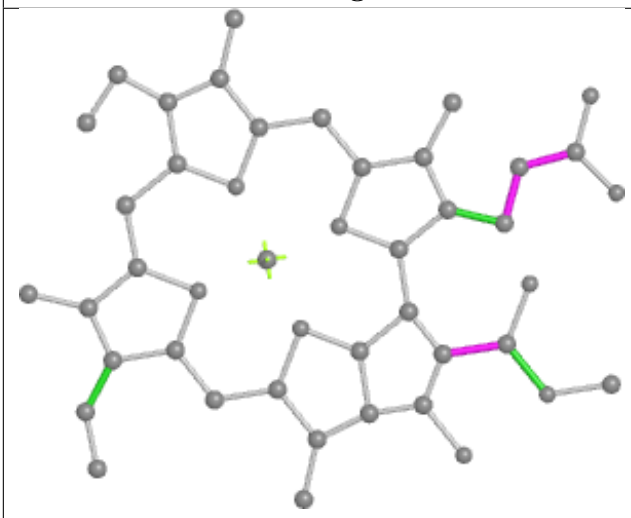
Ligand CLA bB 824



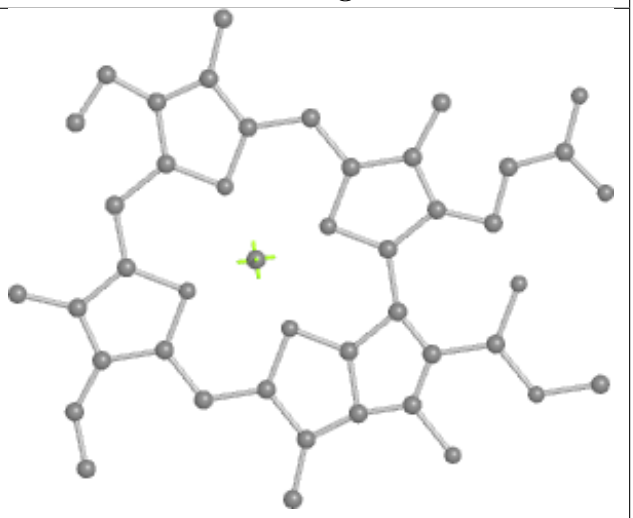
Bond lengths



Bond angles

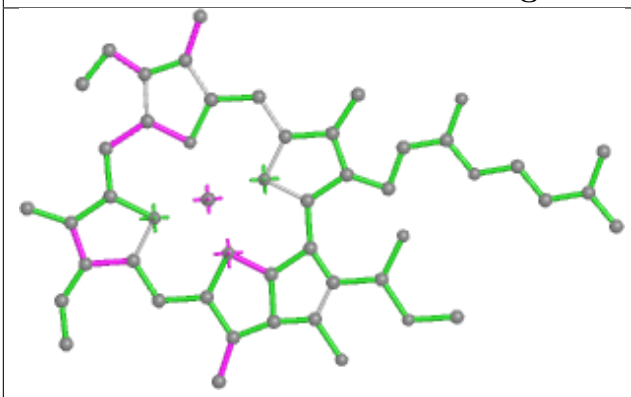


Torsions

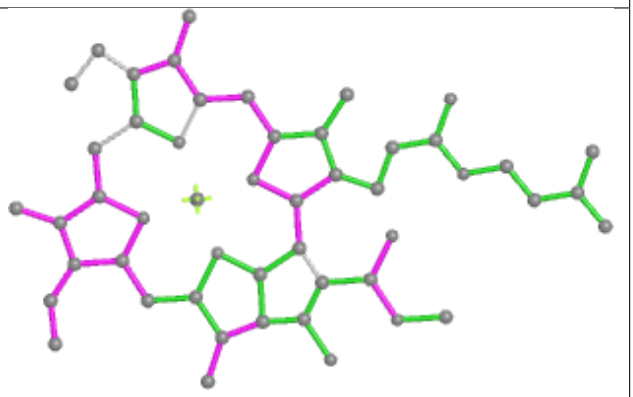


Rings

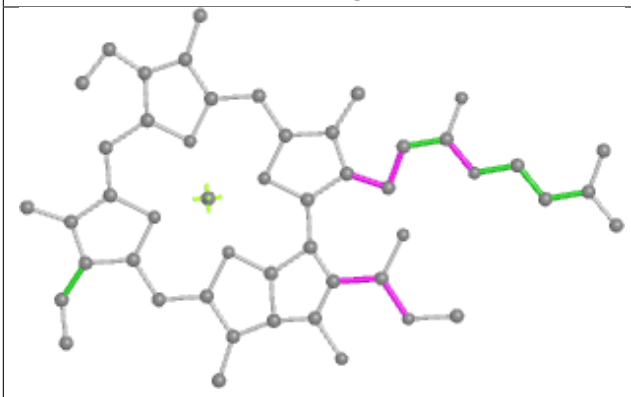
Ligand CLA c4 416



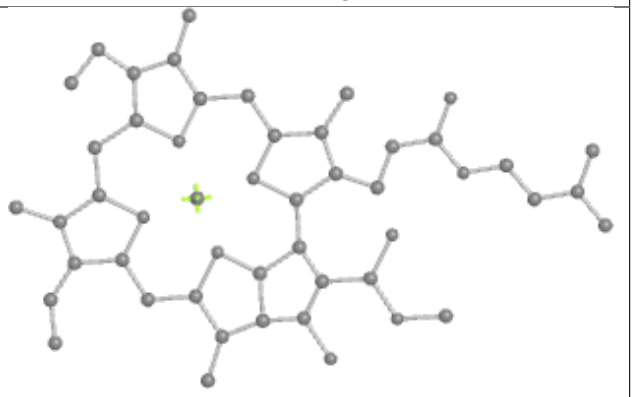
Bond lengths



Bond angles

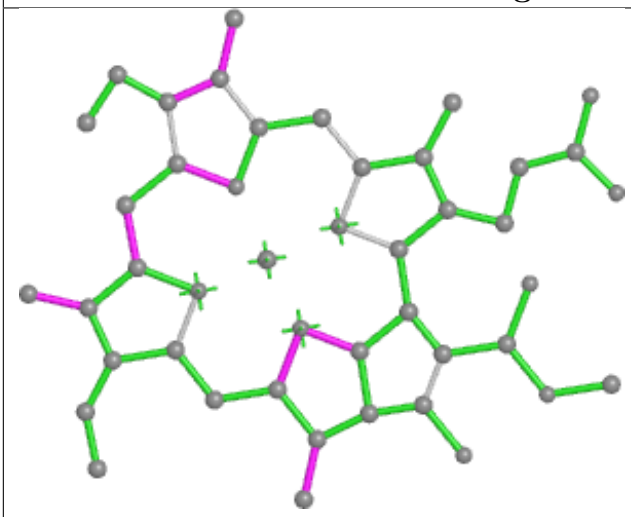


Torsions

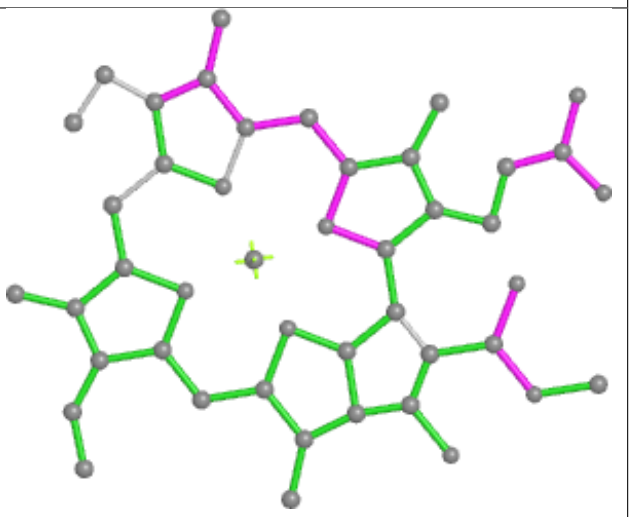


Rings

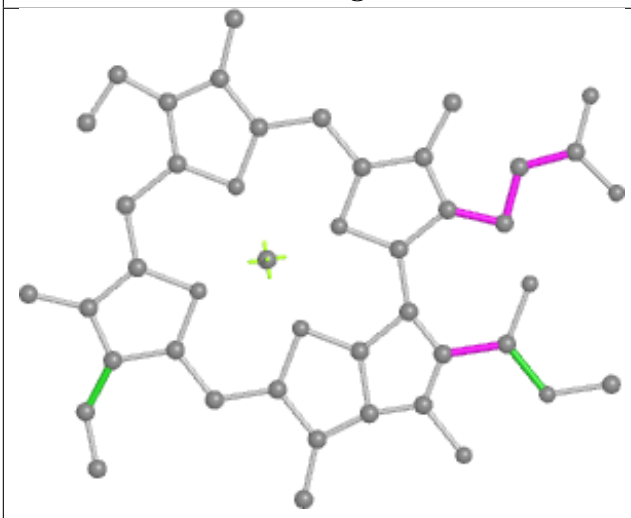
Ligand CLA bA 837



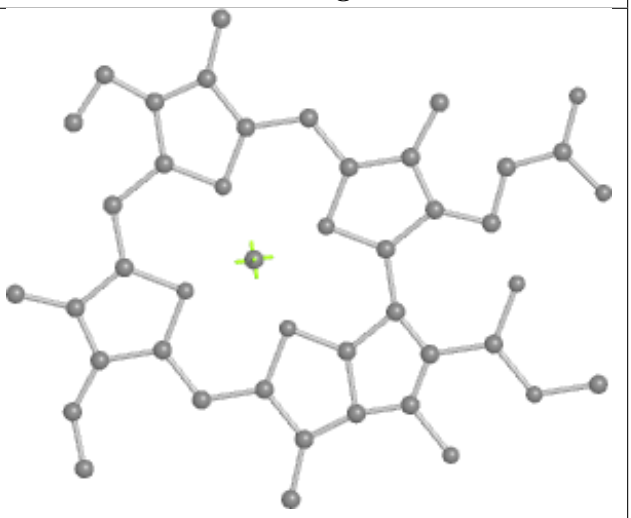
Bond lengths



Bond angles

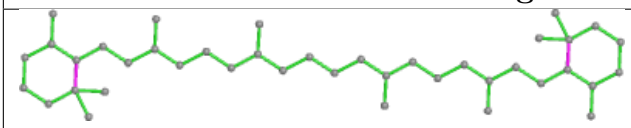


Torsions

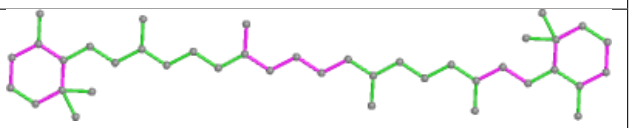


Rings

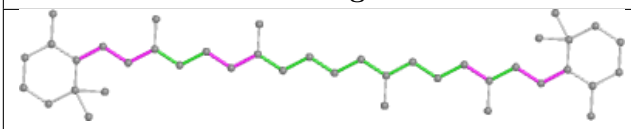
Ligand BCR b2 421



Bond lengths



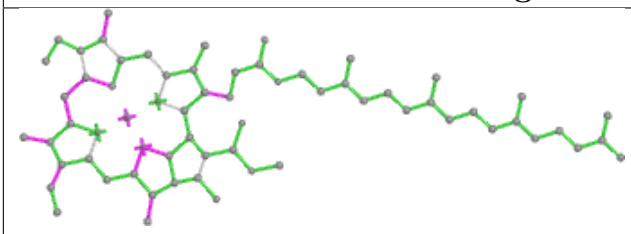
Bond angles



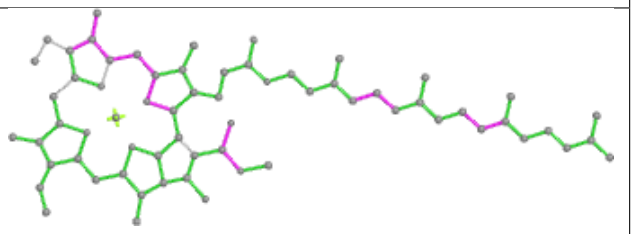
Torsions

Rings

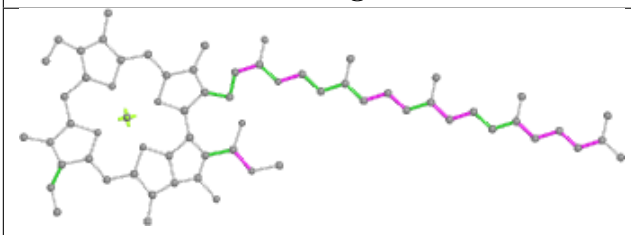
Ligand CLA bB 807



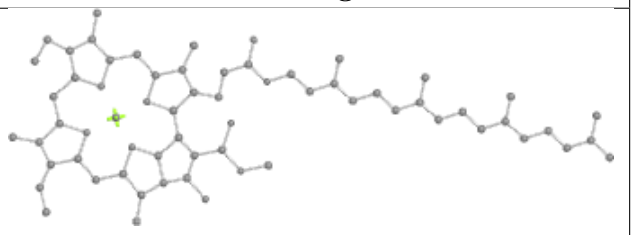
Bond lengths



Bond angles

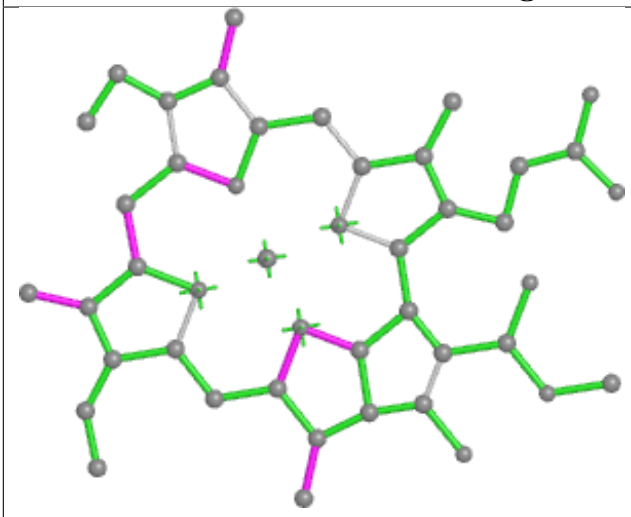


Torsions

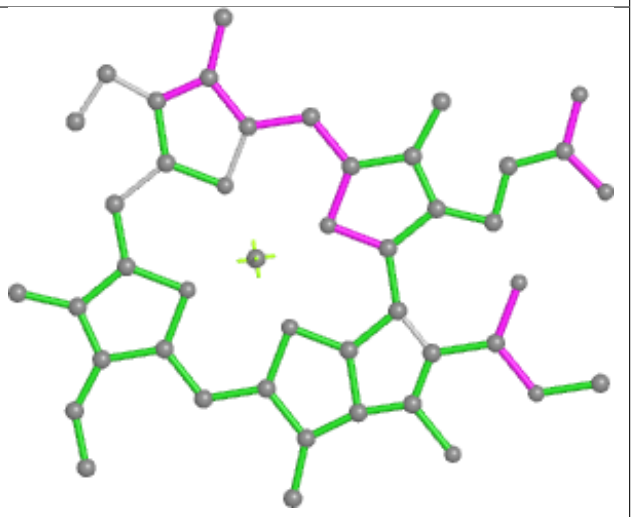


Rings

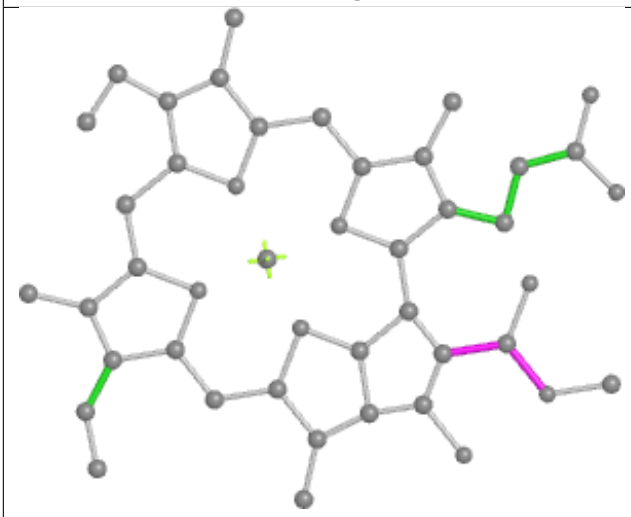
Ligand CLA b3 406



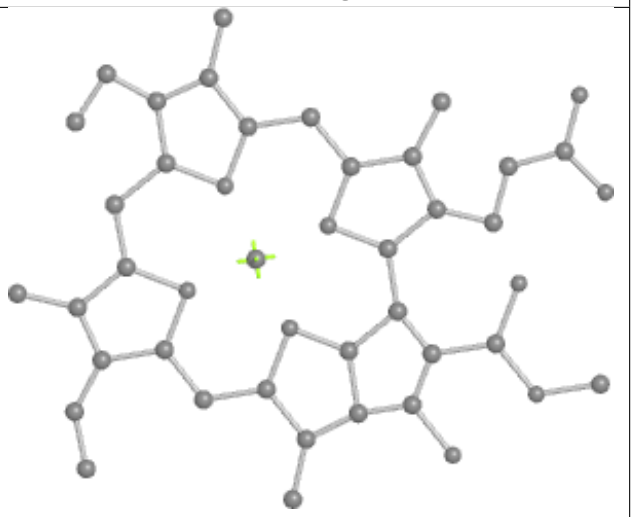
Bond lengths



Bond angles

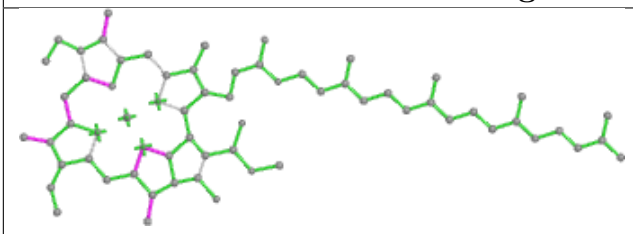


Torsions

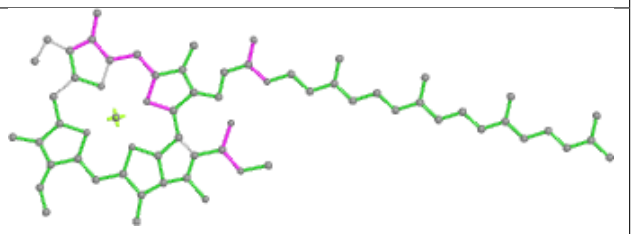


Rings

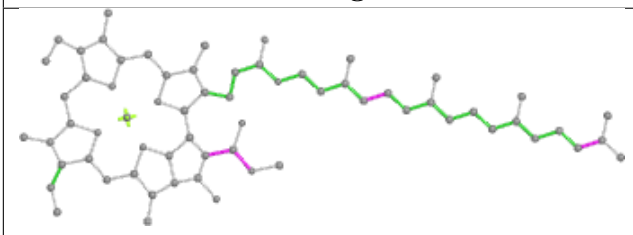
Ligand CLA b5 409



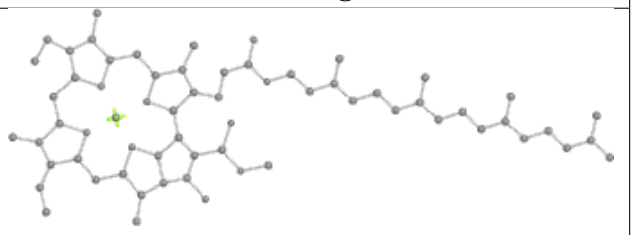
Bond lengths



Bond angles

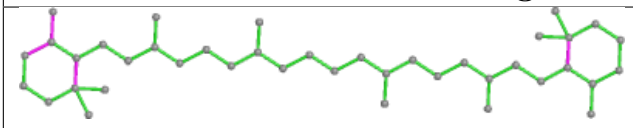


Torsions

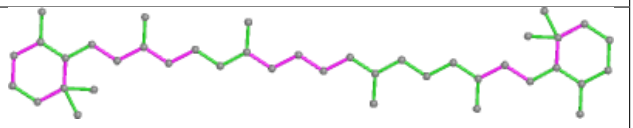


Rings

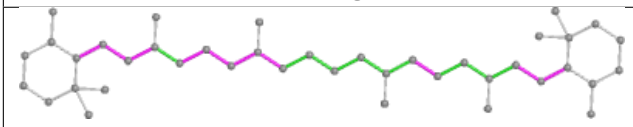
Ligand BCR b3 401



Bond lengths



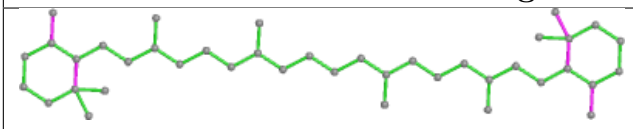
Bond angles



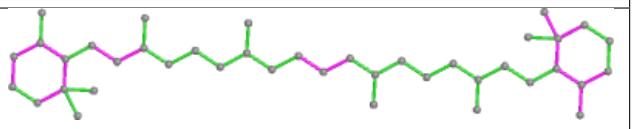
Torsions

Rings

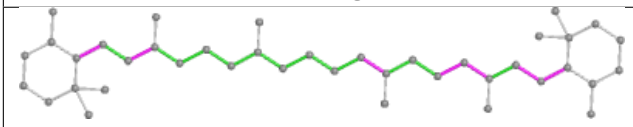
Ligand BCR a6 419



Bond lengths



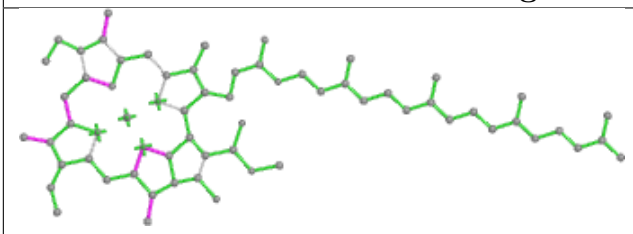
Bond angles



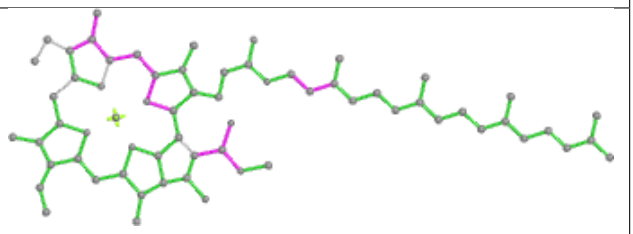
Torsions

Rings

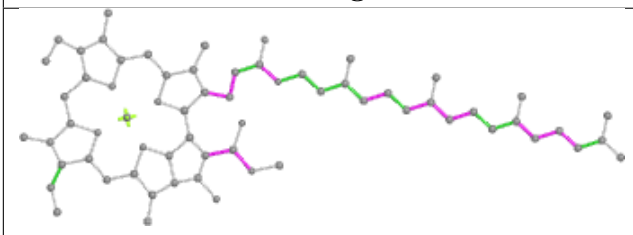
Ligand CLA a4 402



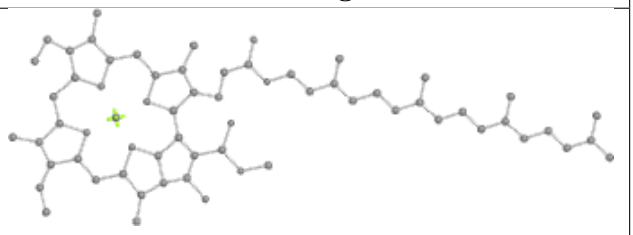
Bond lengths



Bond angles

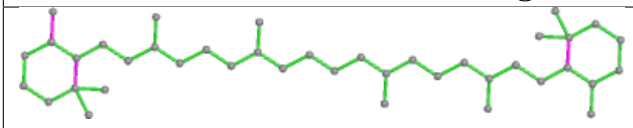


Torsions

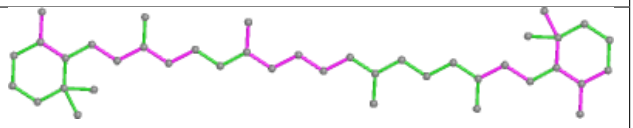


Rings

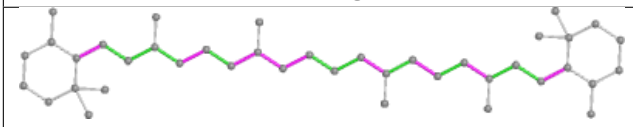
Ligand BCR bJ 103



Bond lengths



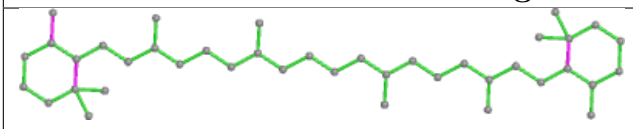
Bond angles



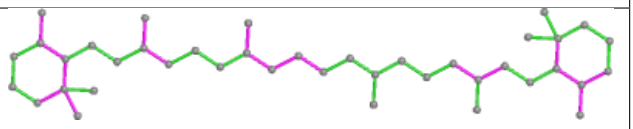
Torsions

Rings

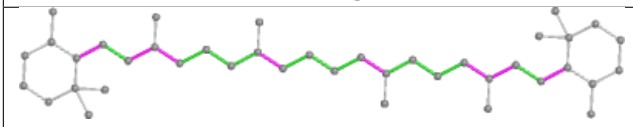
Ligand BCR bF 202



Bond lengths

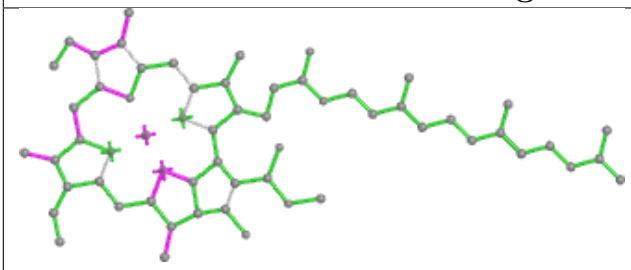
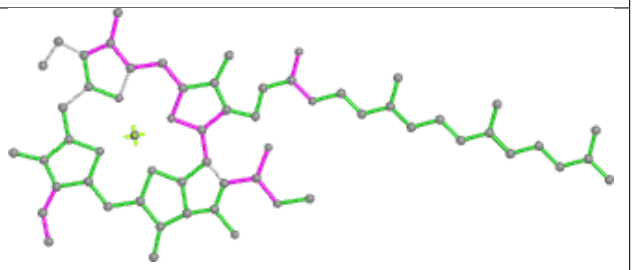
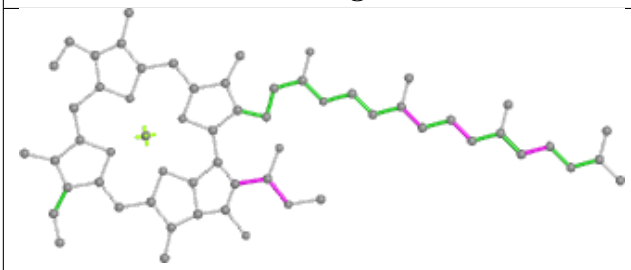
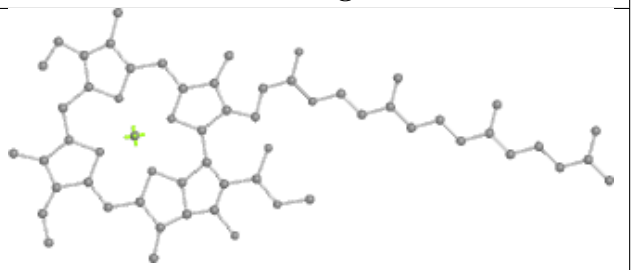


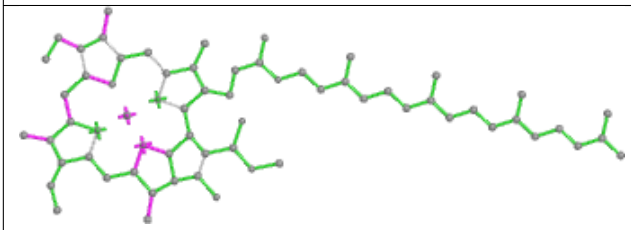
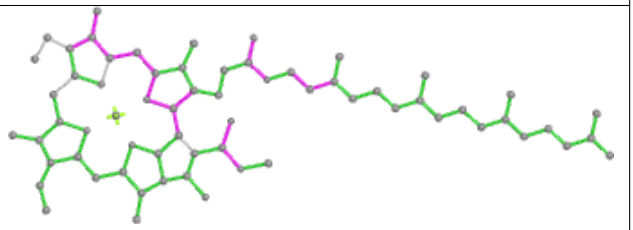
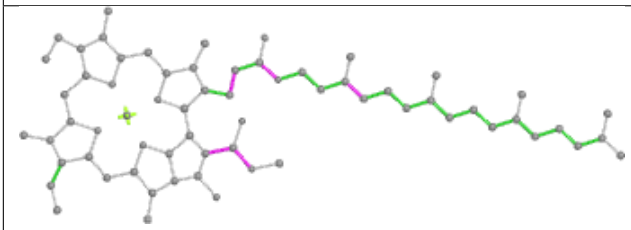
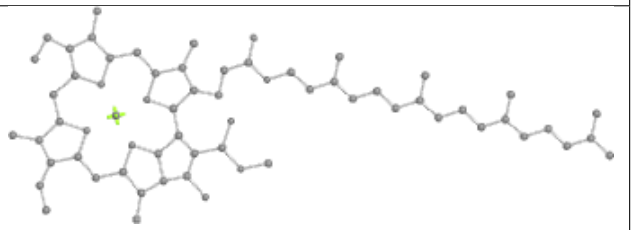
Bond angles



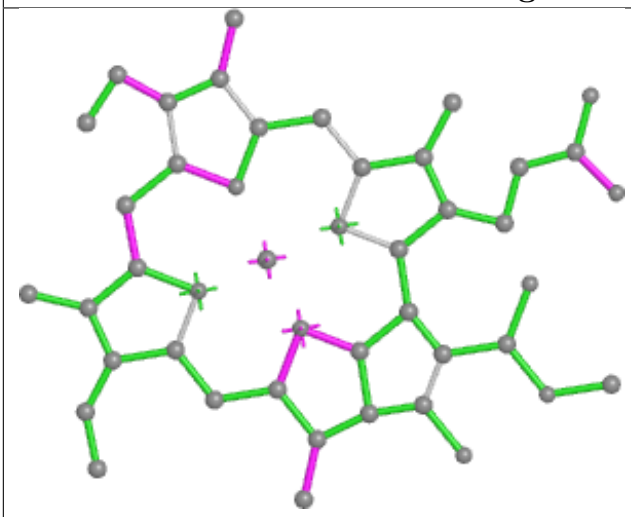
Torsions

Rings

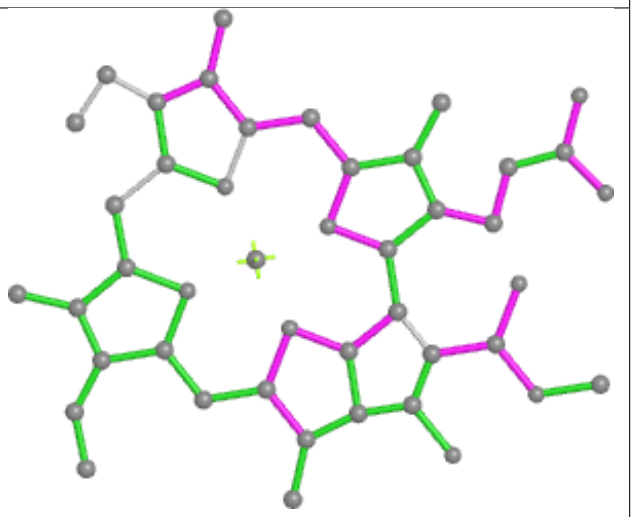
Ligand CLA cB 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c6 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

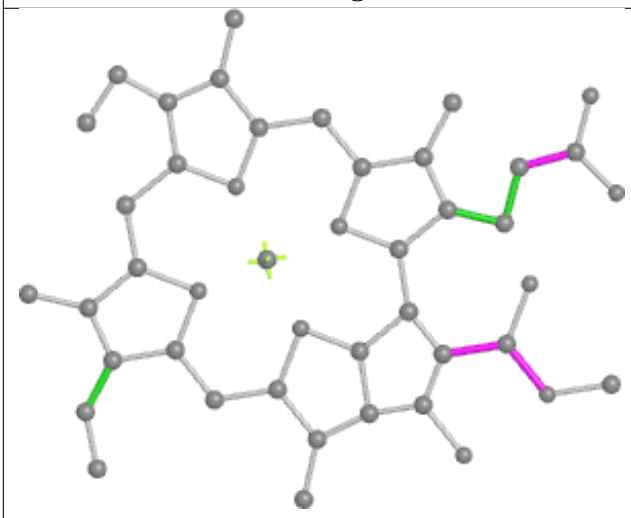
Ligand CLA b5 415



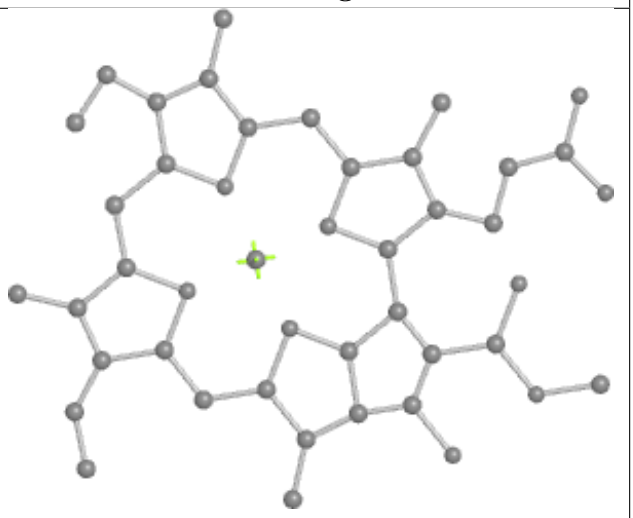
Bond lengths



Bond angles

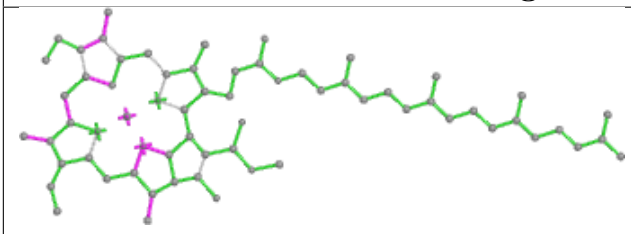


Torsions

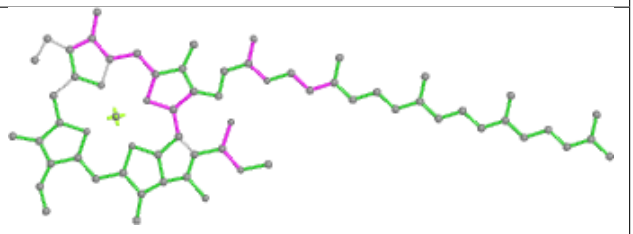


Rings

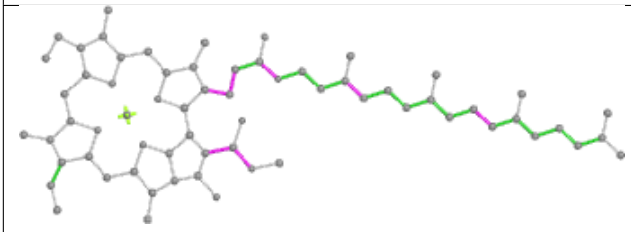
Ligand CLA a3 404



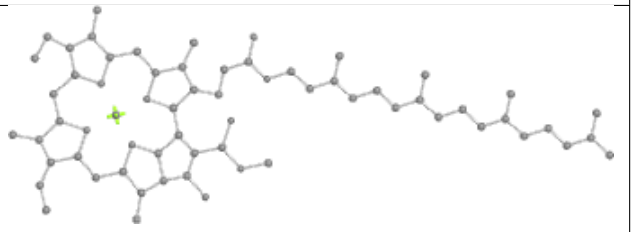
Bond lengths



Bond angles

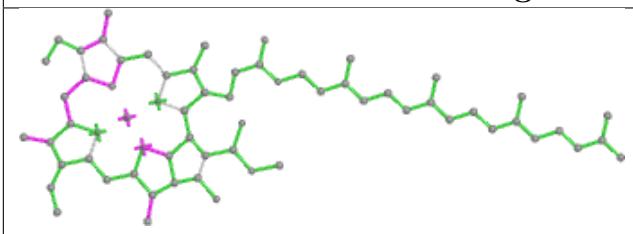


Torsions

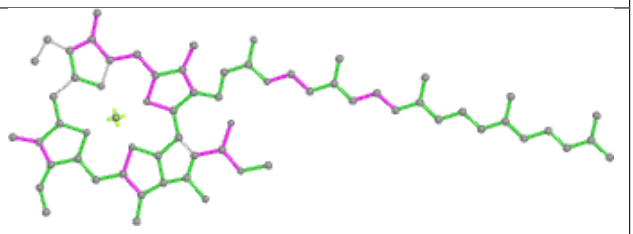


Rings

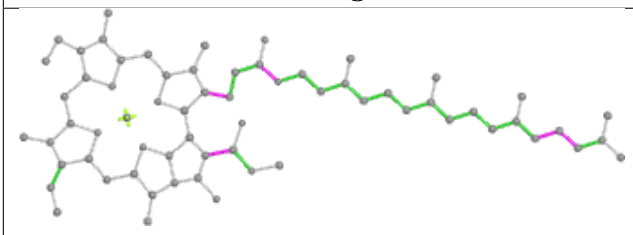
Ligand CLA bB 830



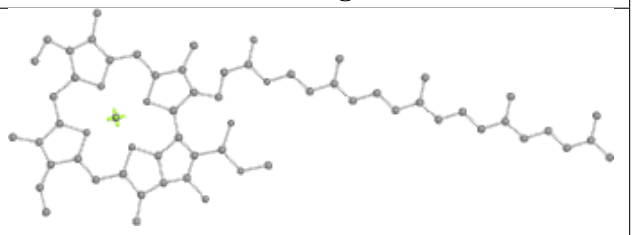
Bond lengths



Bond angles

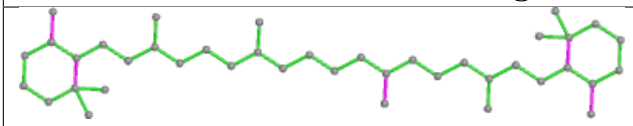


Torsions

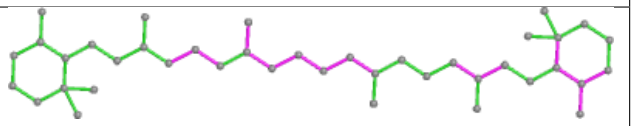


Rings

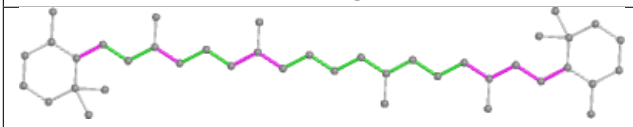
Ligand BCR bB 850



Bond lengths



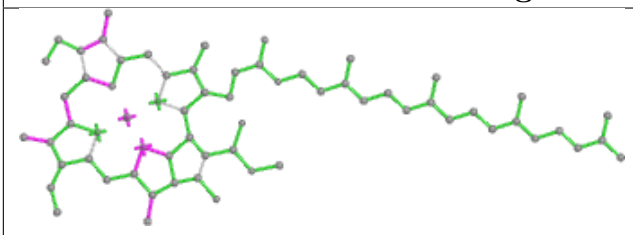
Bond angles



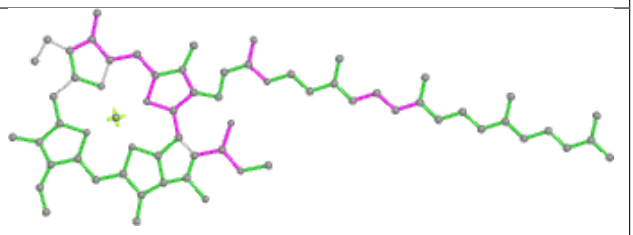
Torsions

Rings

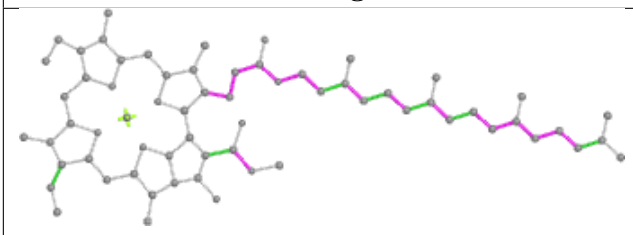
Ligand CLA aA 829



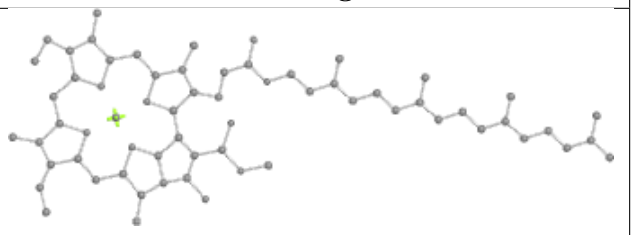
Bond lengths



Bond angles

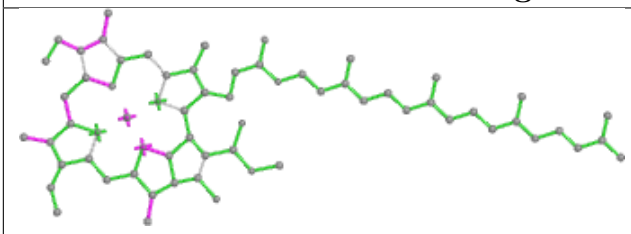


Torsions

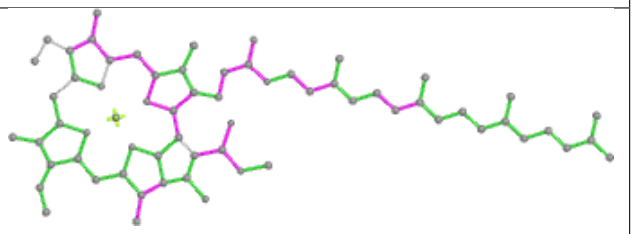


Rings

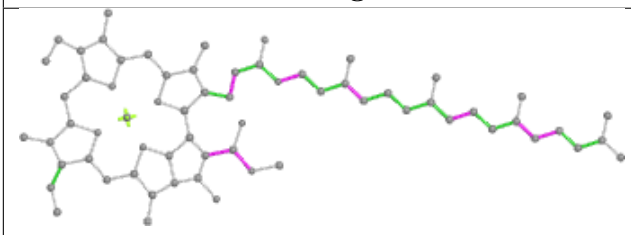
Ligand CLA bB 803



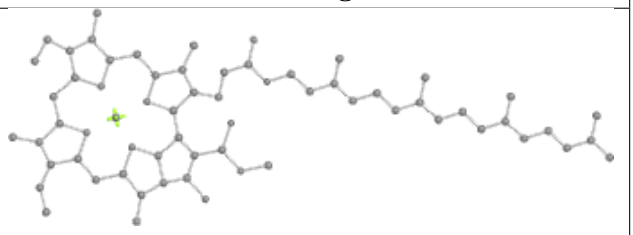
Bond lengths



Bond angles

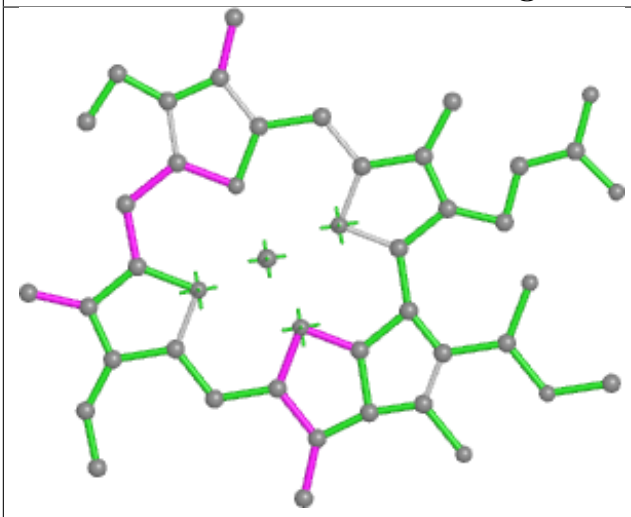


Torsions

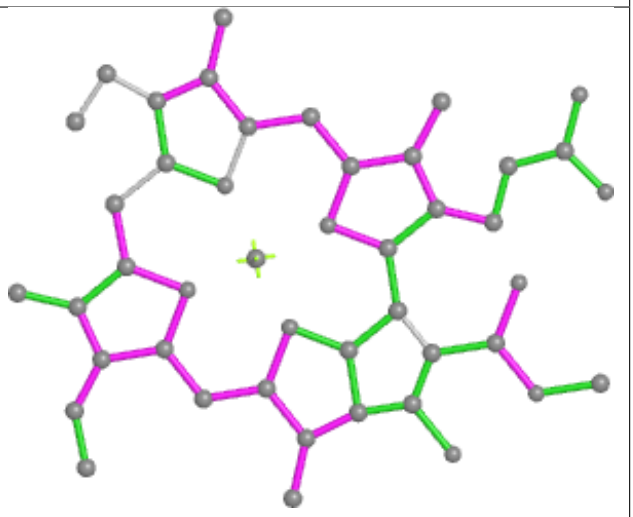


Rings

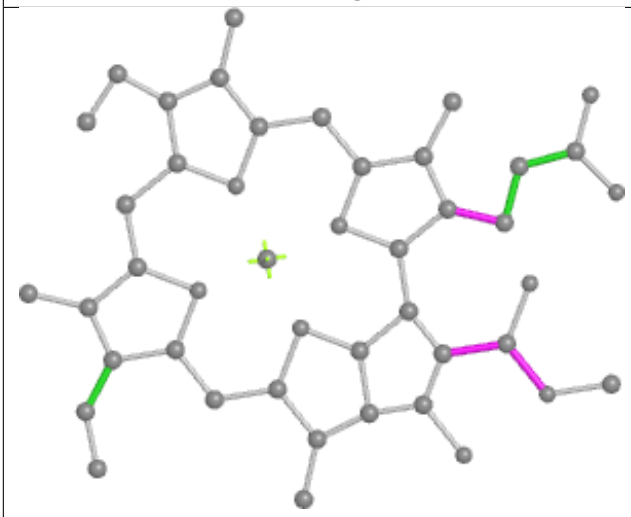
Ligand CLA b4 405



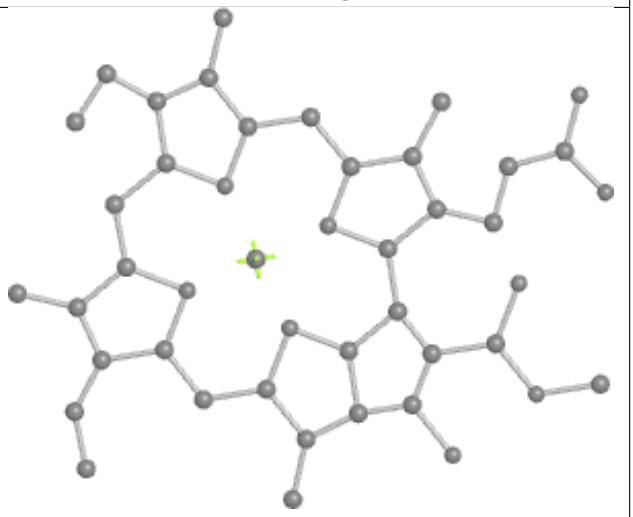
Bond lengths



Bond angles

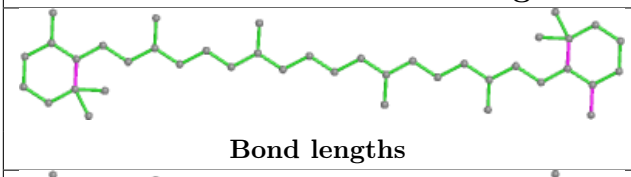


Torsions

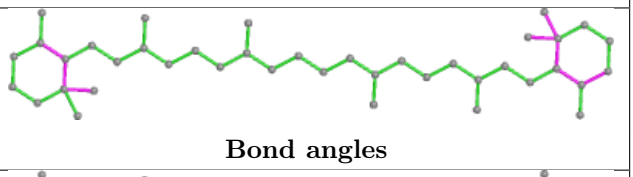


Rings

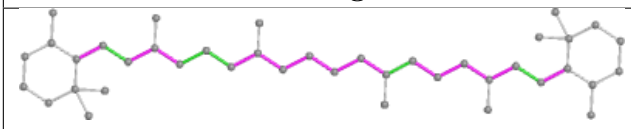
Ligand BCR aA 852



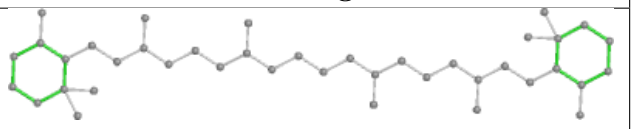
Bond lengths



Bond angles

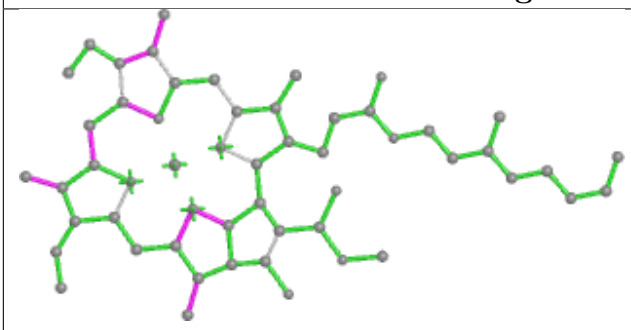


Torsions

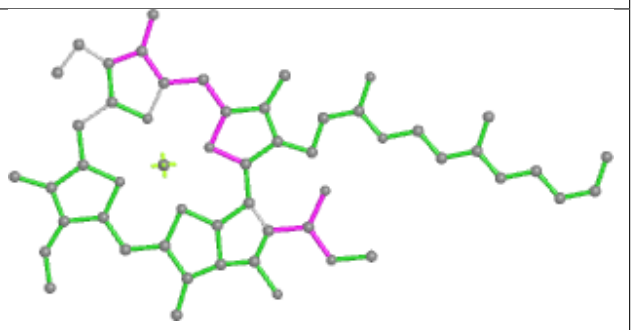


Rings

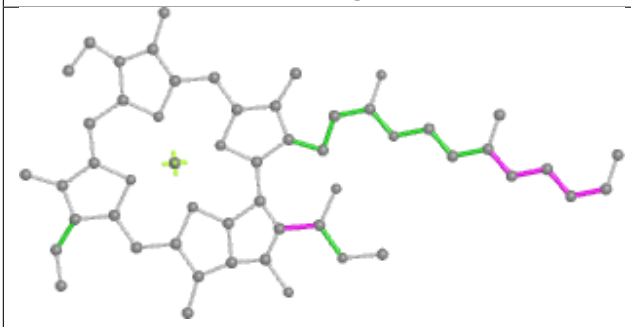
Ligand CLA aA 818



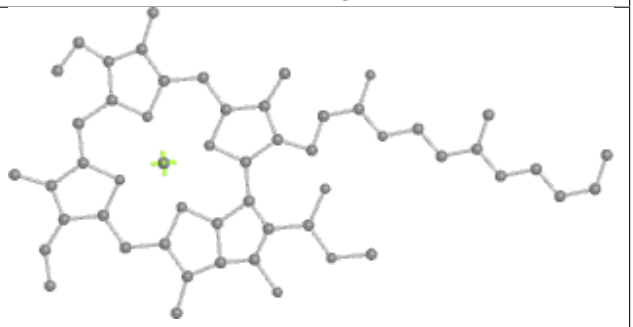
Bond lengths



Bond angles

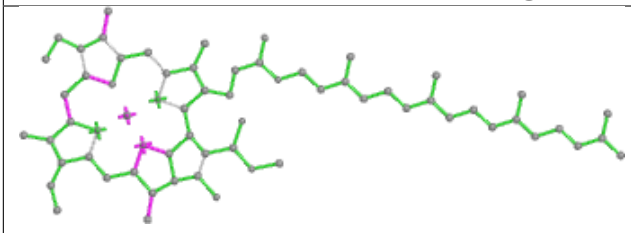


Torsions

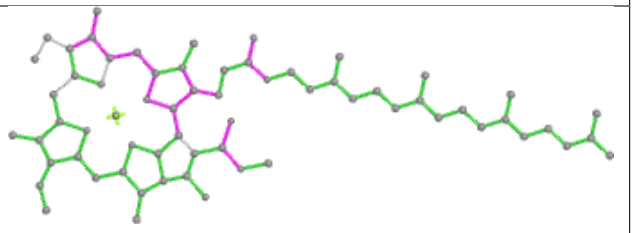


Rings

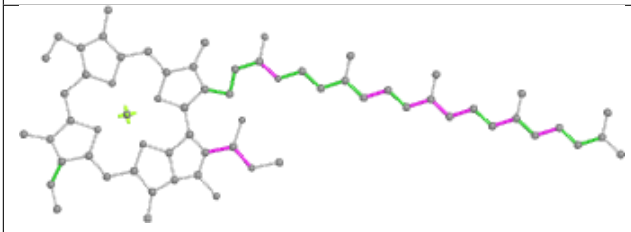
Ligand CLA c5 403



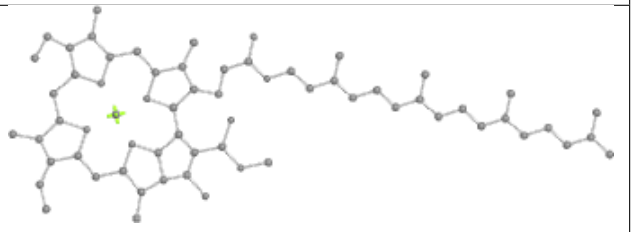
Bond lengths



Bond angles

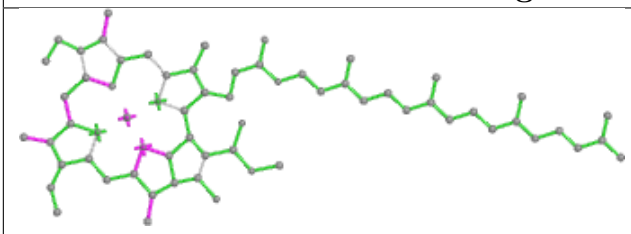


Torsions

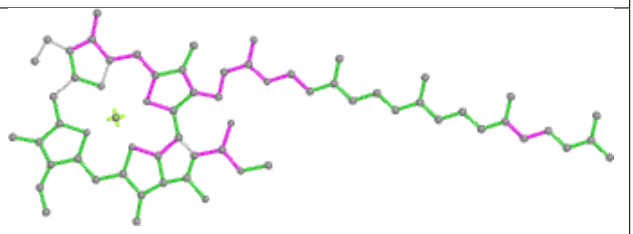


Rings

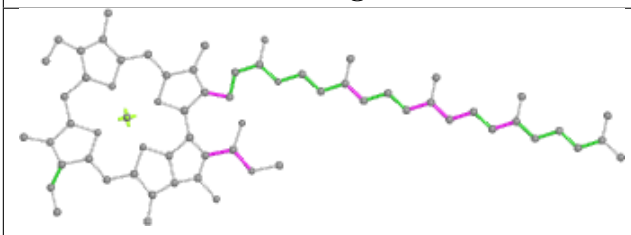
Ligand CLA aB 827



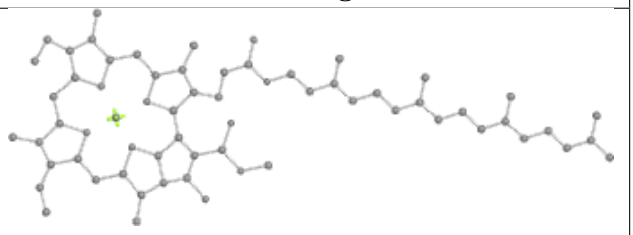
Bond lengths



Bond angles

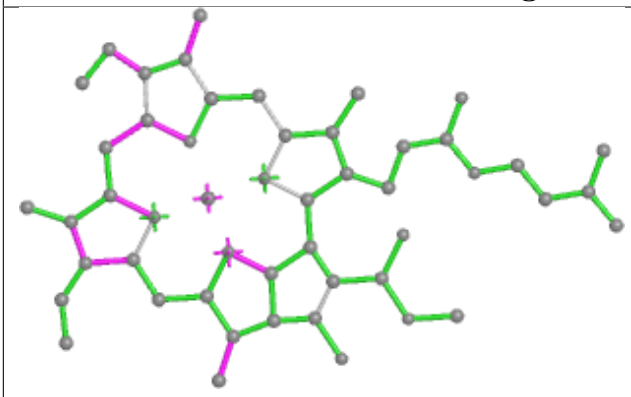


Torsions

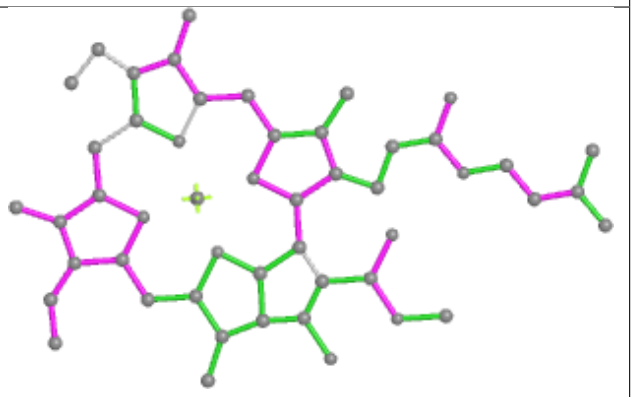


Rings

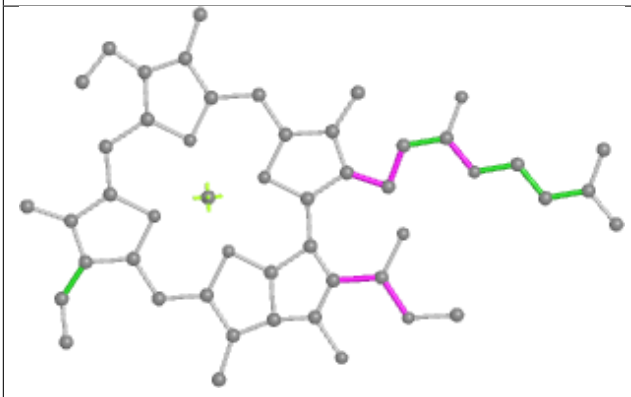
Ligand CLA c3 416



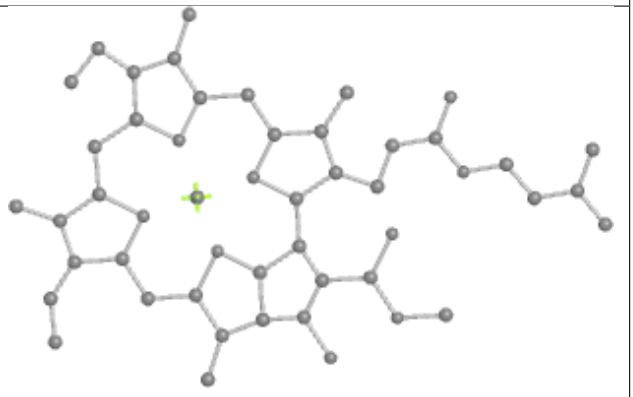
Bond lengths



Bond angles

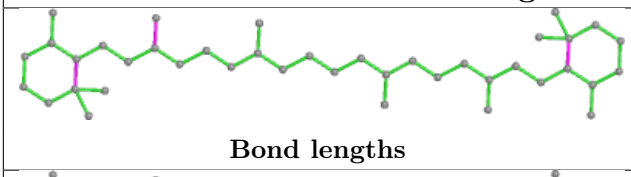


Torsions

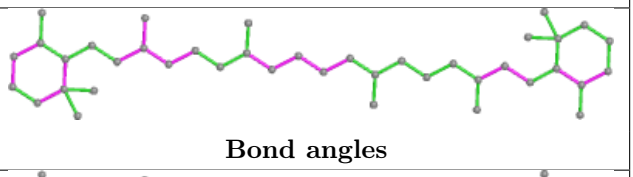


Rings

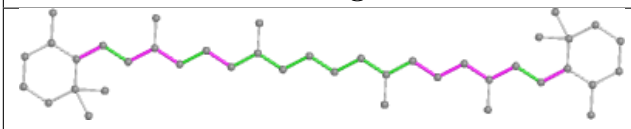
Ligand BCR c1 401



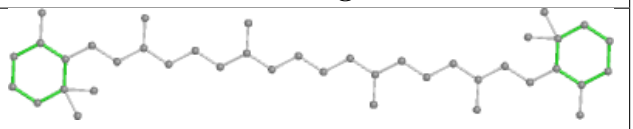
Bond lengths



Bond angles

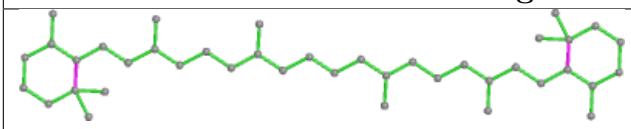


Torsions

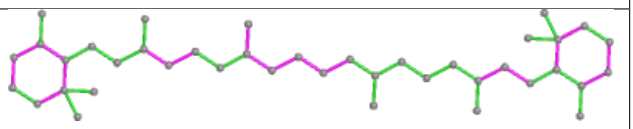


Rings

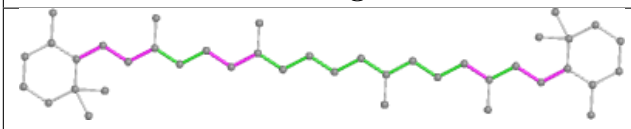
Ligand BCR b4 420



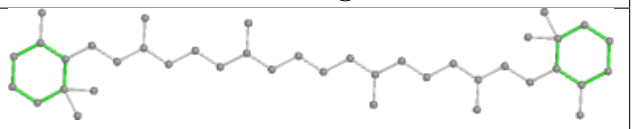
Bond lengths



Bond angles

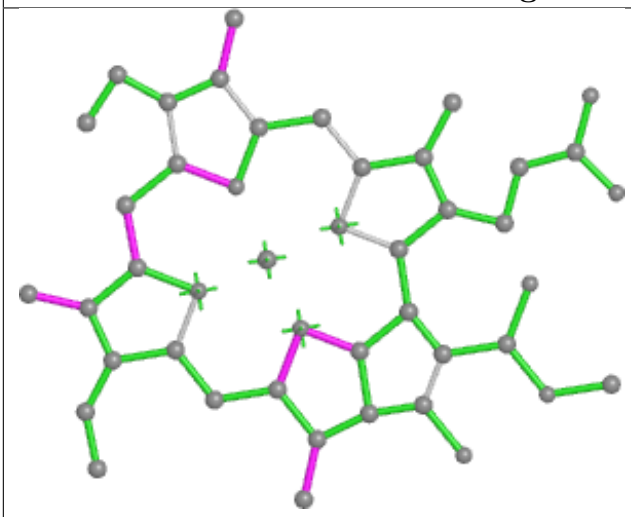


Torsions

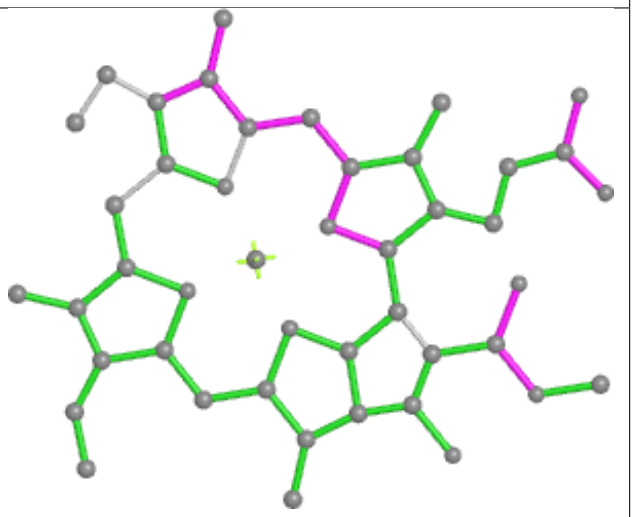


Rings

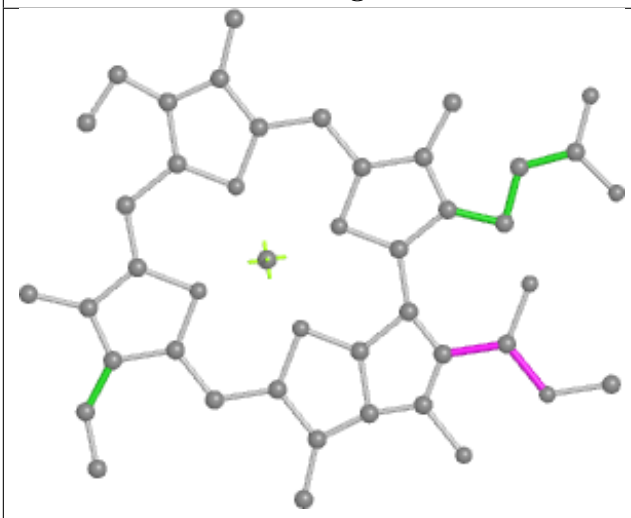
Ligand CLA a4 406



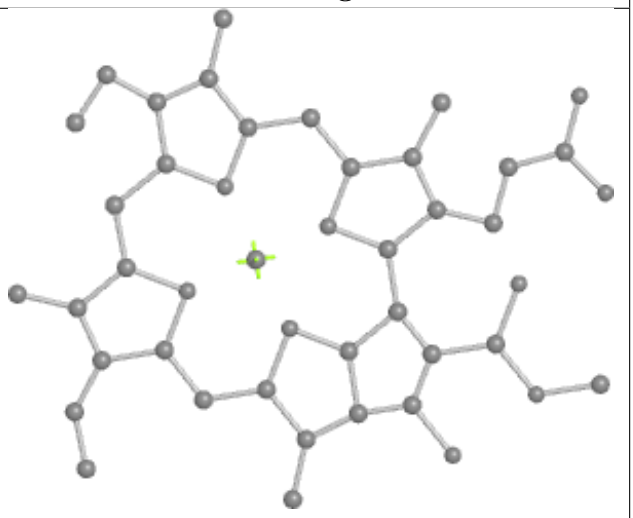
Bond lengths



Bond angles

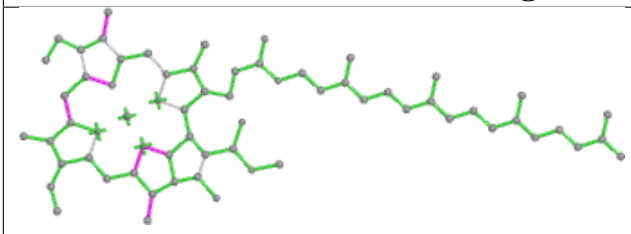


Torsions

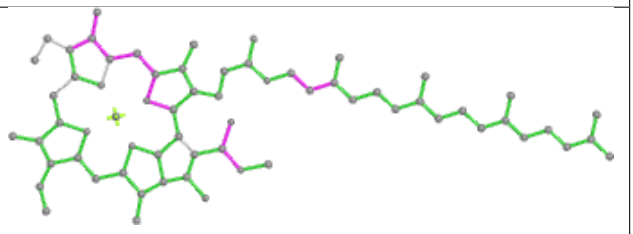


Rings

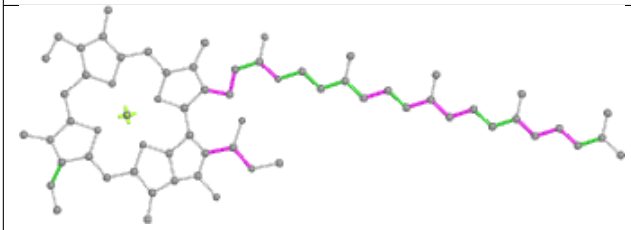
Ligand CLA a2 402



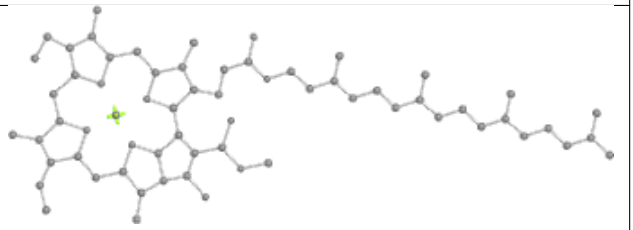
Bond lengths



Bond angles

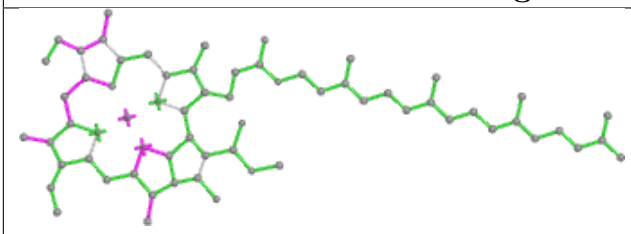


Torsions

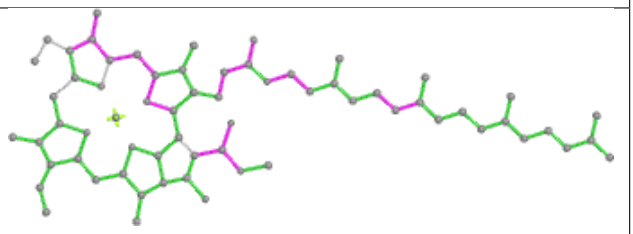


Rings

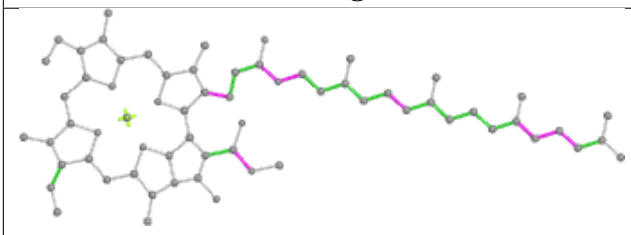
Ligand CLA bA 812



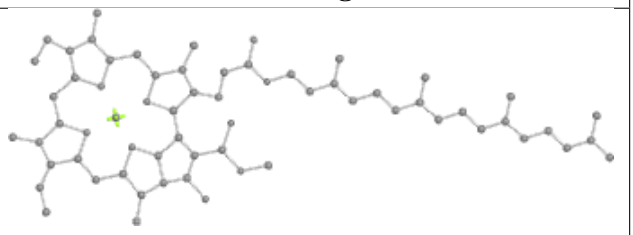
Bond lengths



Bond angles

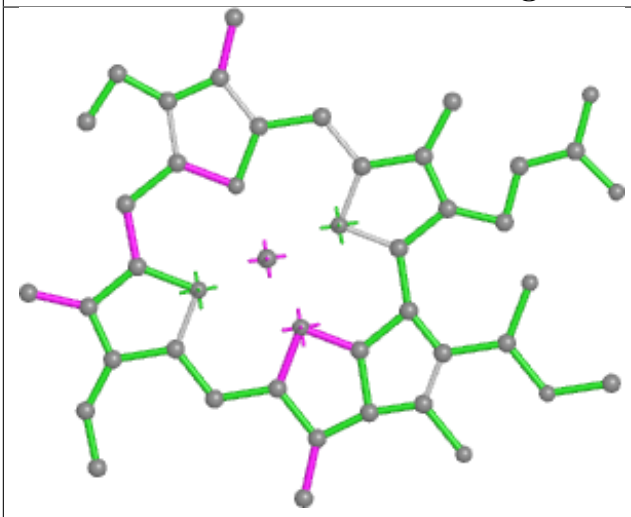


Torsions

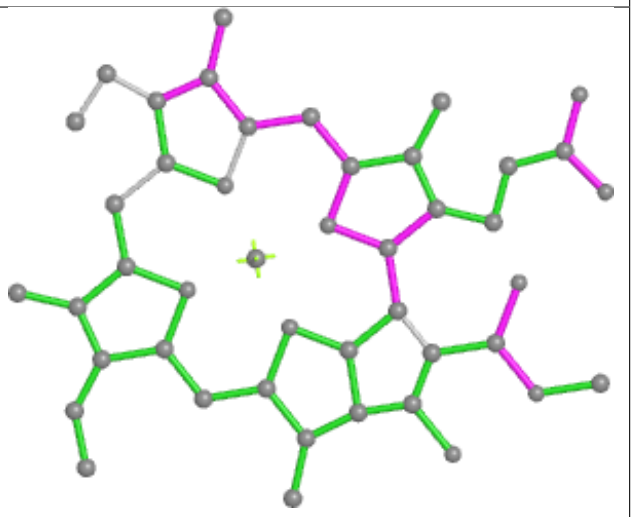


Rings

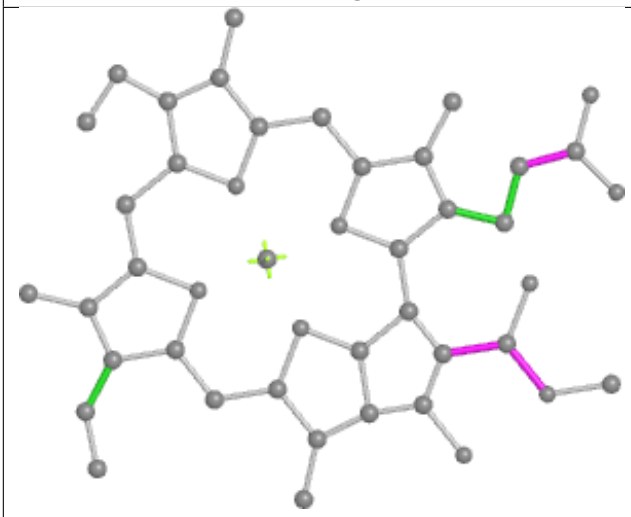
Ligand CLA c1 407



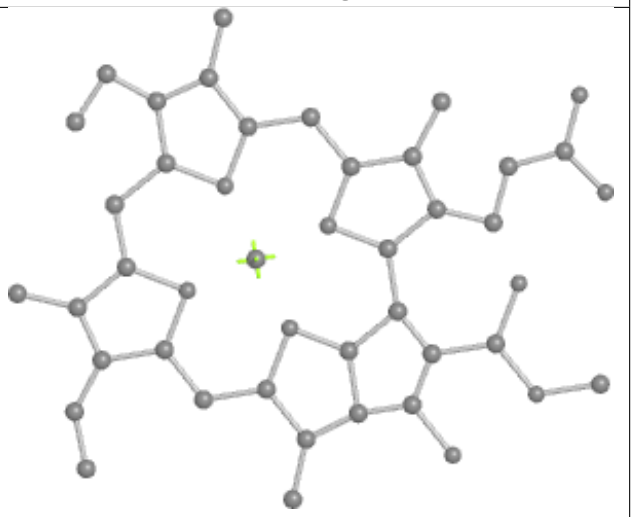
Bond lengths



Bond angles

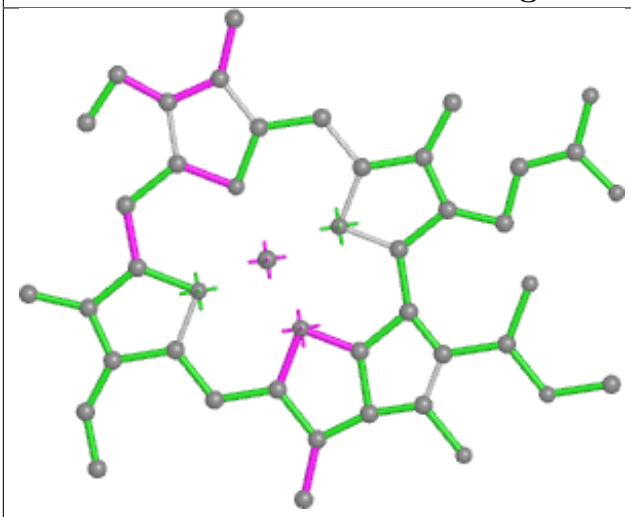


Torsions

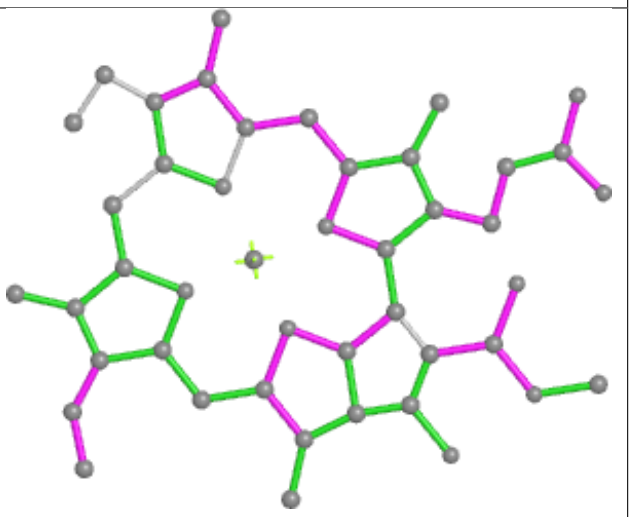


Rings

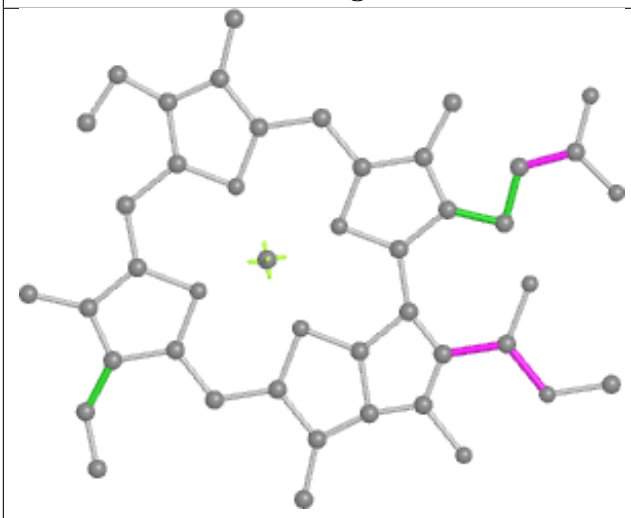
Ligand CLA a4 415



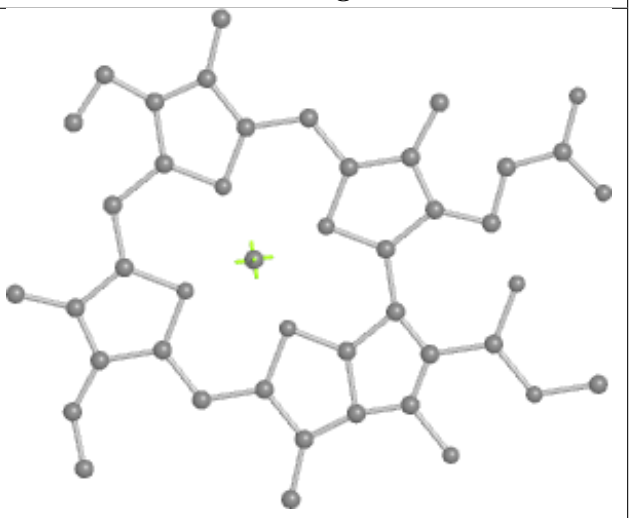
Bond lengths



Bond angles

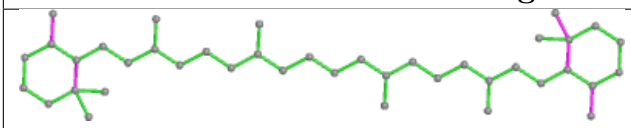


Torsions

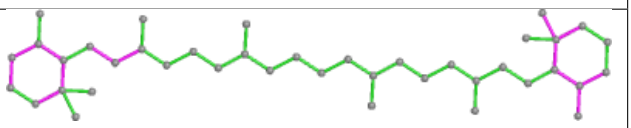


Rings

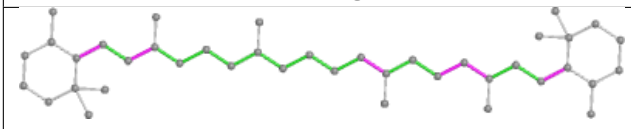
Ligand BCR a4 418



Bond lengths



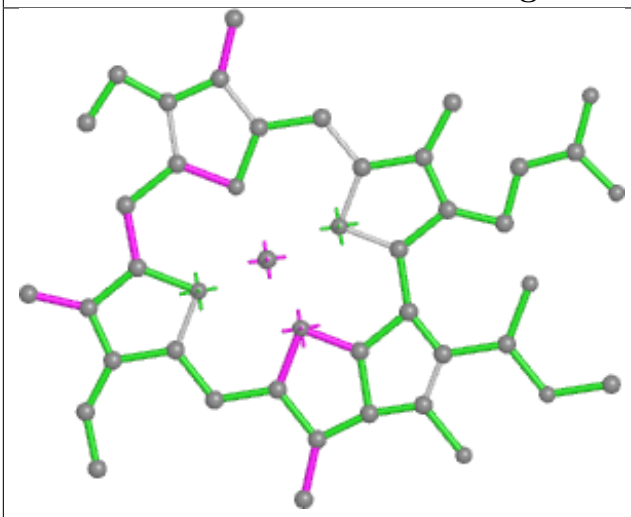
Bond angles



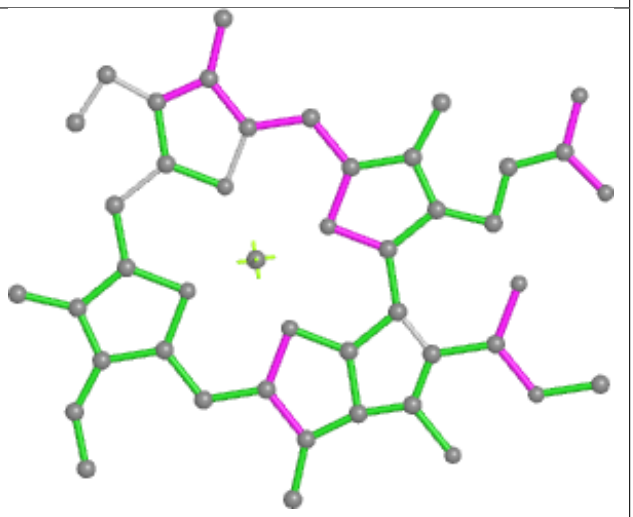
Torsions

Rings

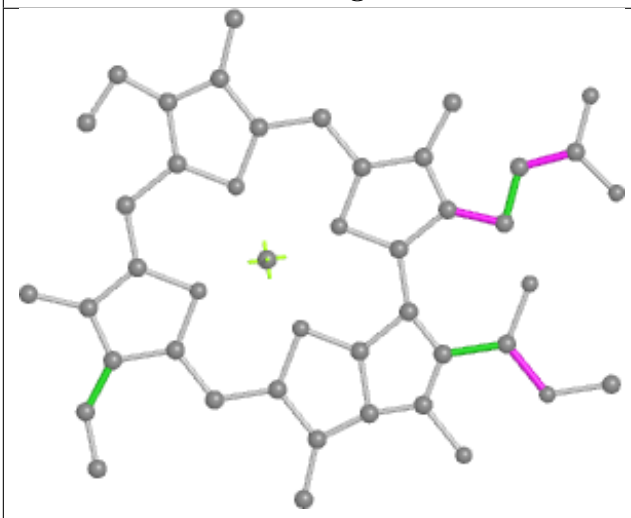
Ligand CLA a2 409



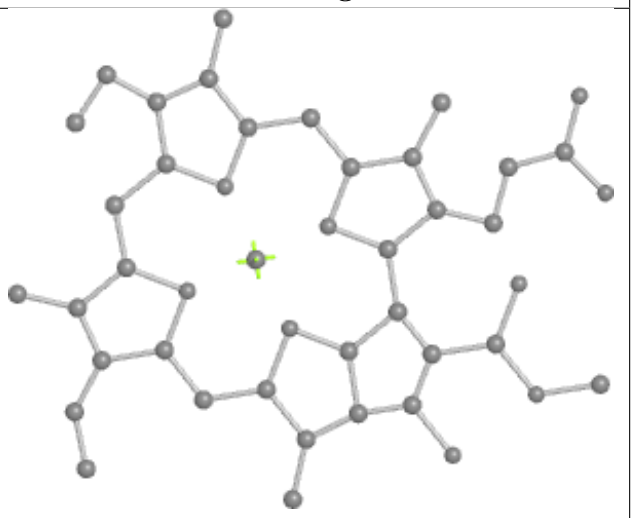
Bond lengths



Bond angles

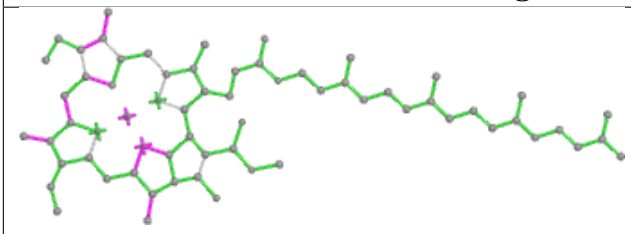


Torsions

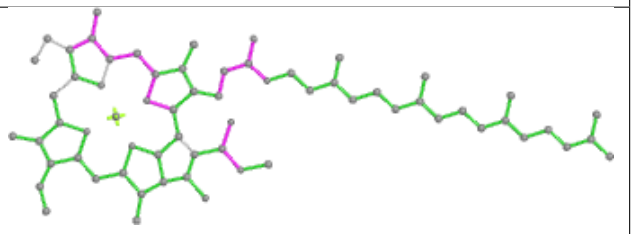


Rings

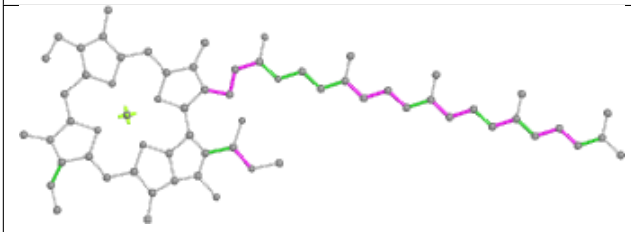
Ligand CLA bA 810



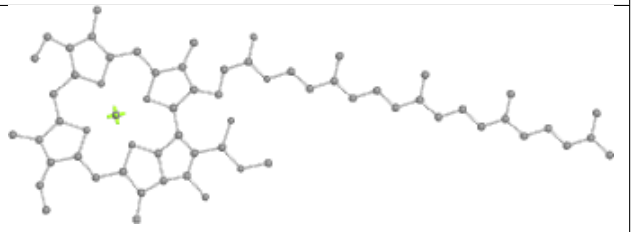
Bond lengths



Bond angles

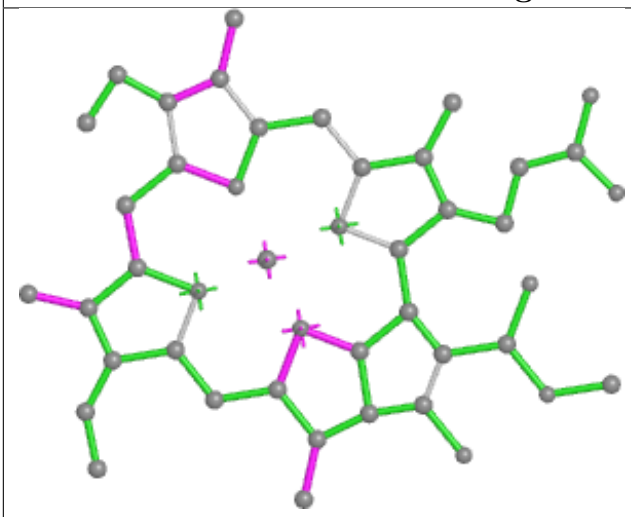


Torsions

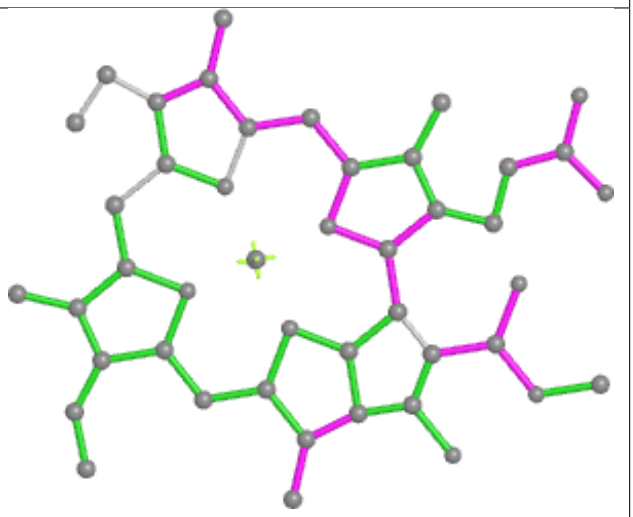


Rings

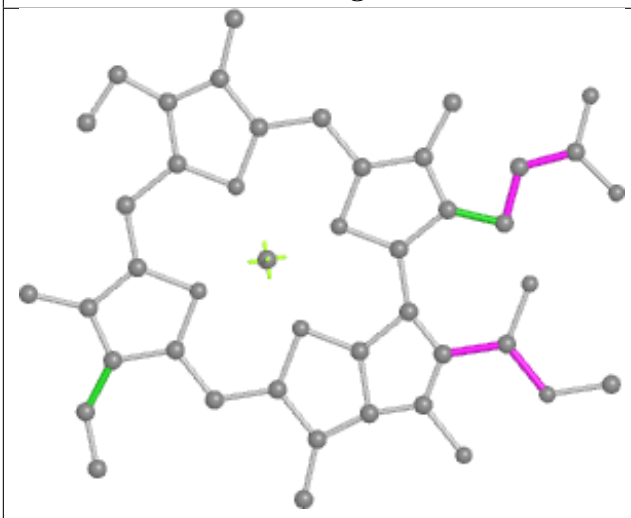
Ligand CLA aX 102



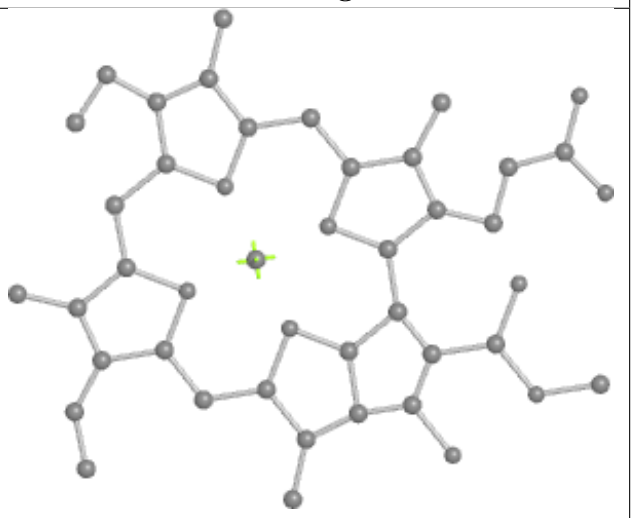
Bond lengths



Bond angles

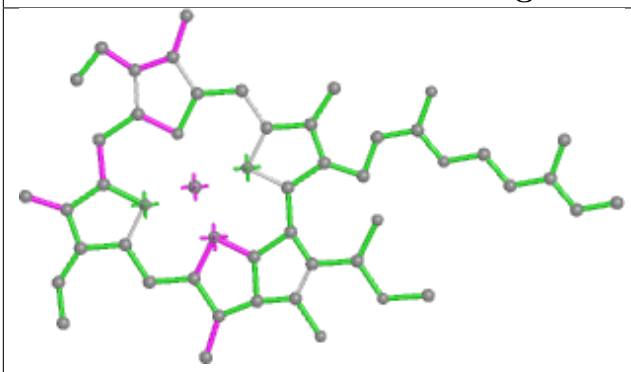


Torsions

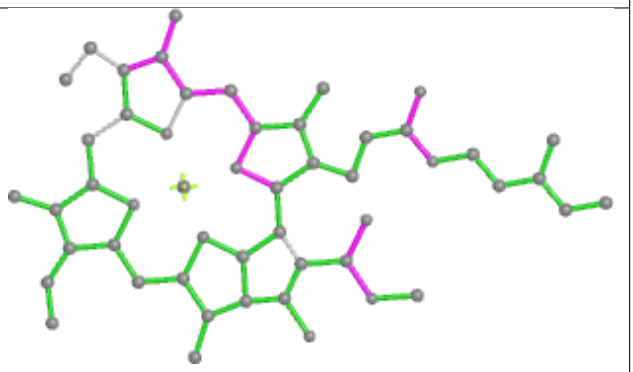


Rings

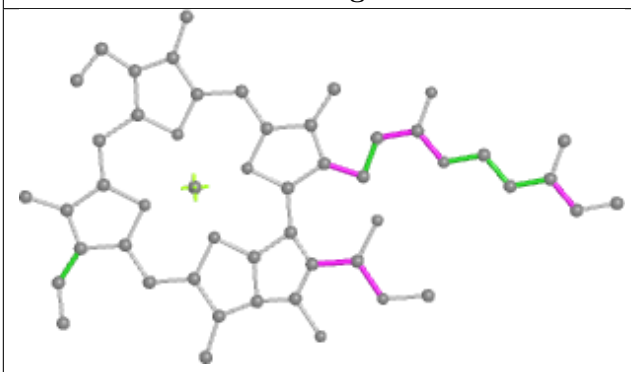
Ligand CLA cA 824



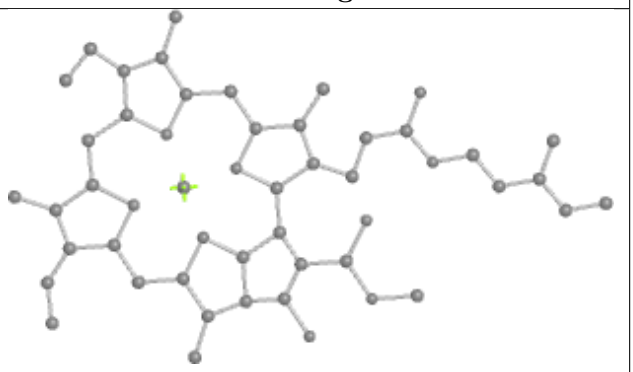
Bond lengths



Bond angles

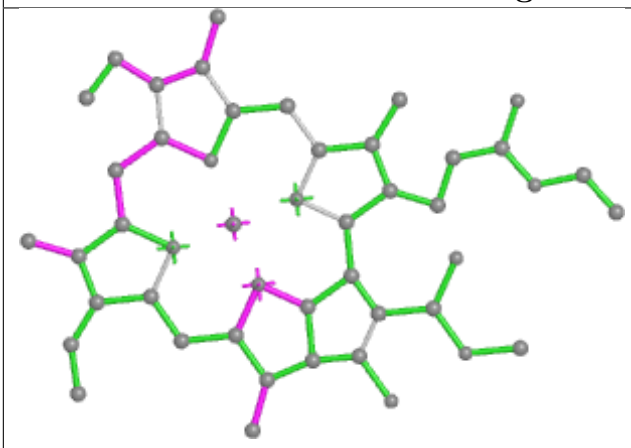


Torsions

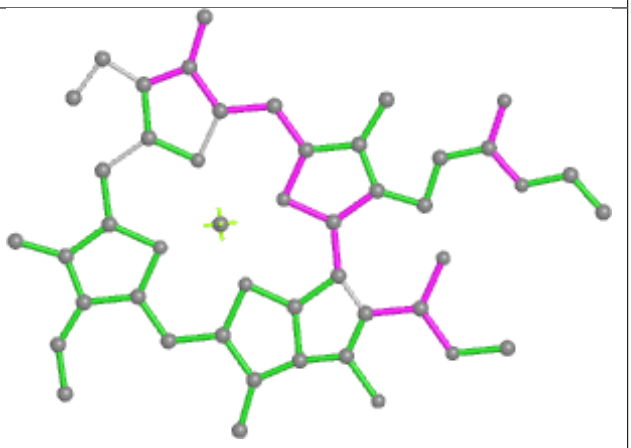


Rings

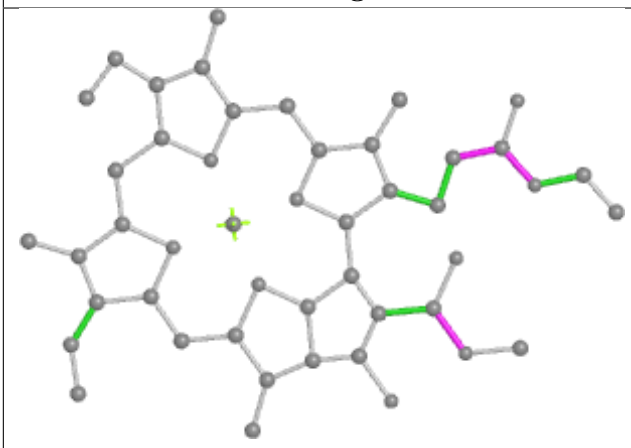
Ligand CLA cA 840



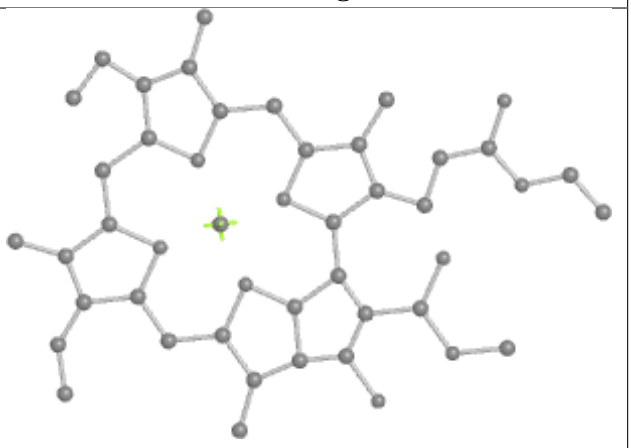
Bond lengths



Bond angles

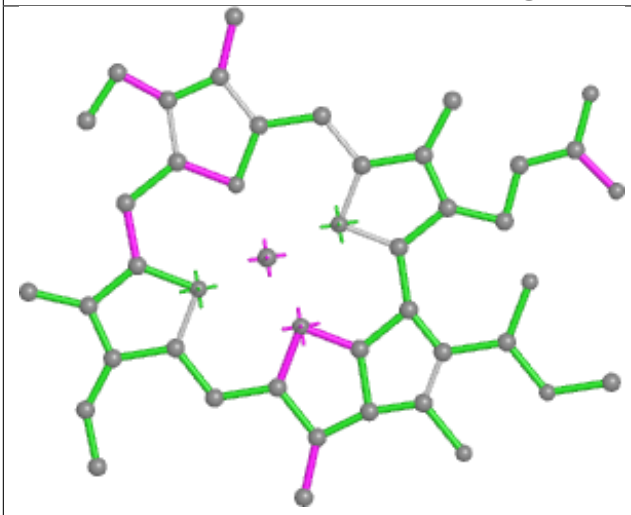


Torsions

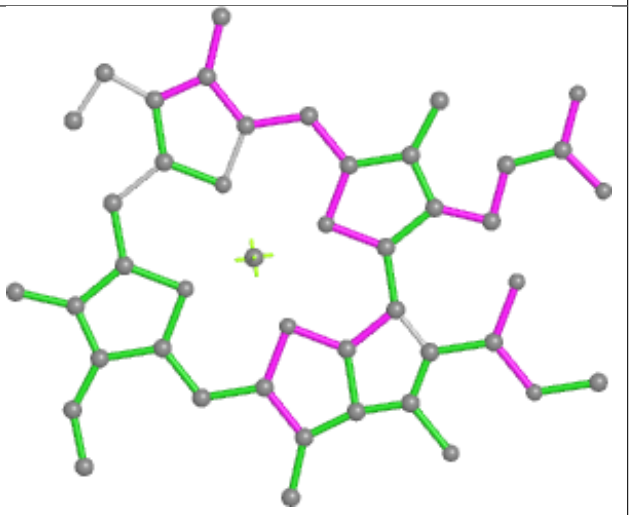


Rings

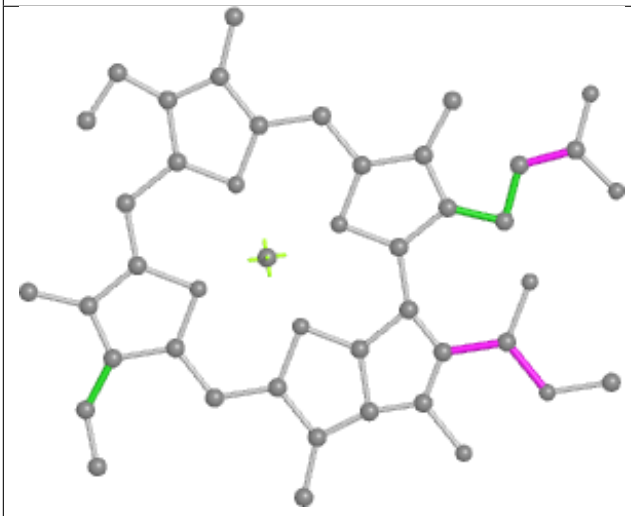
Ligand CLA c1 415



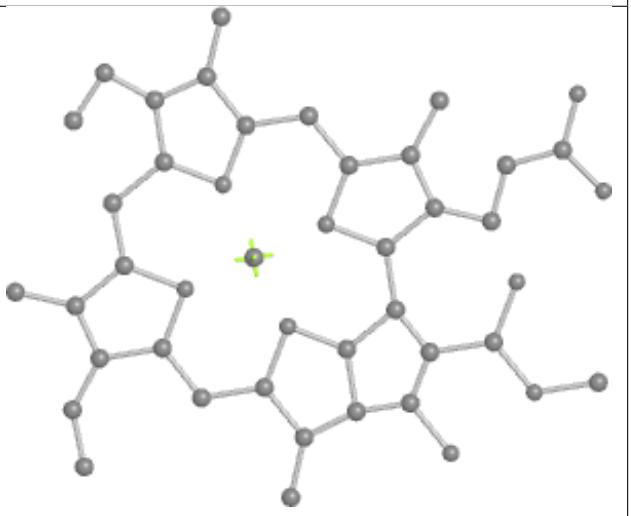
Bond lengths



Bond angles

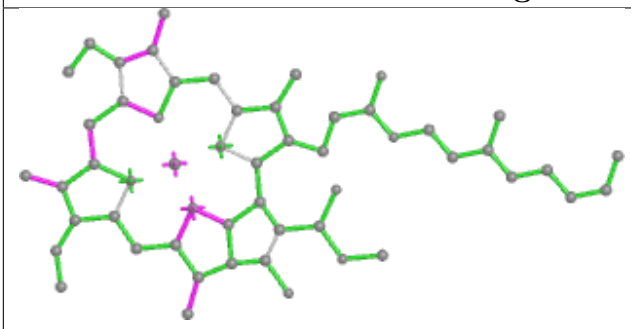


Torsions

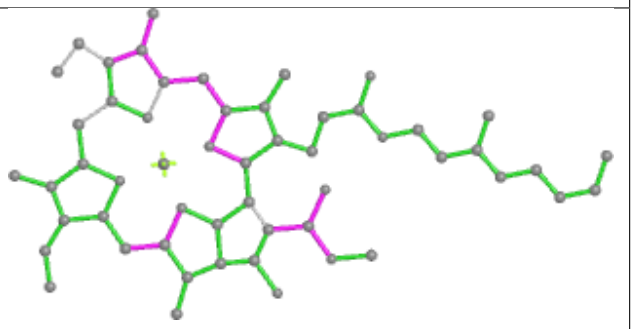


Rings

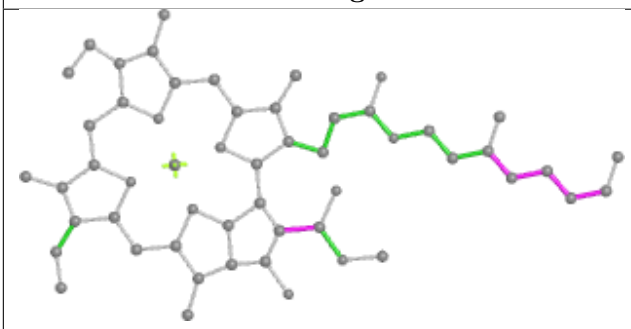
Ligand CLA bA 818



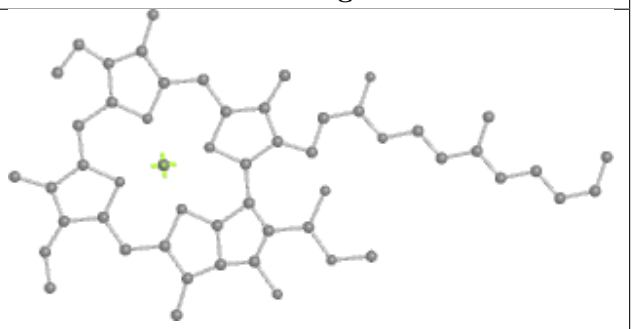
Bond lengths



Bond angles

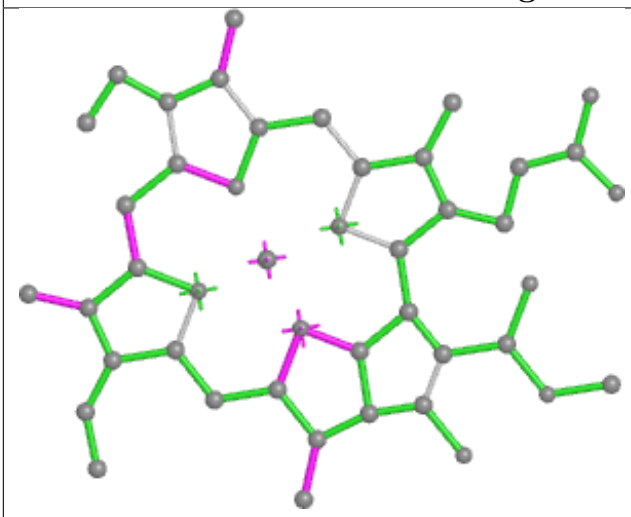


Torsions

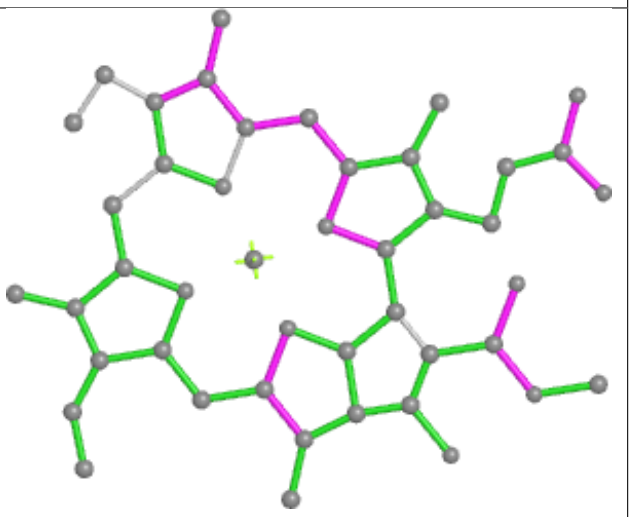


Rings

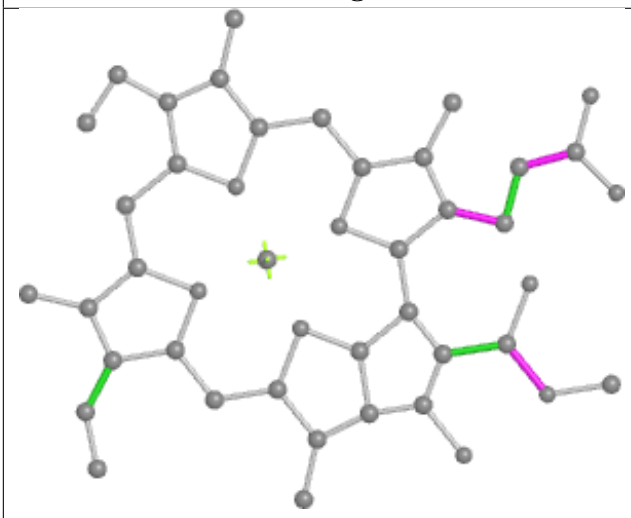
Ligand CLA b4 408



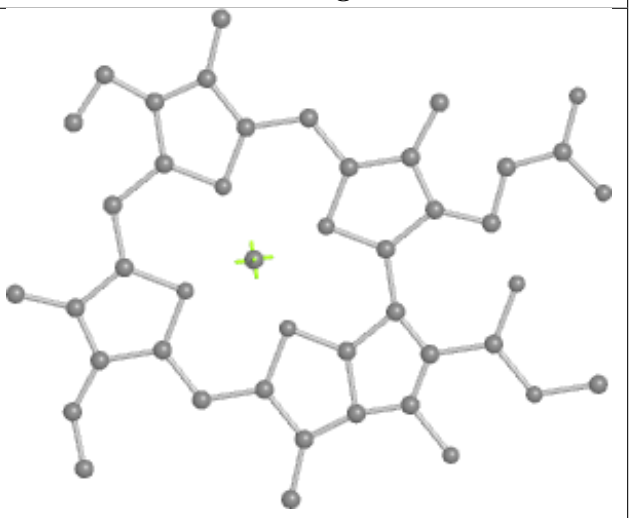
Bond lengths



Bond angles

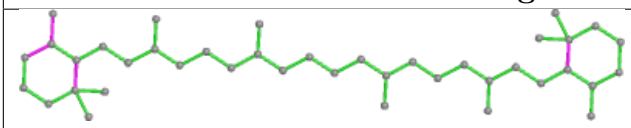


Torsions

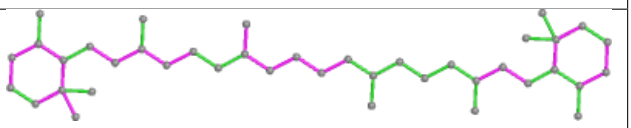


Rings

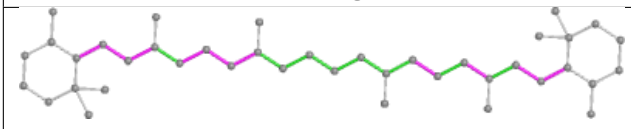
Ligand BCR a2 401



Bond lengths



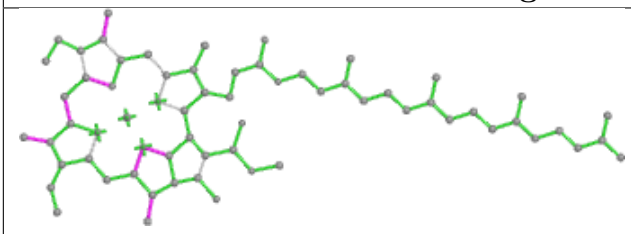
Bond angles



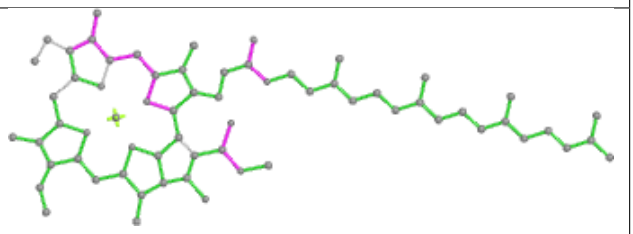
Torsions

Rings

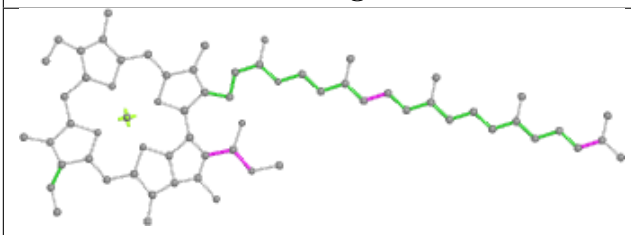
Ligand CLA a5 409



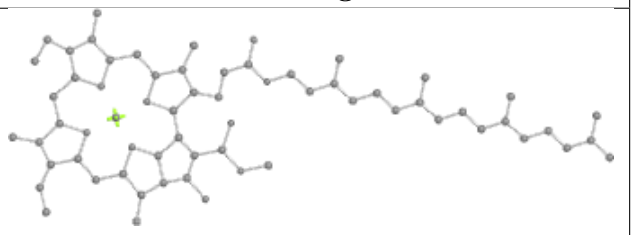
Bond lengths



Bond angles

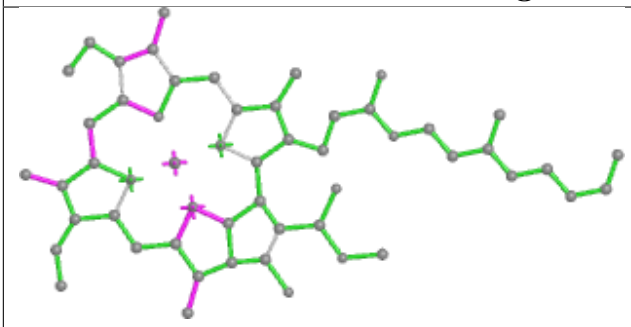


Torsions

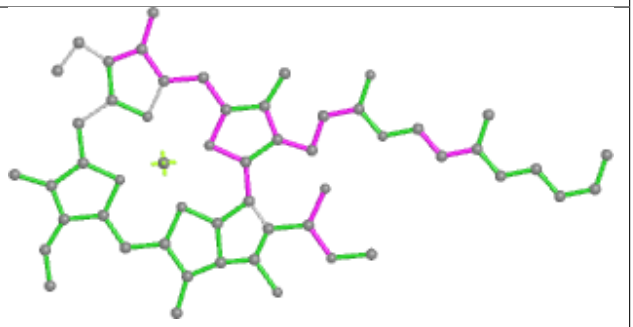


Rings

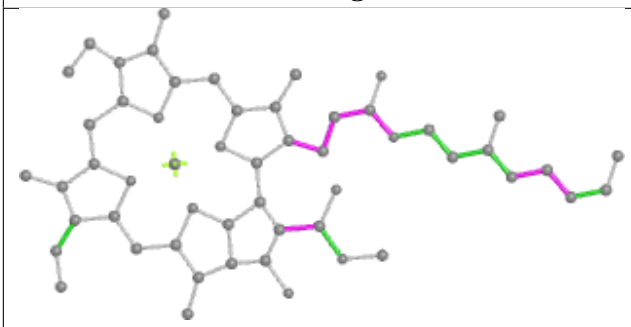
Ligand CLA cA 813



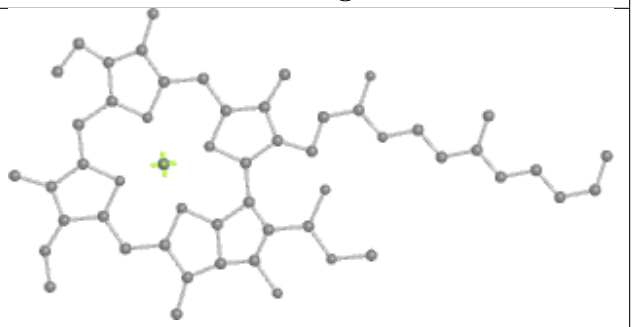
Bond lengths



Bond angles

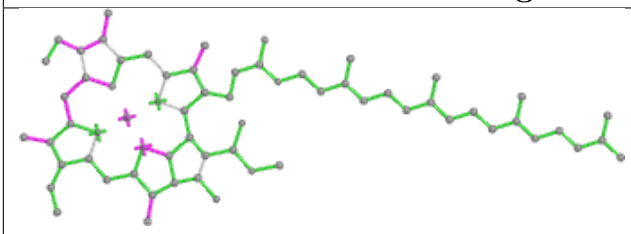


Torsions

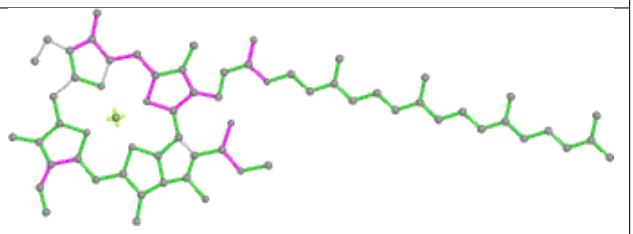


Rings

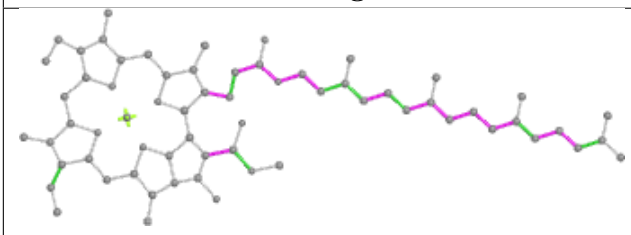
Ligand CLA cA 806



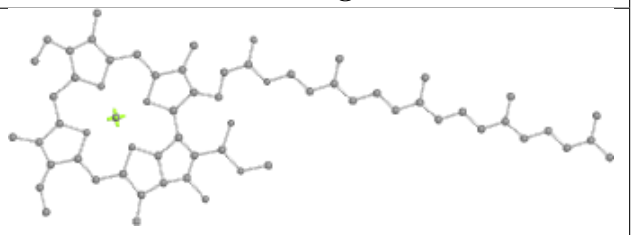
Bond lengths



Bond angles

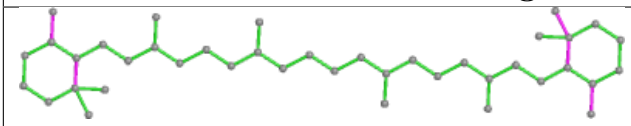


Torsions

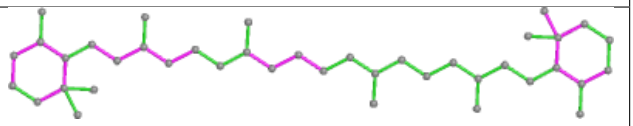


Rings

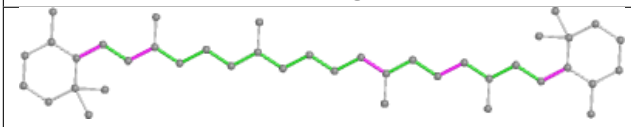
Ligand BCR c1 418



Bond lengths



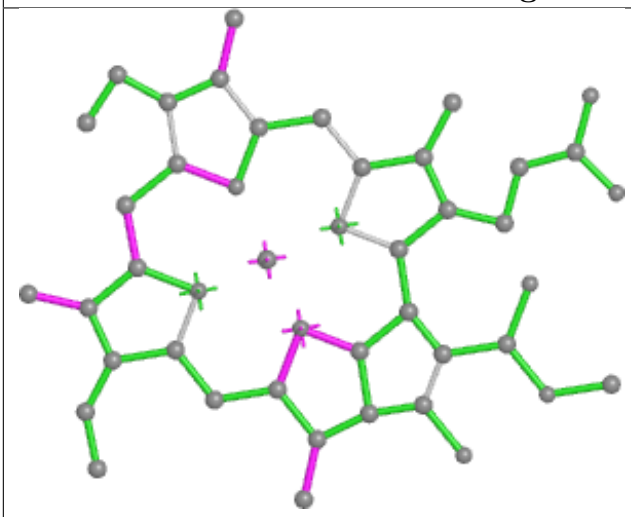
Bond angles



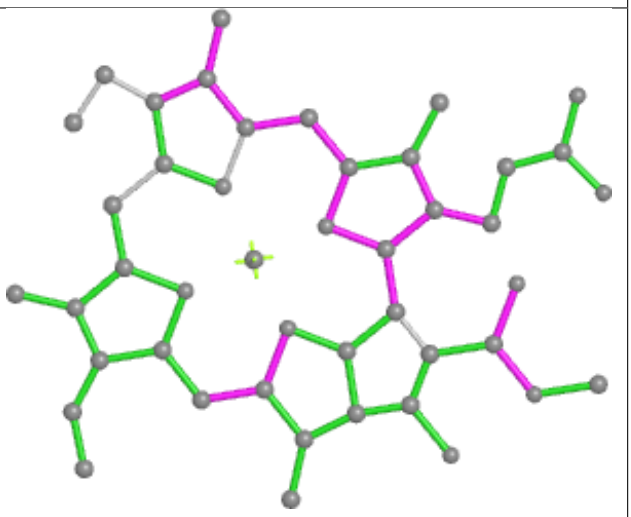
Torsions

Rings

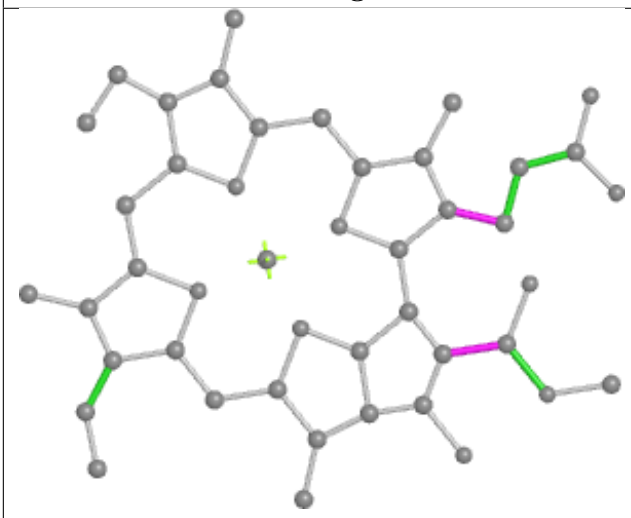
Ligand CLA a5 411



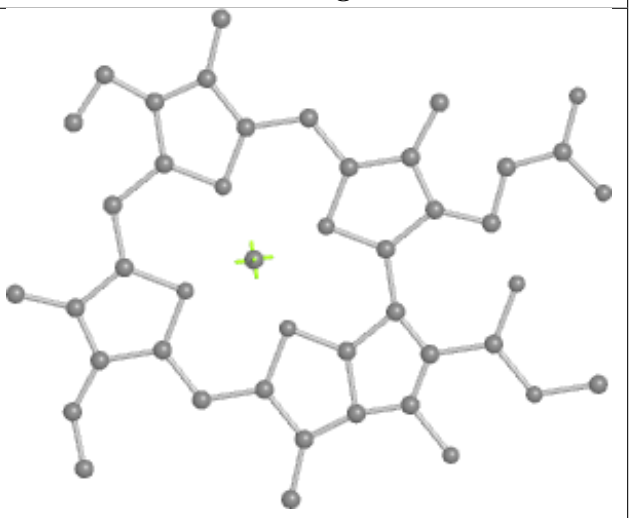
Bond lengths



Bond angles

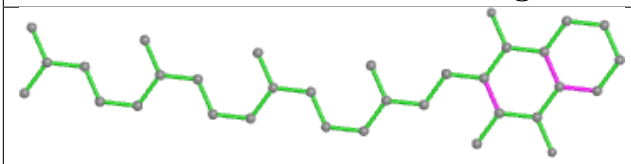


Torsions

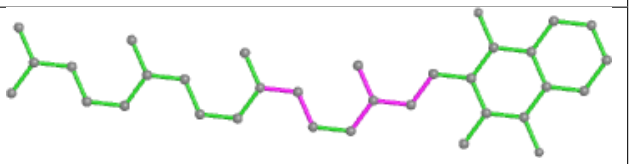


Rings

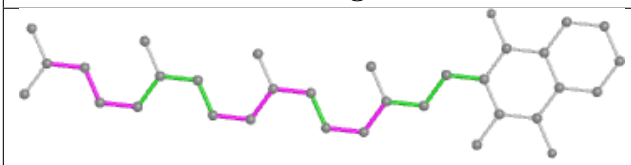
Ligand PQN aB 843



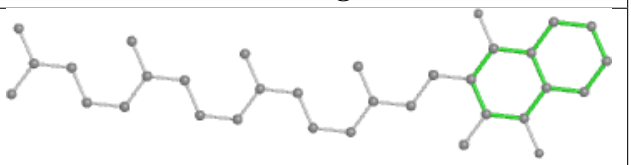
Bond lengths



Bond angles

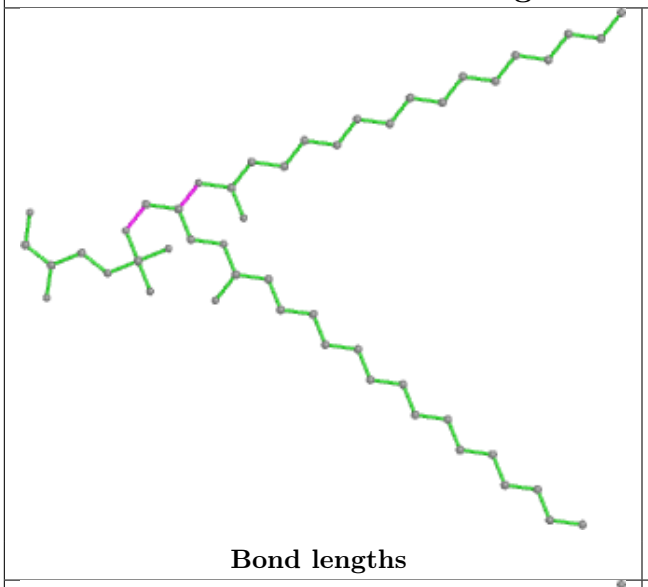


Torsions

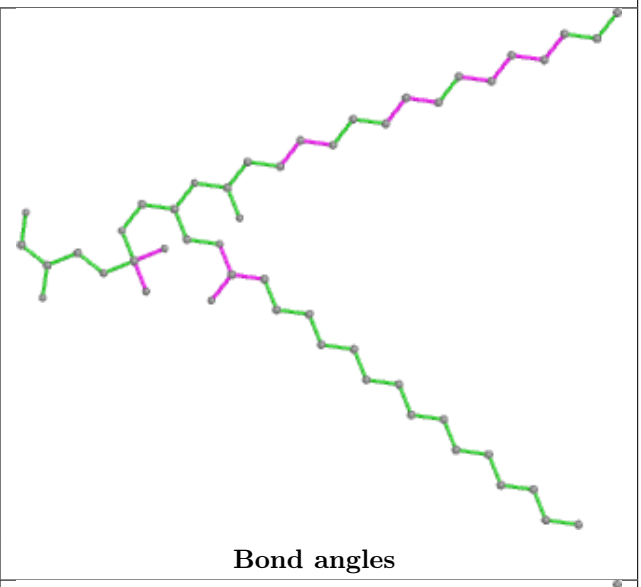


Rings

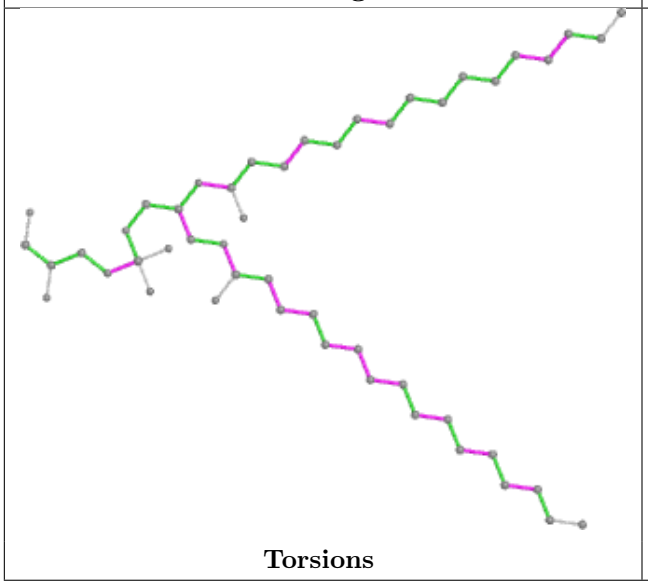
Ligand LHG aA 853



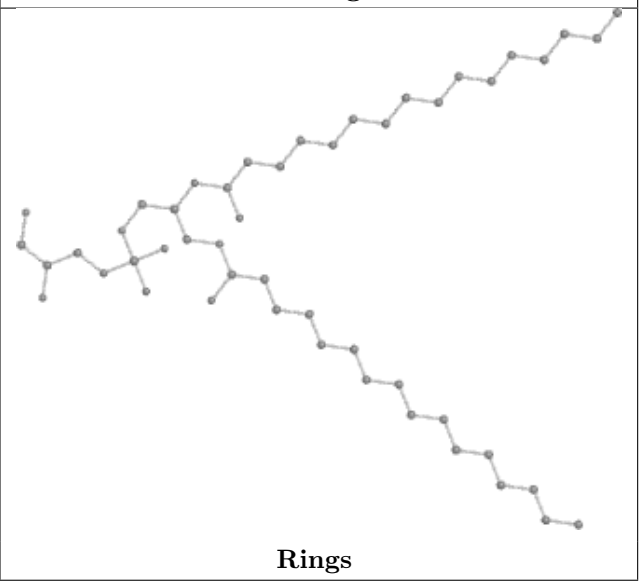
Bond lengths



Bond angles

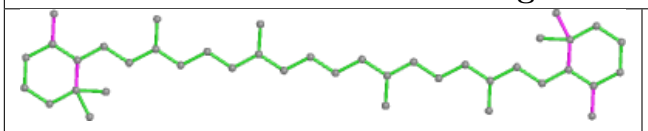


Torsions

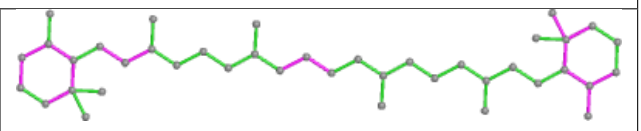


Rings

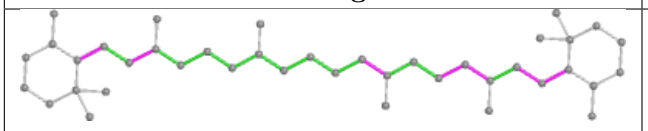
Ligand BCR b3 418



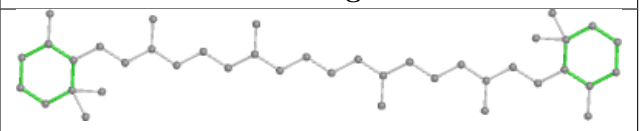
Bond lengths



Bond angles

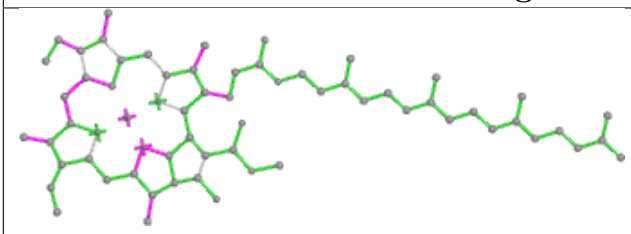


Torsions

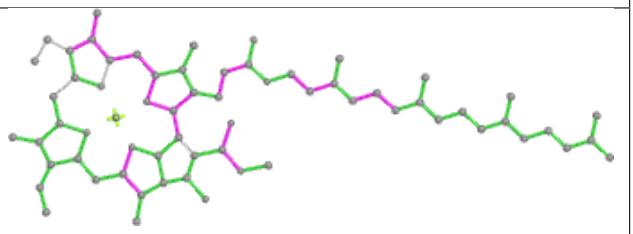


Rings

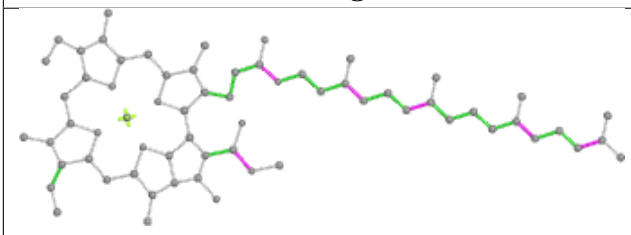
Ligand CLA aA 834



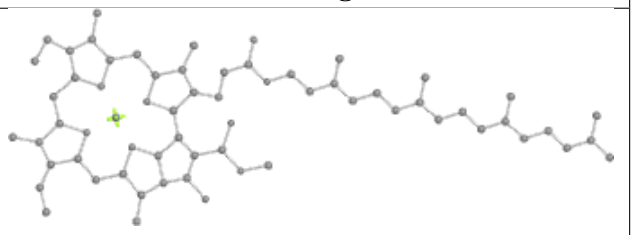
Bond lengths



Bond angles

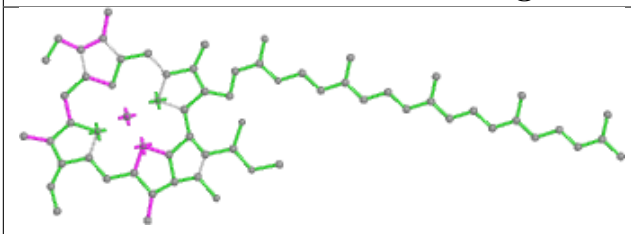


Torsions

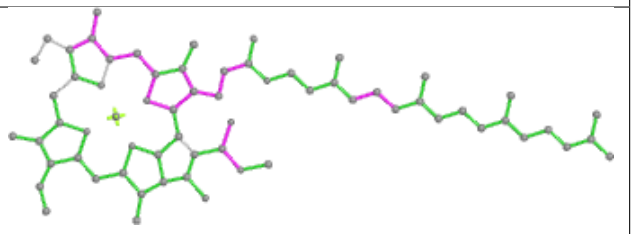


Rings

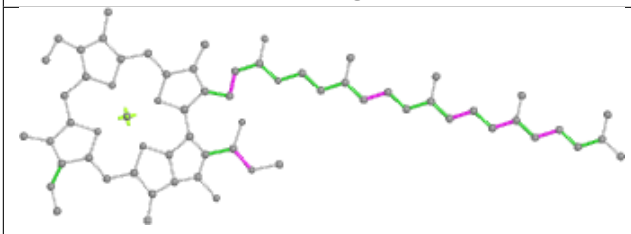
Ligand CLA aB 839



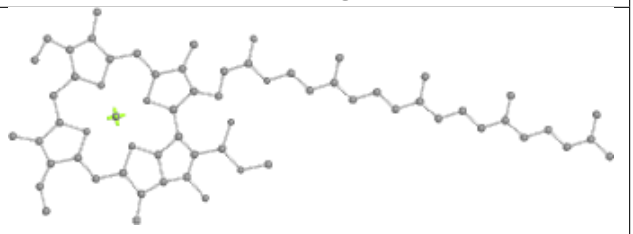
Bond lengths



Bond angles

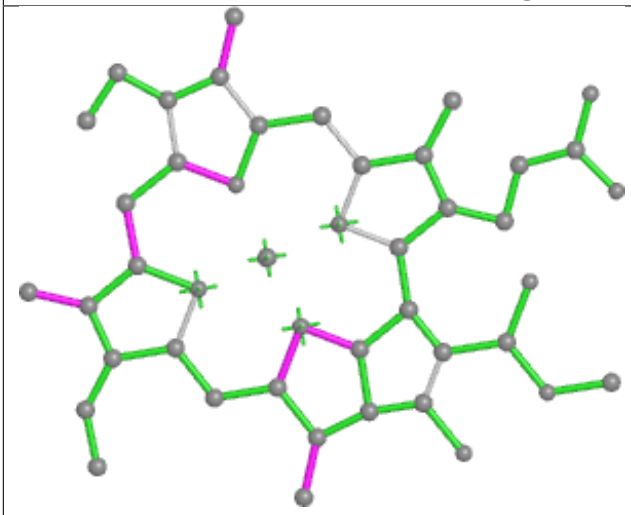


Torsions

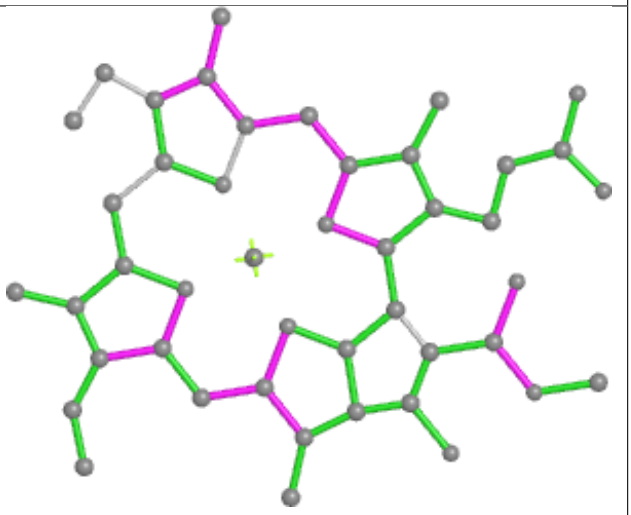


Rings

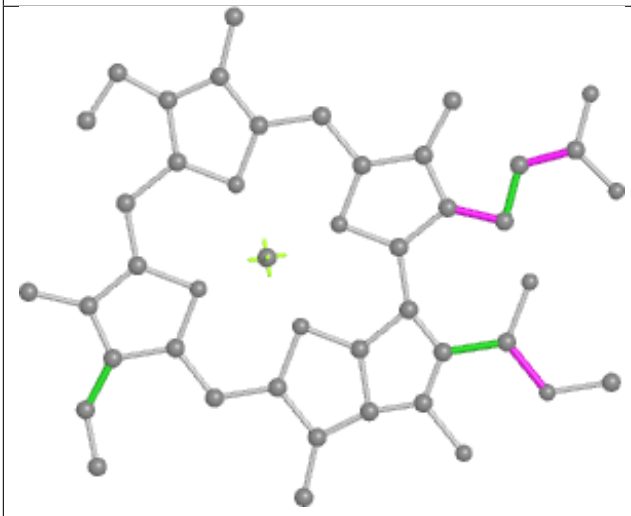
Ligand CLA b1 408



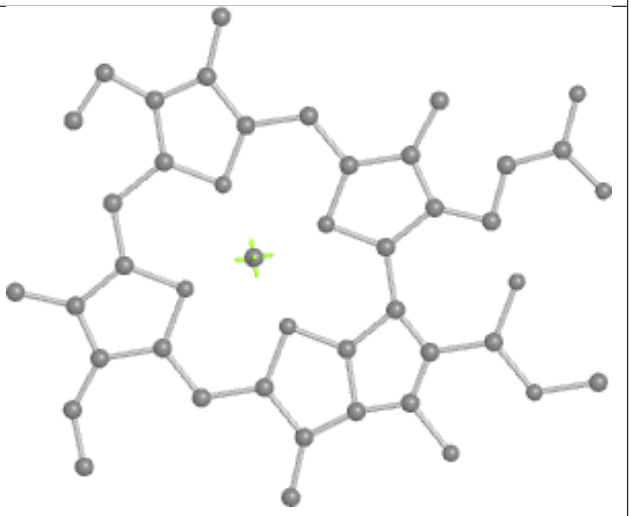
Bond lengths



Bond angles

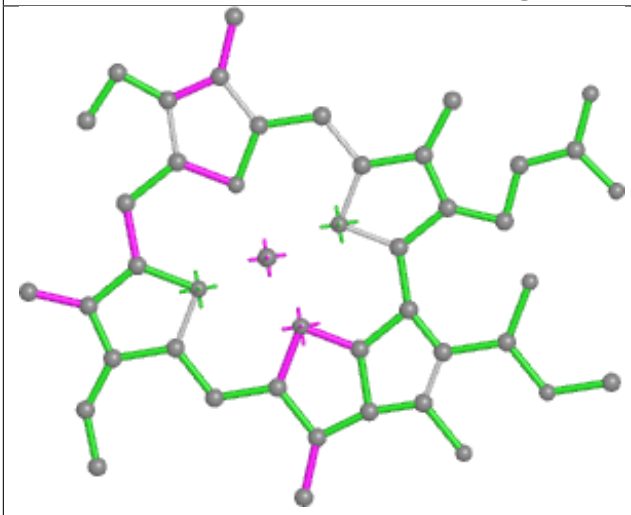


Torsions

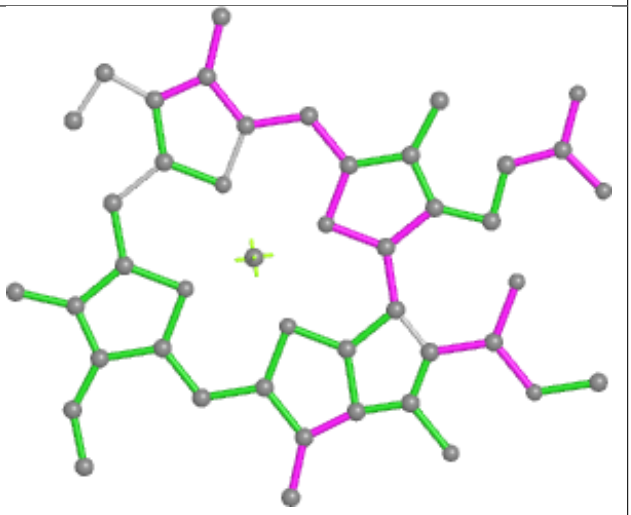


Rings

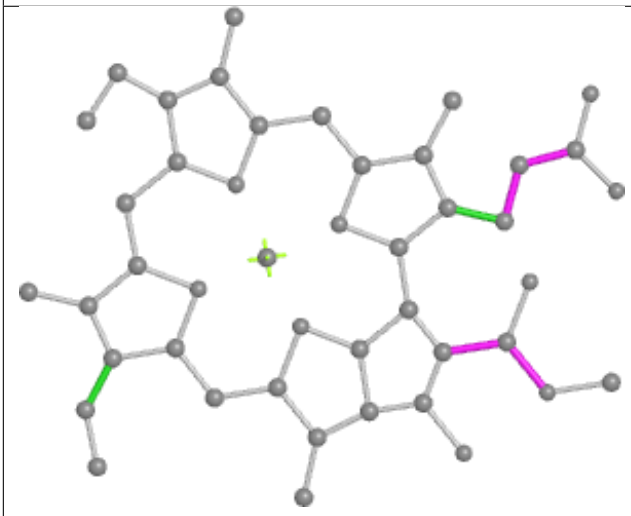
Ligand CLA cX 102



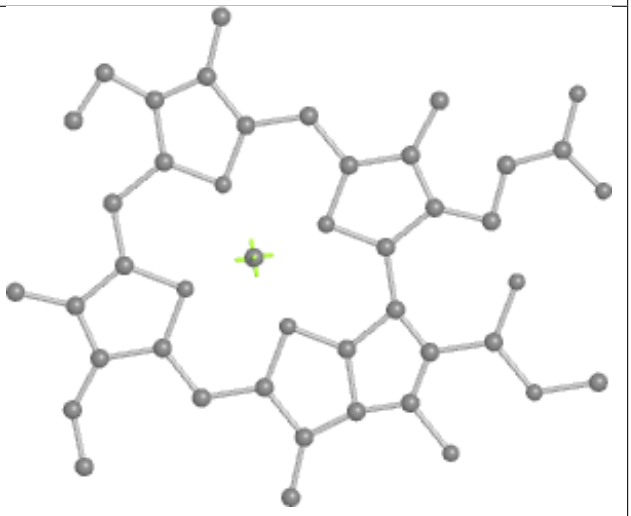
Bond lengths



Bond angles

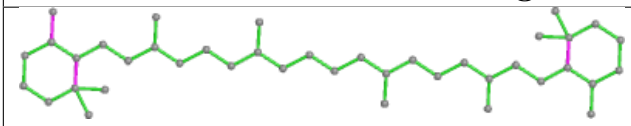


Torsions

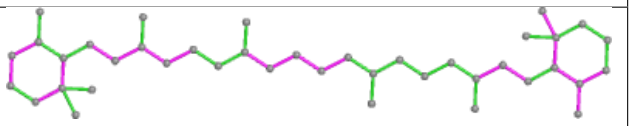


Rings

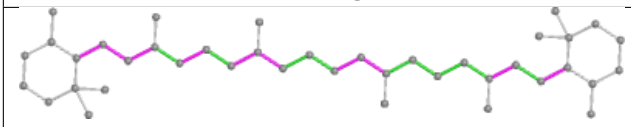
Ligand BCR aL 205



Bond lengths



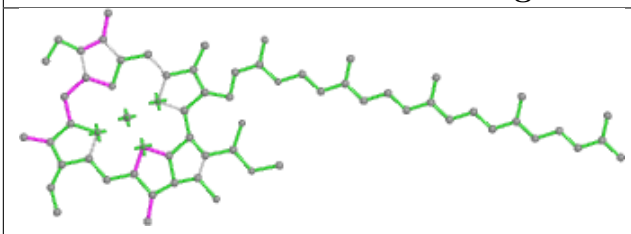
Bond angles



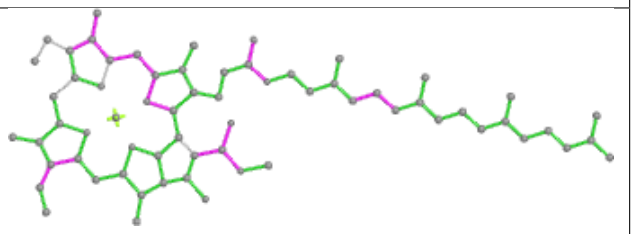
Torsions

Rings

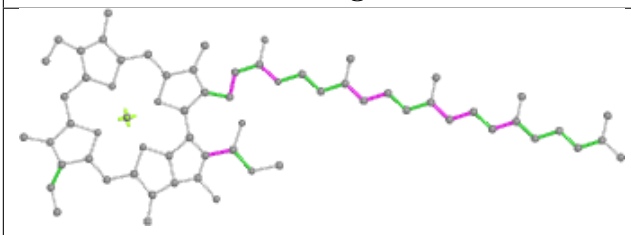
Ligand CLA bB 808



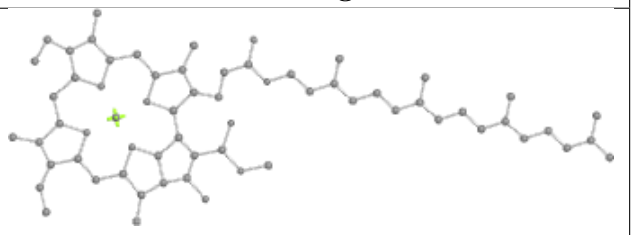
Bond lengths



Bond angles

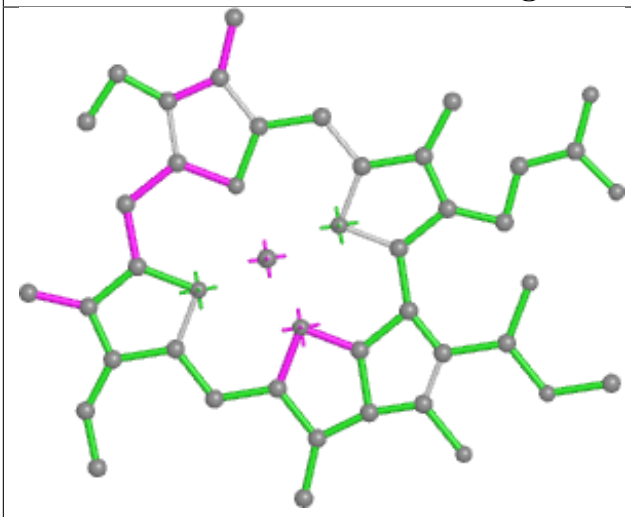


Torsions

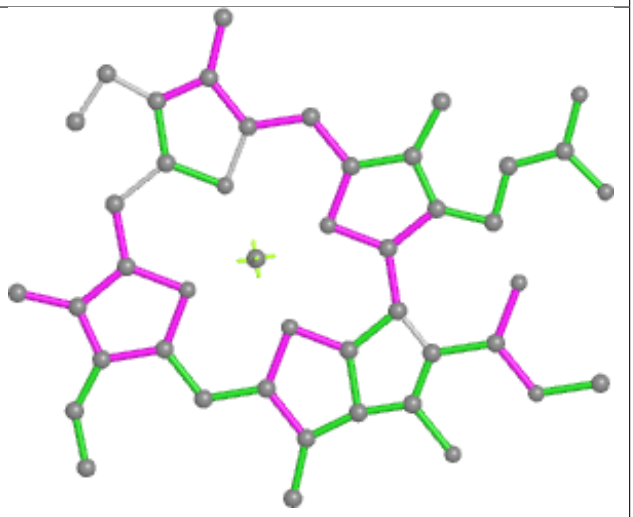


Rings

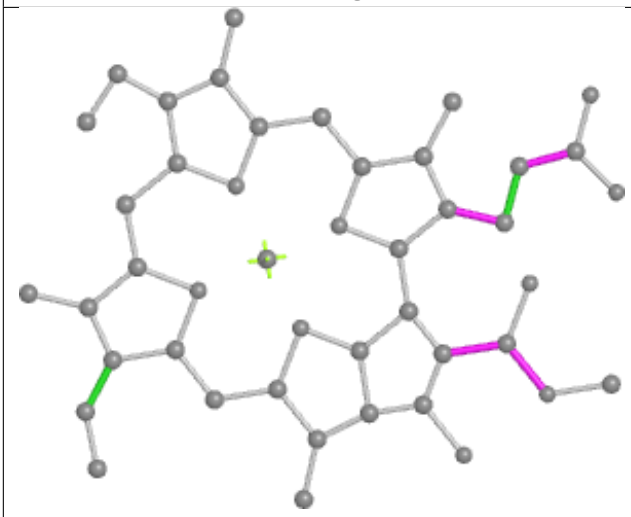
Ligand CLA c5 412



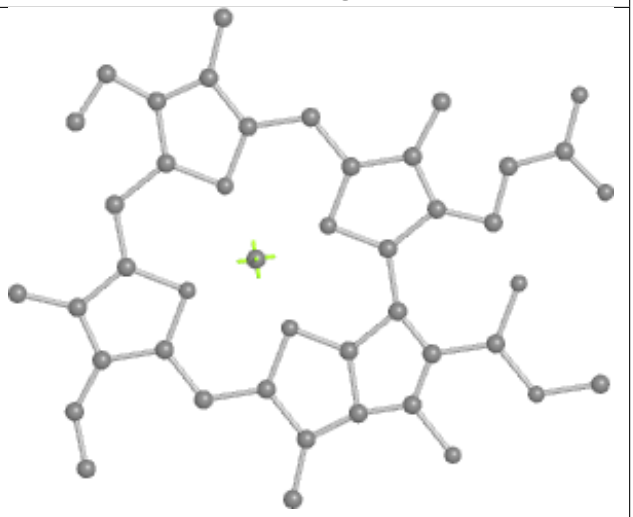
Bond lengths



Bond angles

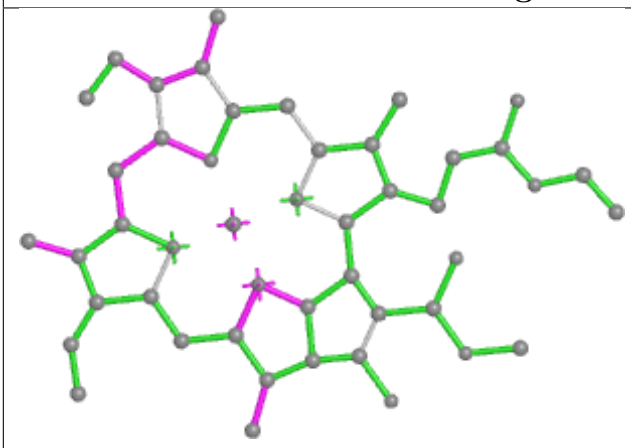


Torsions

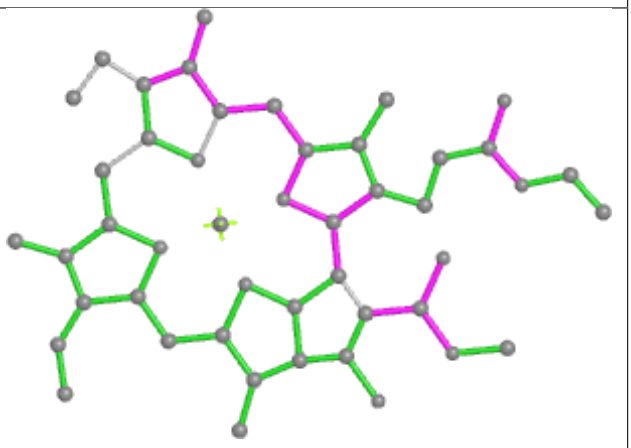


Rings

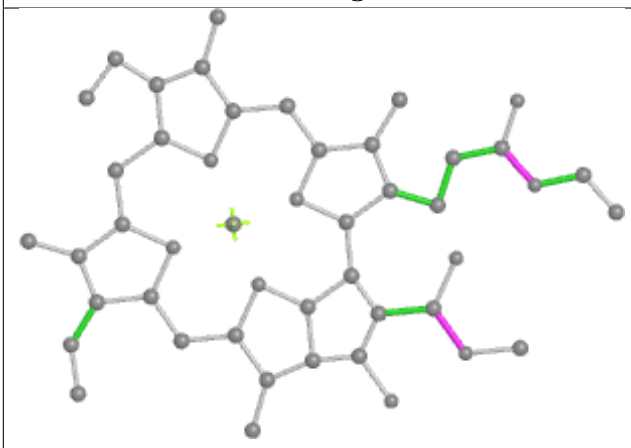
Ligand CLA aA 840



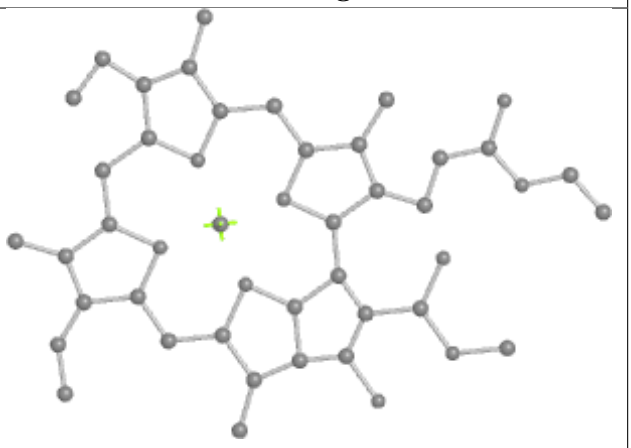
Bond lengths



Bond angles

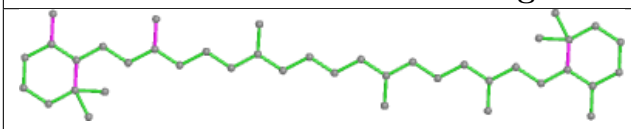


Torsions

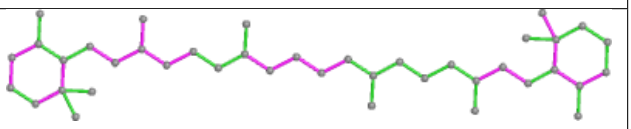


Rings

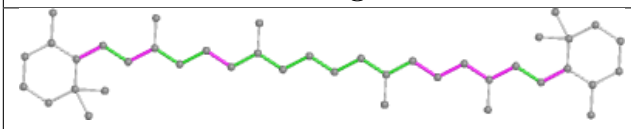
Ligand BCR a1 418



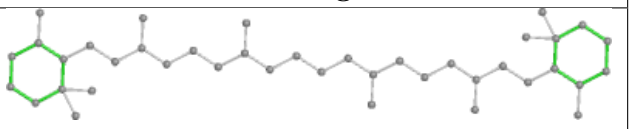
Bond lengths



Bond angles

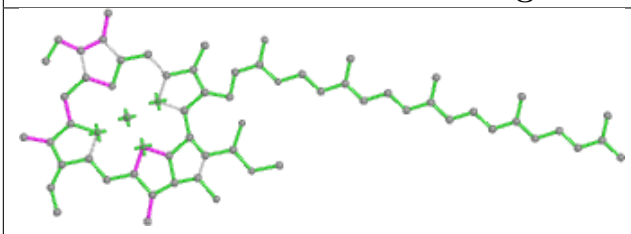


Torsions

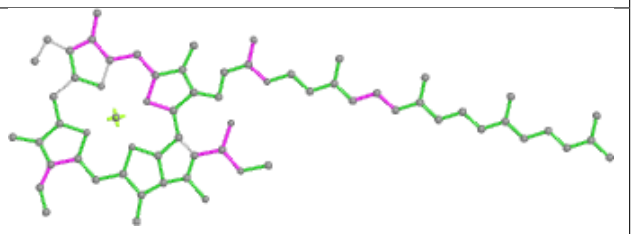


Rings

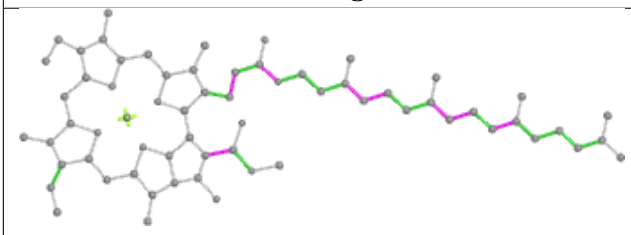
Ligand CLA cB 808



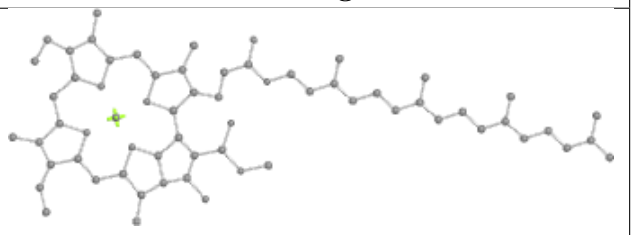
Bond lengths



Bond angles

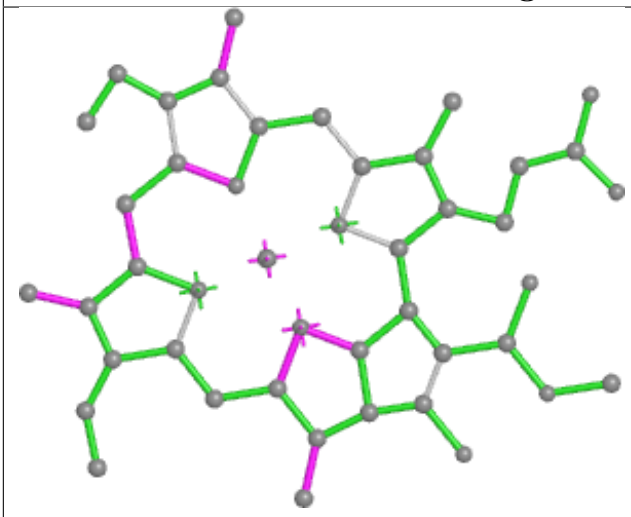


Torsions

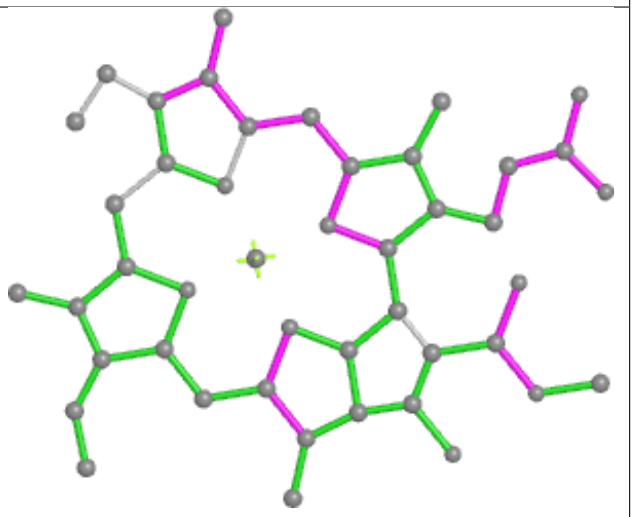


Rings

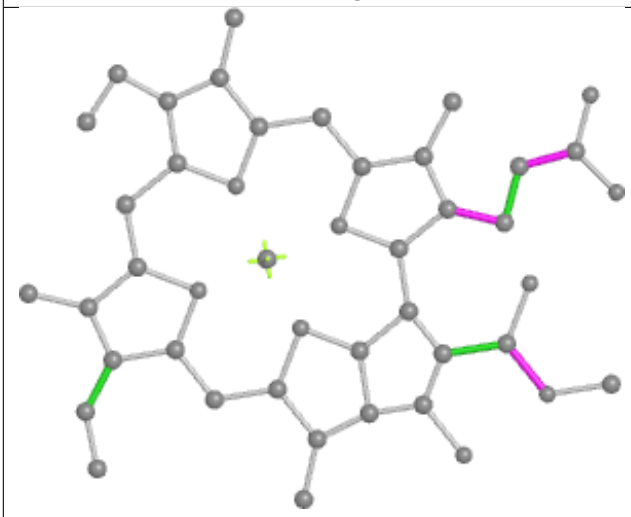
Ligand CLA b5 408



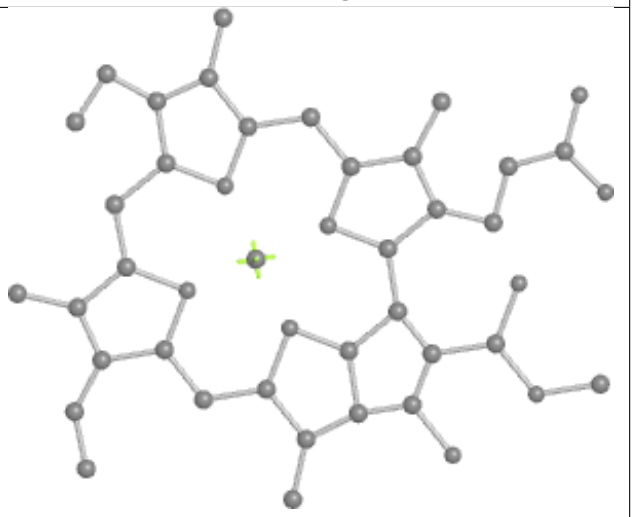
Bond lengths



Bond angles

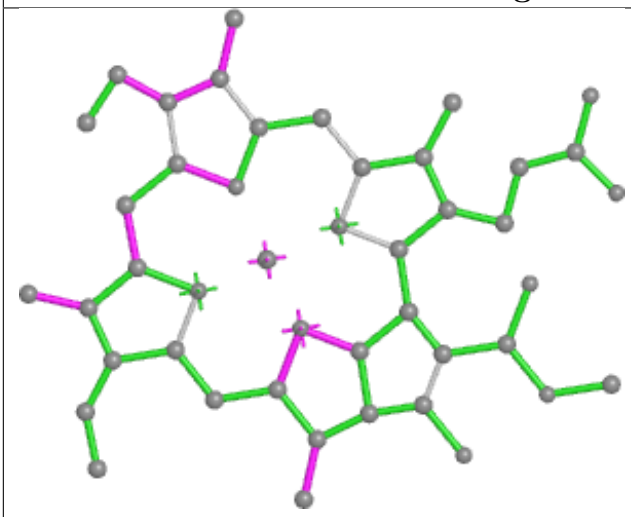


Torsions

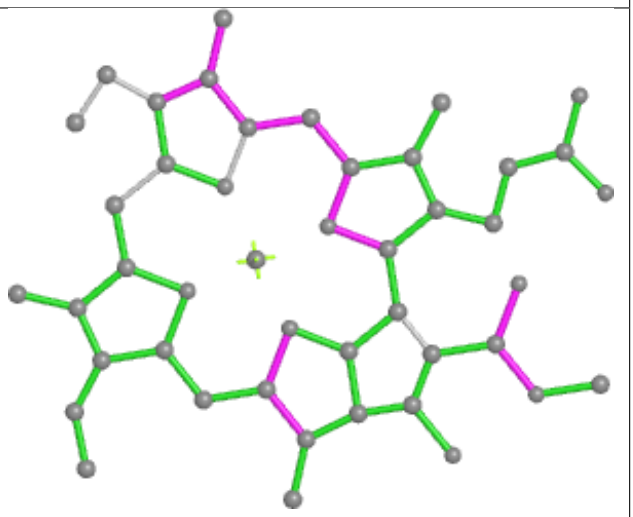


Rings

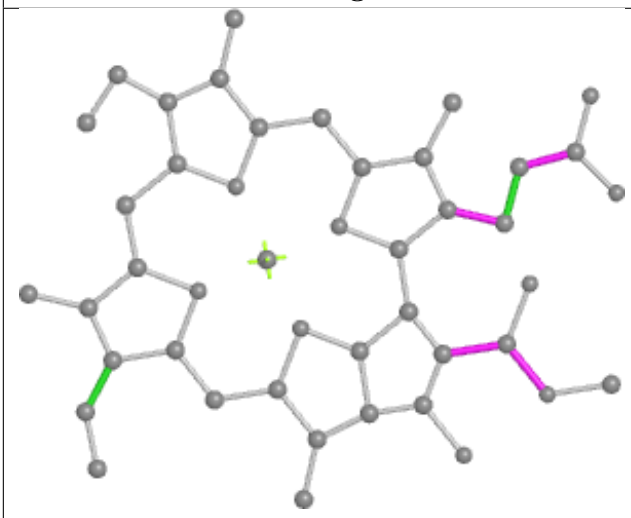
Ligand CLA bA 811



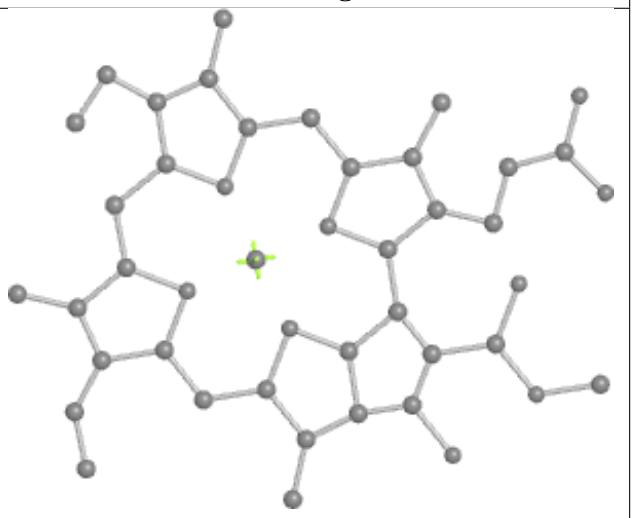
Bond lengths



Bond angles

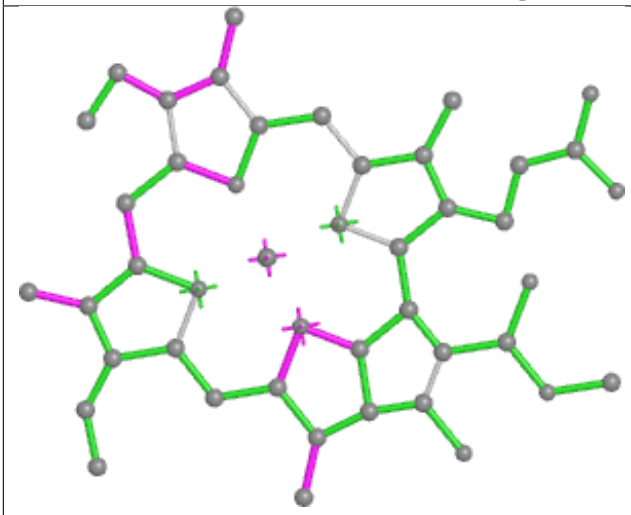


Torsions

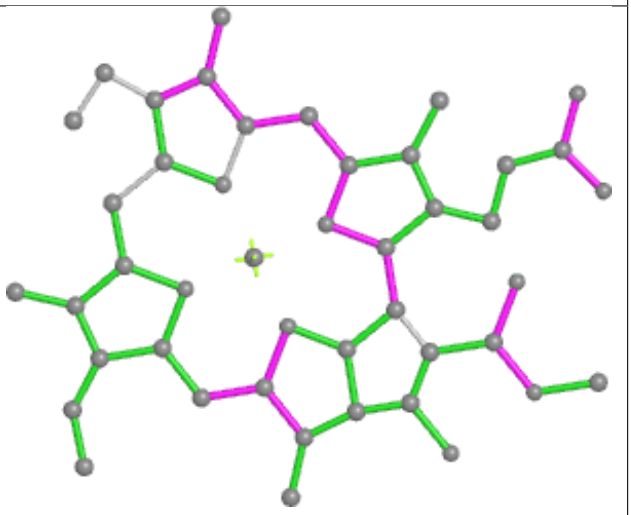


Rings

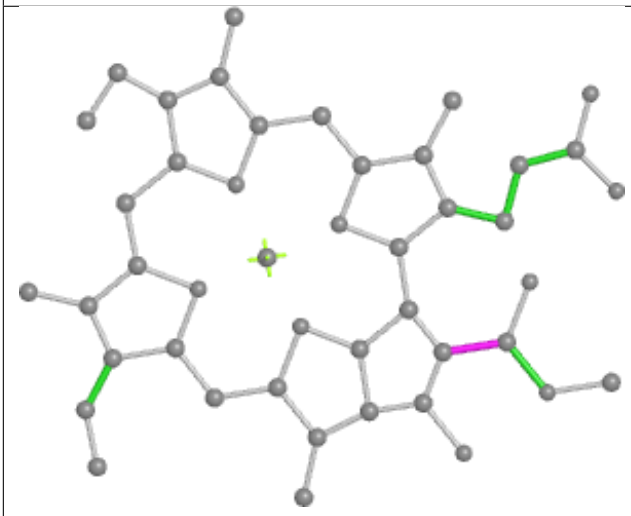
Ligand CLA bA 815



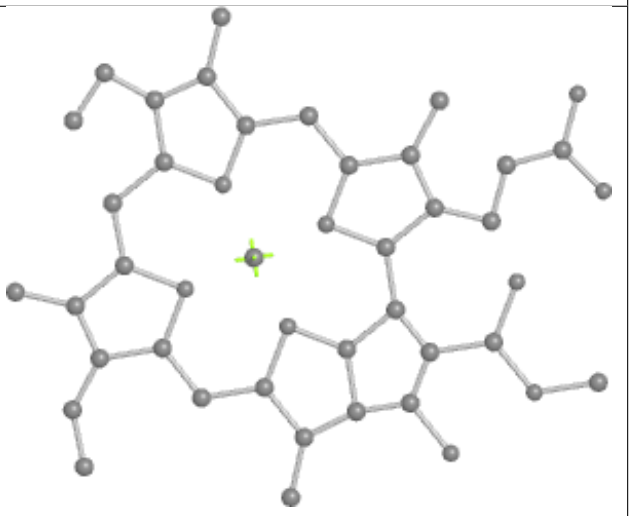
Bond lengths



Bond angles

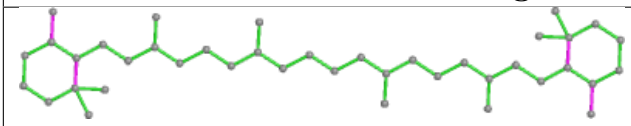


Torsions

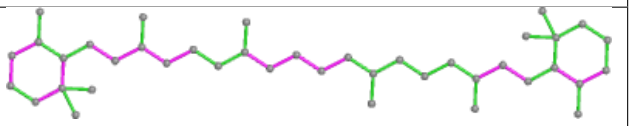


Rings

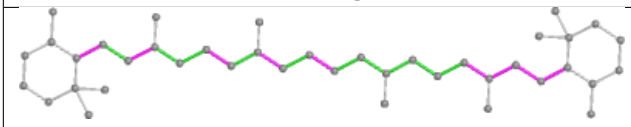
Ligand BCR bB 848



Bond lengths



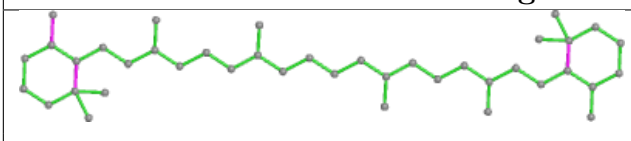
Bond angles

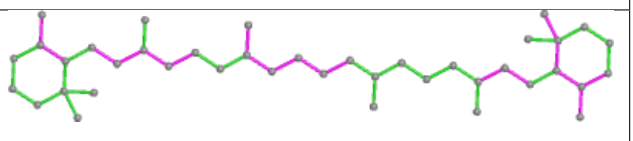


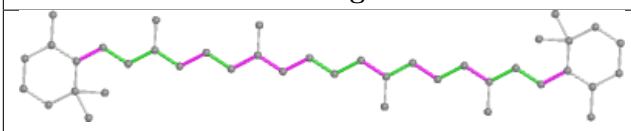
Torsions

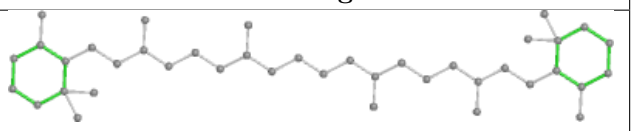
Rings

Ligand BCR cJ 103

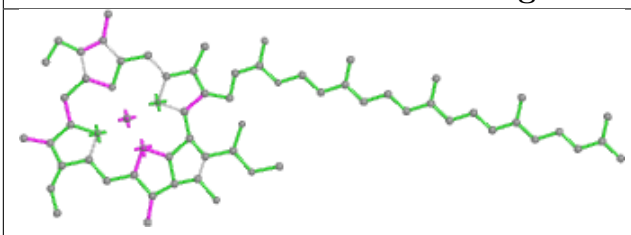

Bond lengths

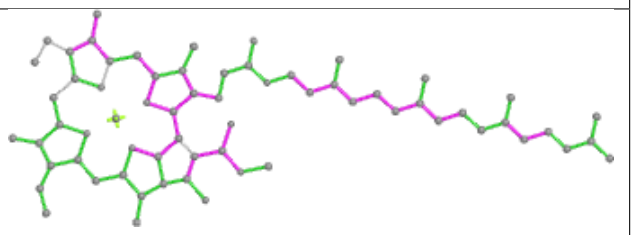

Bond angles

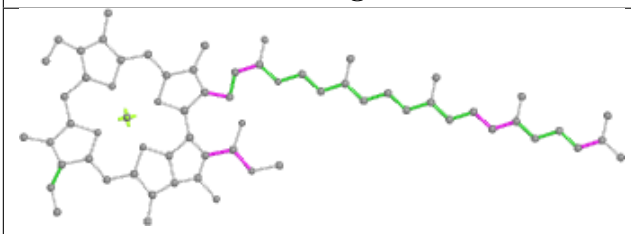

Torsions

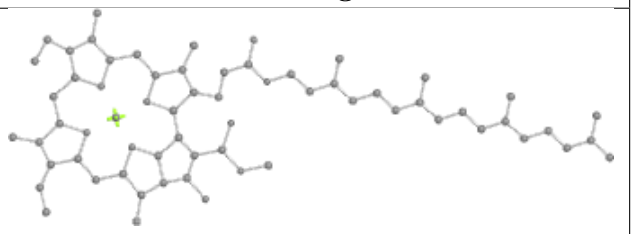

Rings

Ligand CLA b5 420

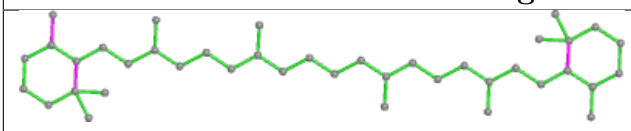

Bond lengths

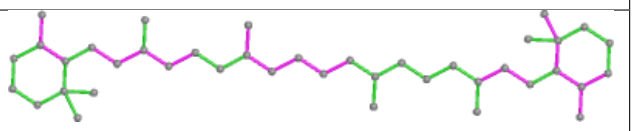

Bond angles

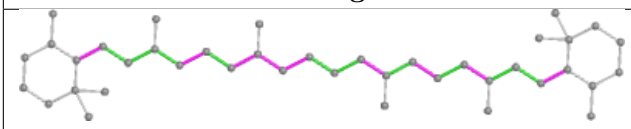

Torsions

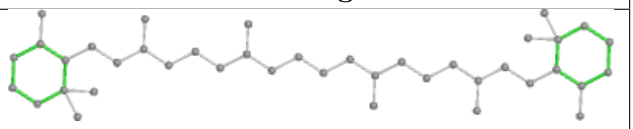

Rings

Ligand BCR aJ 204

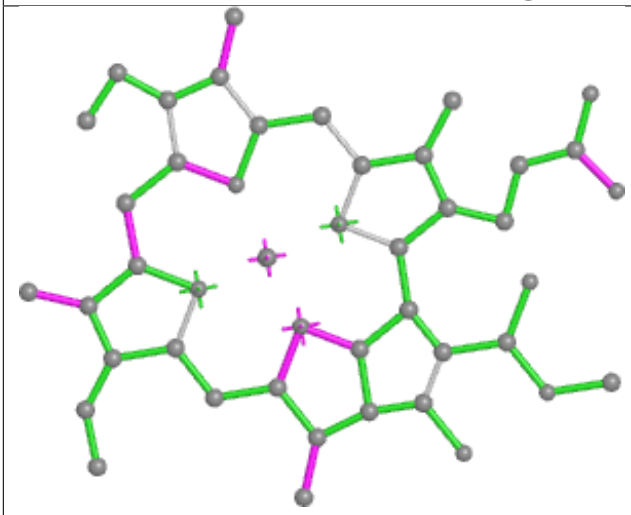

Bond lengths


Bond angles

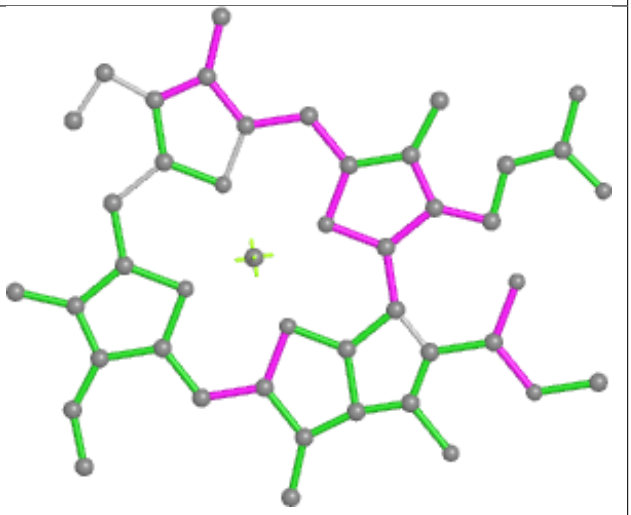

Torsions


Rings

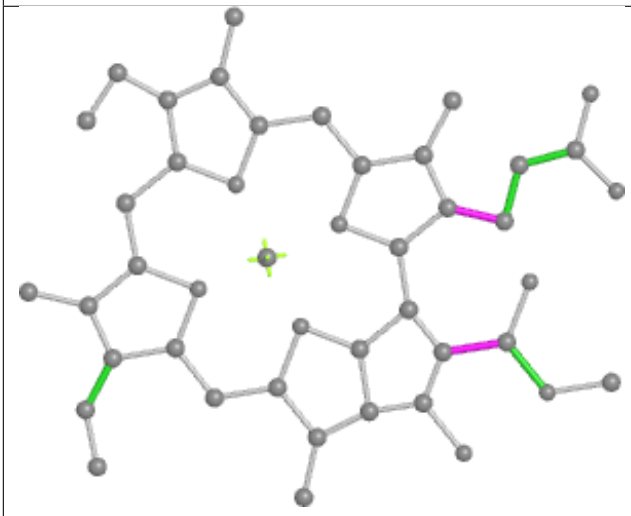
Ligand CLA a2 412



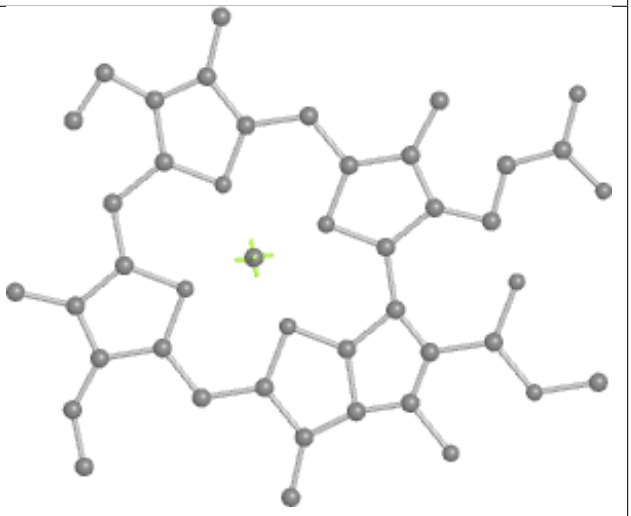
Bond lengths



Bond angles

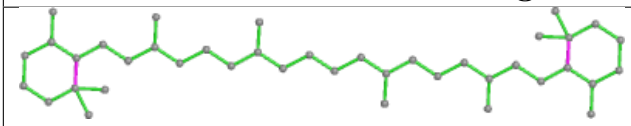


Torsions

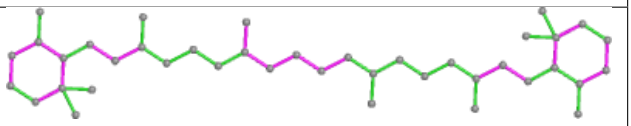


Rings

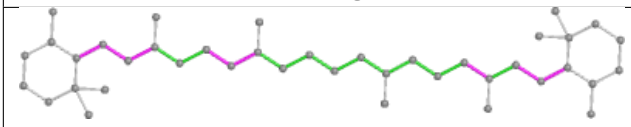
Ligand BCR b6 420



Bond lengths



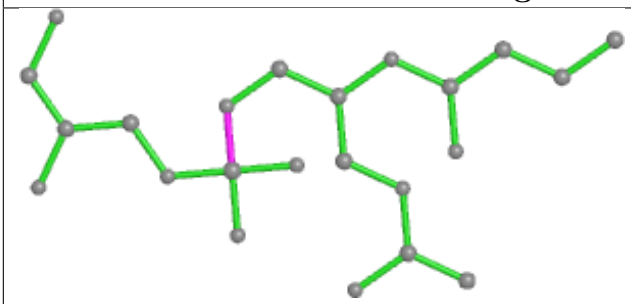
Bond angles



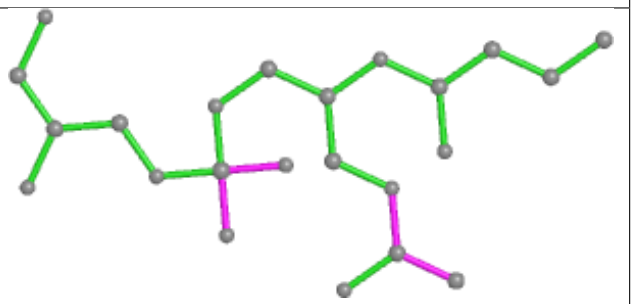
Torsions

Rings

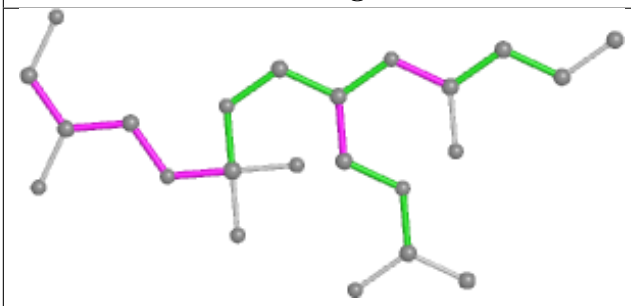
Ligand LHG cX 101



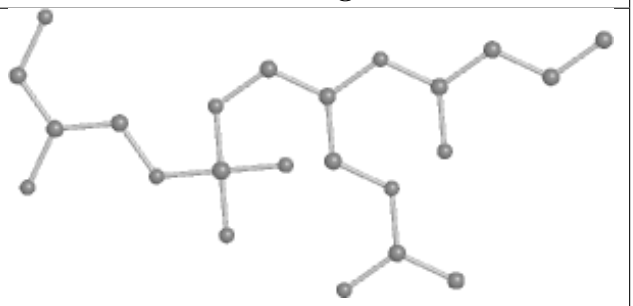
Bond lengths



Bond angles

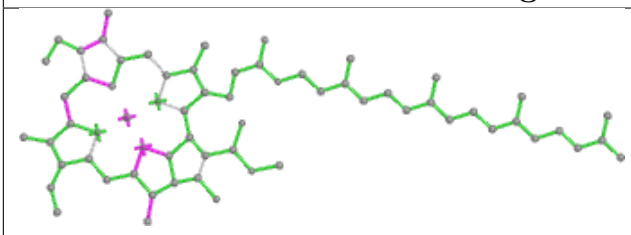


Torsions

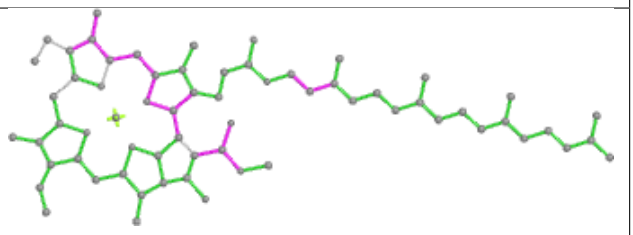


Rings

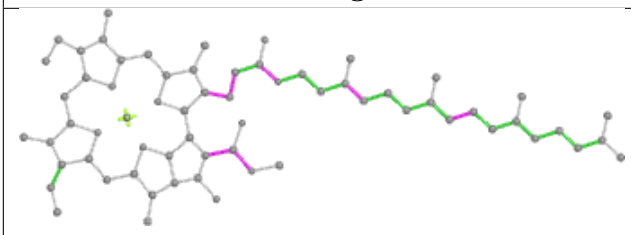
Ligand CLA a1 403



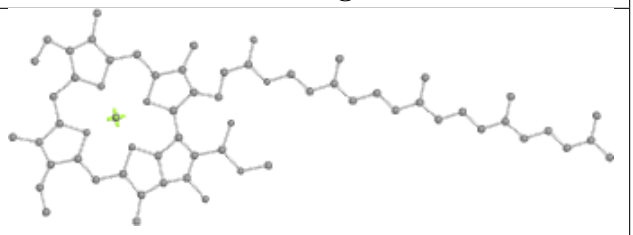
Bond lengths



Bond angles

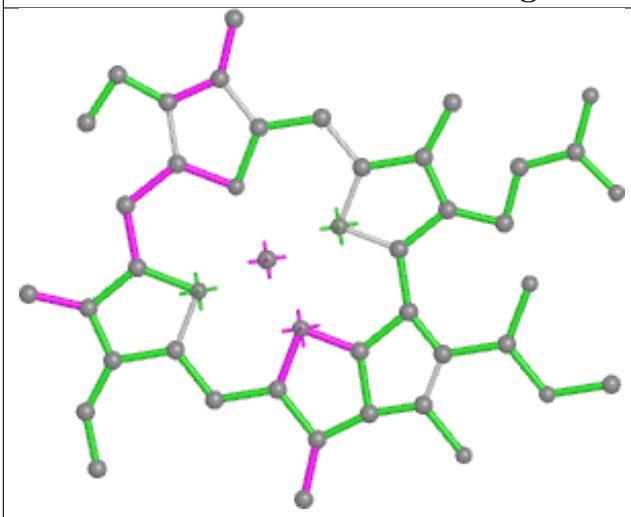


Torsions

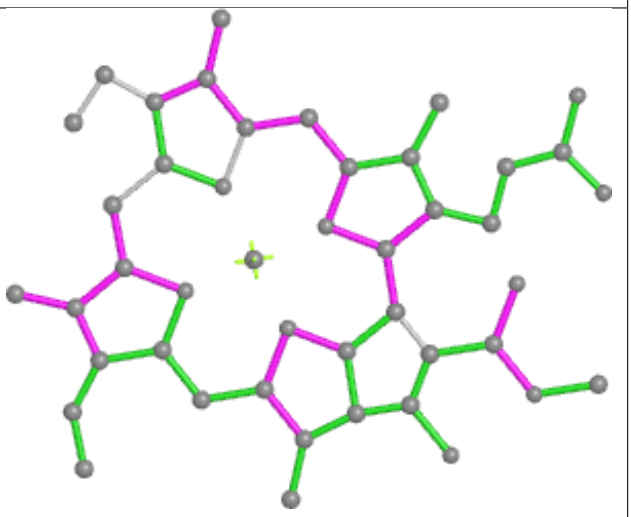


Rings

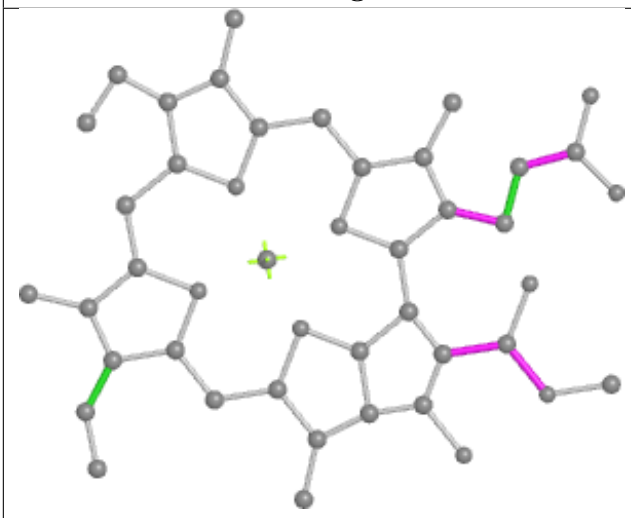
Ligand CLA a5 412



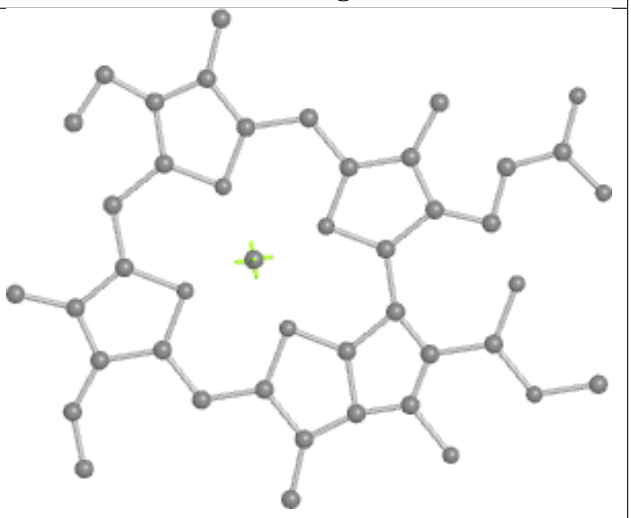
Bond lengths



Bond angles

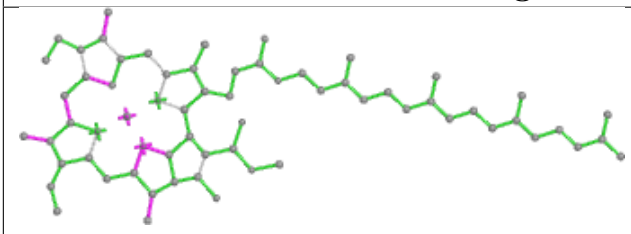


Torsions

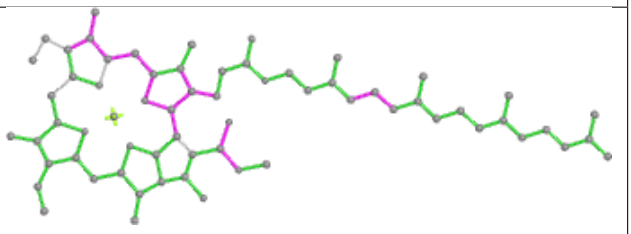


Rings

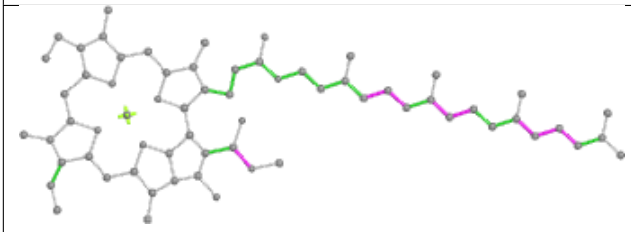
Ligand CLA bA 826



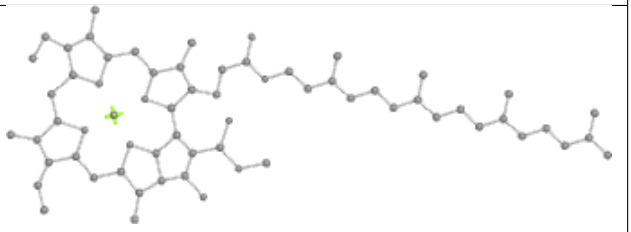
Bond lengths



Bond angles

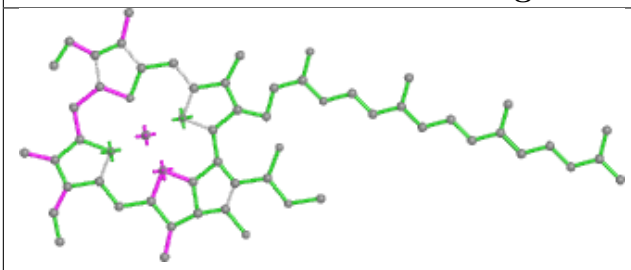


Torsions

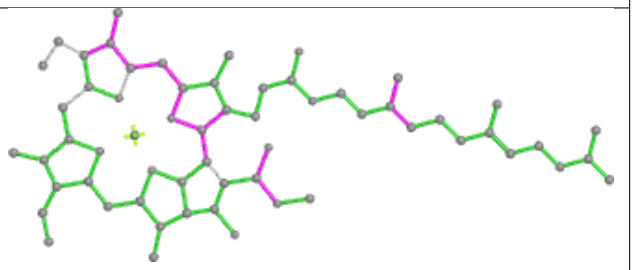


Rings

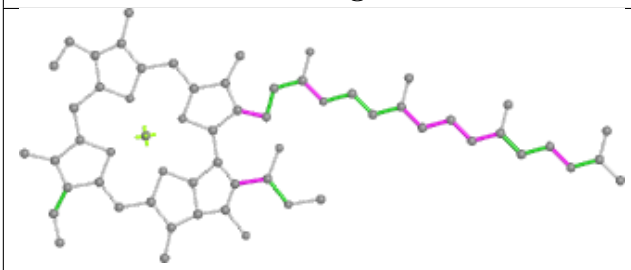
Ligand CLA bB 819



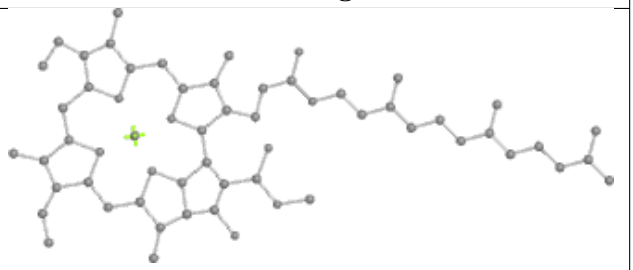
Bond lengths



Bond angles

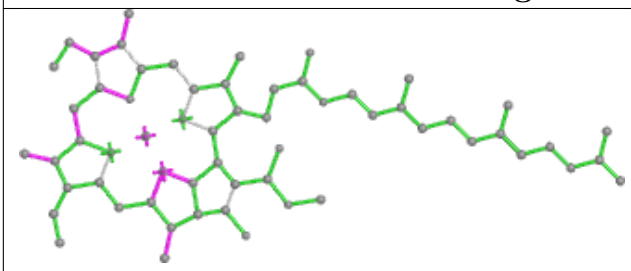


Torsions

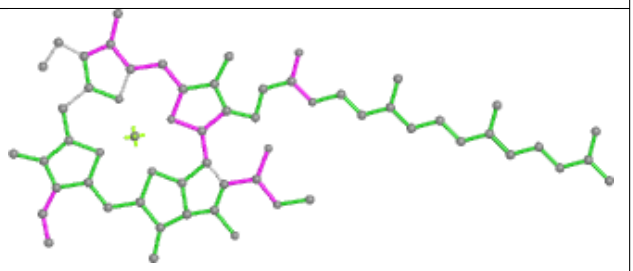


Rings

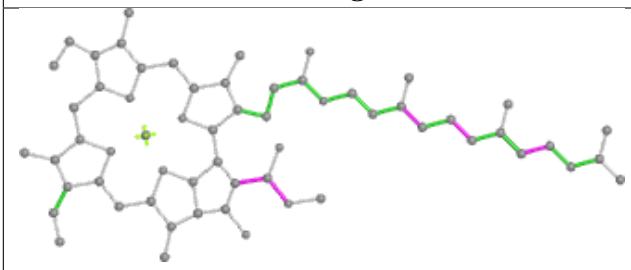
Ligand CLA bB 836



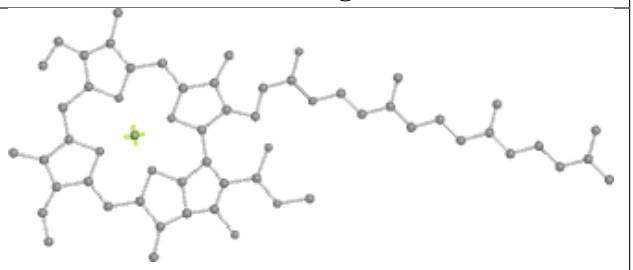
Bond lengths



Bond angles

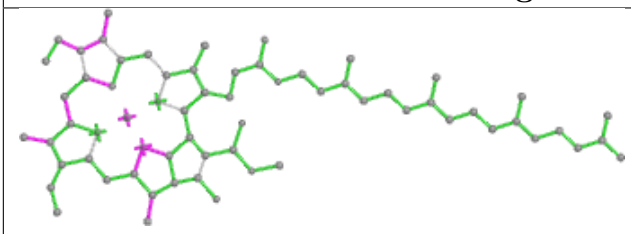


Torsions

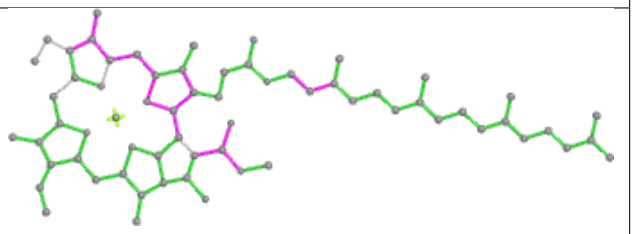


Rings

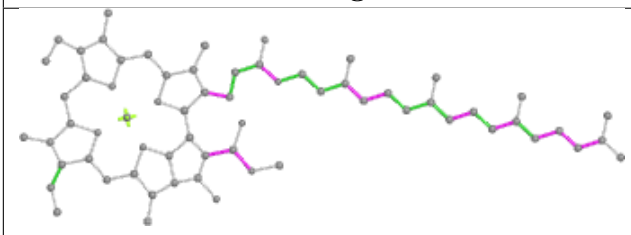
Ligand CLA cA 820



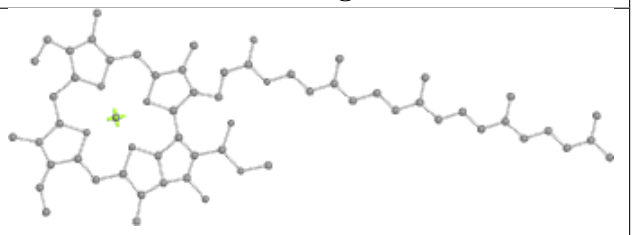
Bond lengths



Bond angles

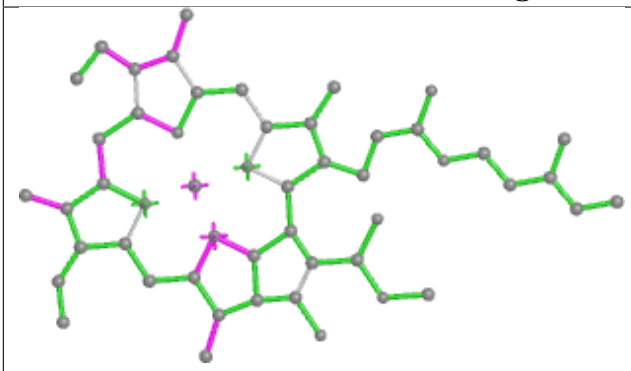


Torsions

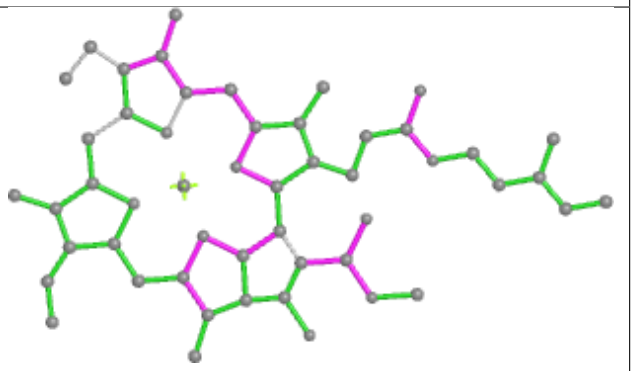


Rings

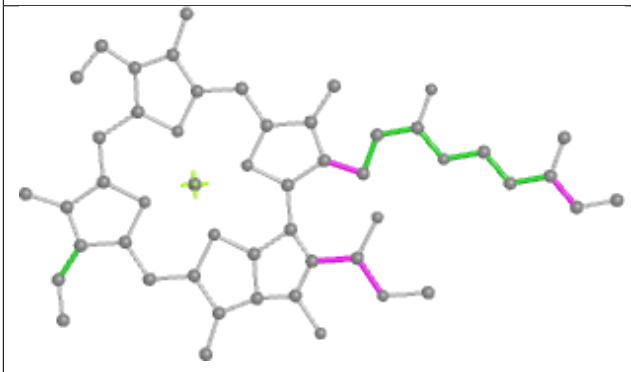
Ligand CLA bA 842



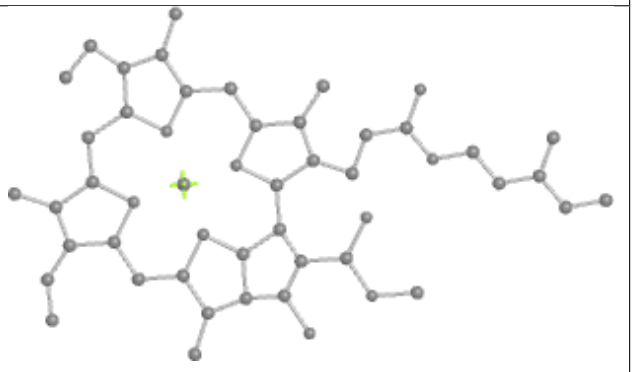
Bond lengths



Bond angles

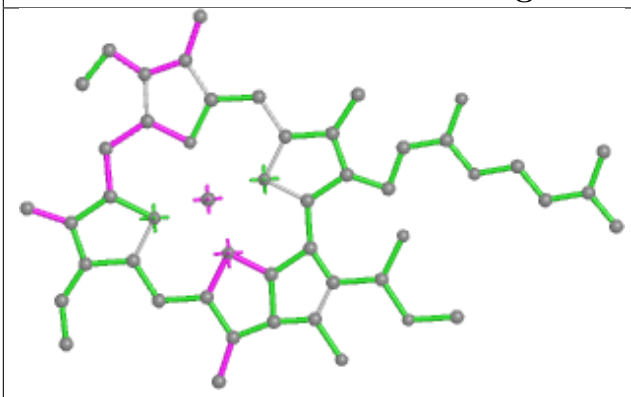


Torsions

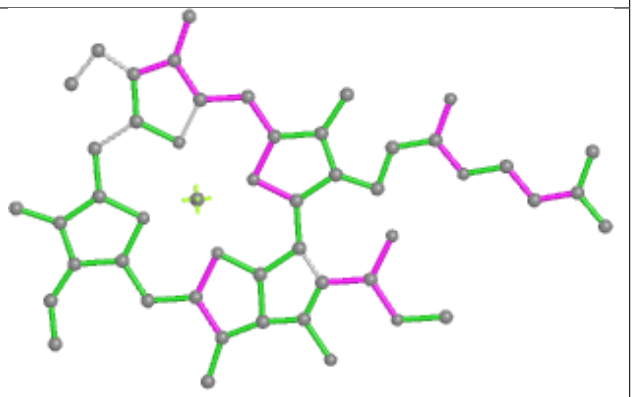


Rings

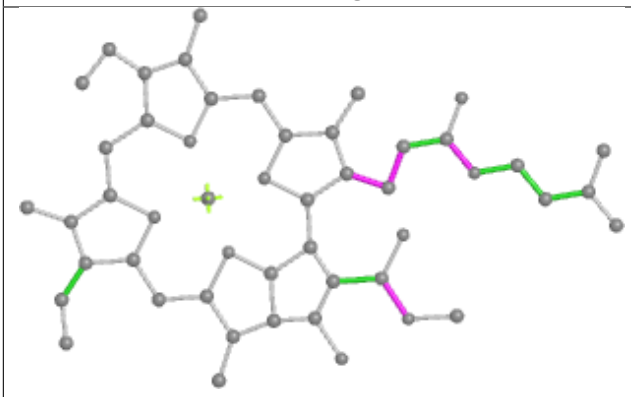
Ligand CLA cA 832



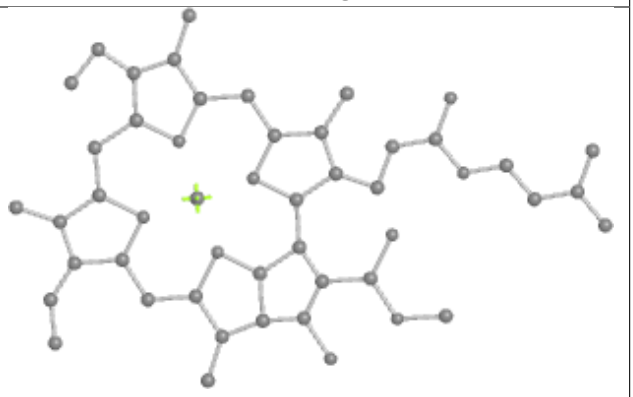
Bond lengths



Bond angles

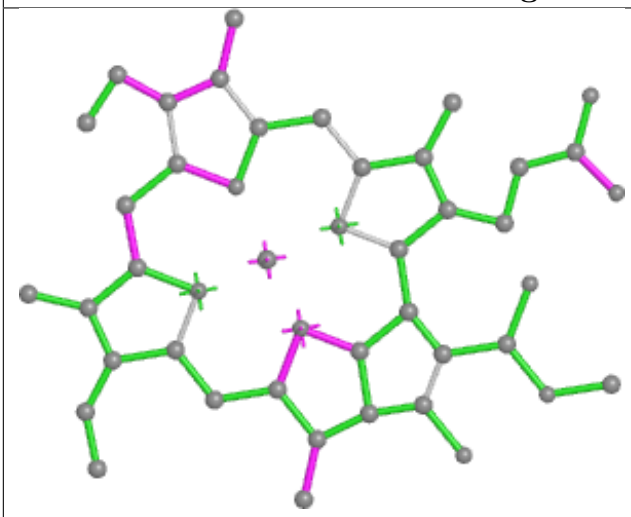


Torsions

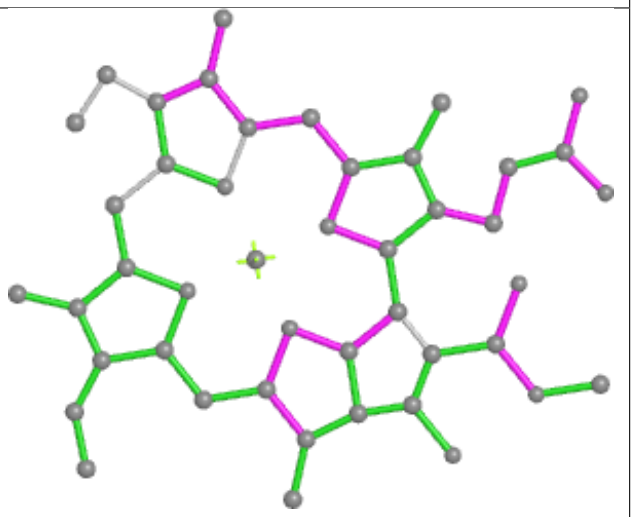


Rings

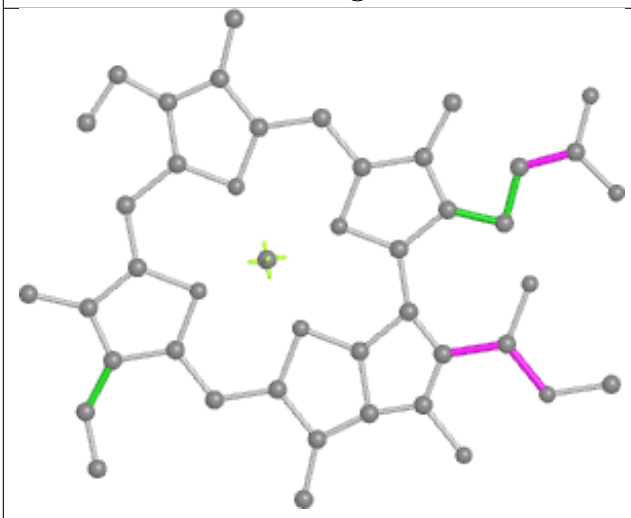
Ligand CLA c2 416



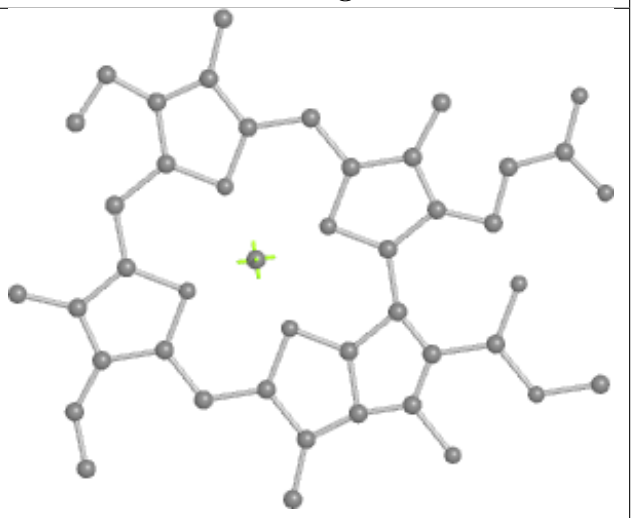
Bond lengths



Bond angles

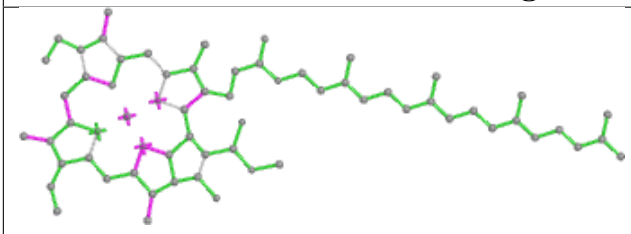


Torsions

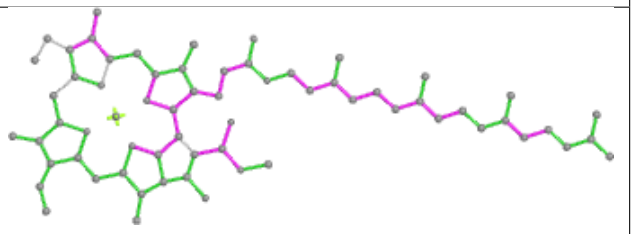


Rings

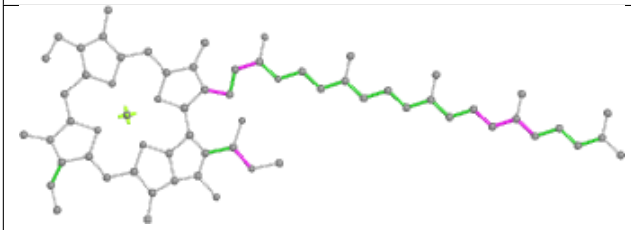
Ligand CLA c3 421



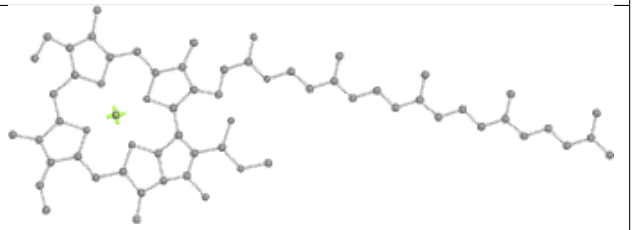
Bond lengths



Bond angles

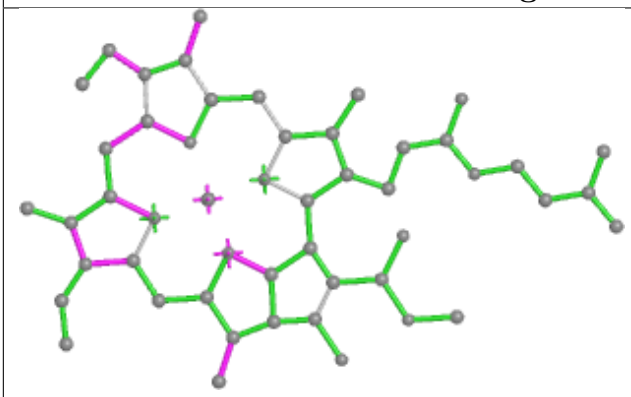


Torsions

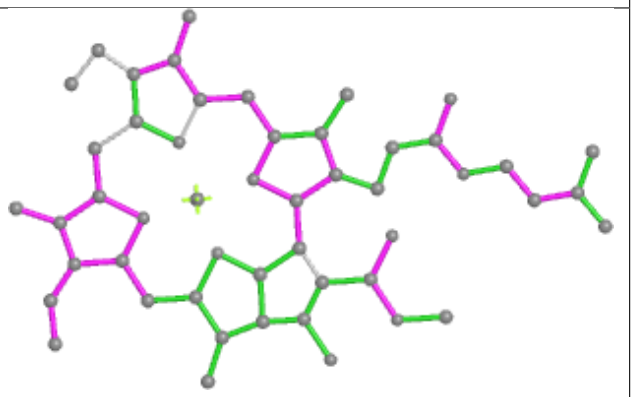


Rings

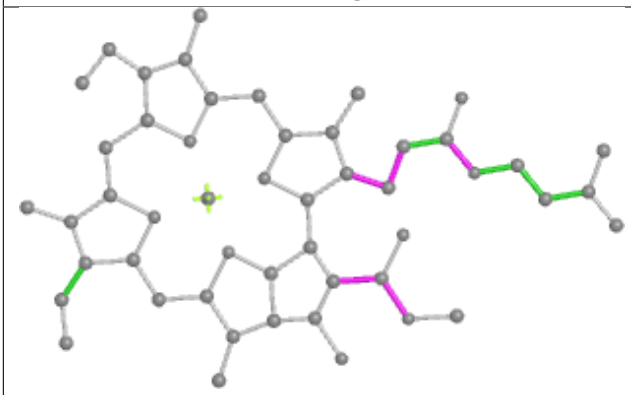
Ligand CLA a1 415



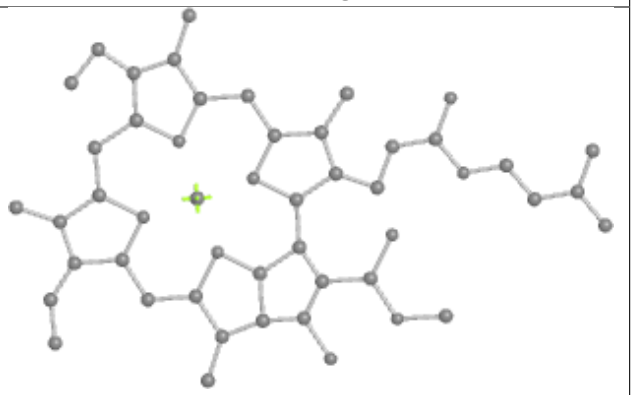
Bond lengths



Bond angles

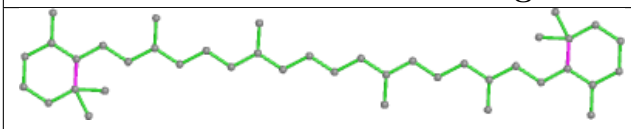


Torsions

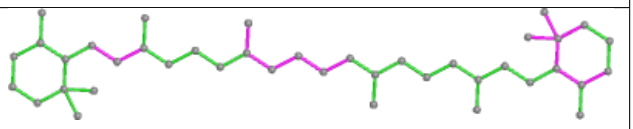


Rings

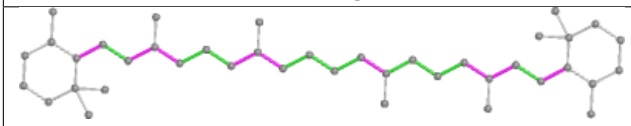
Ligand BCR cB 846



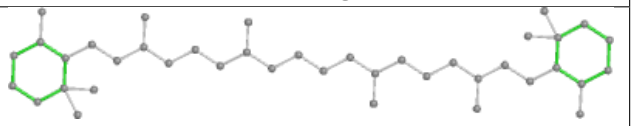
Bond lengths



Bond angles

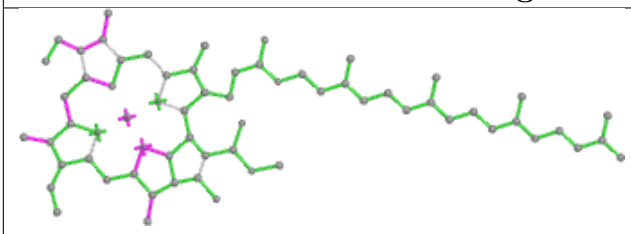


Torsions

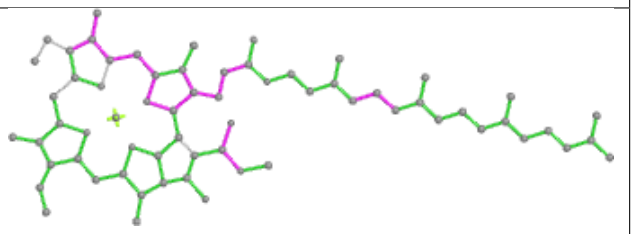


Rings

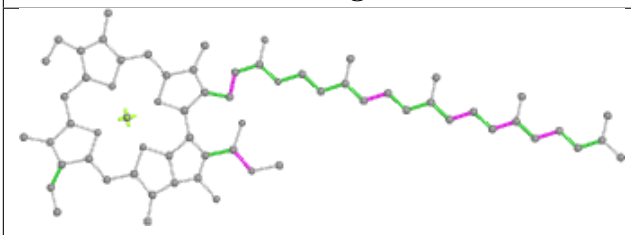
Ligand CLA cB 839



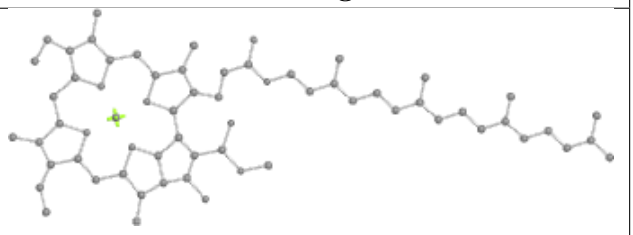
Bond lengths



Bond angles

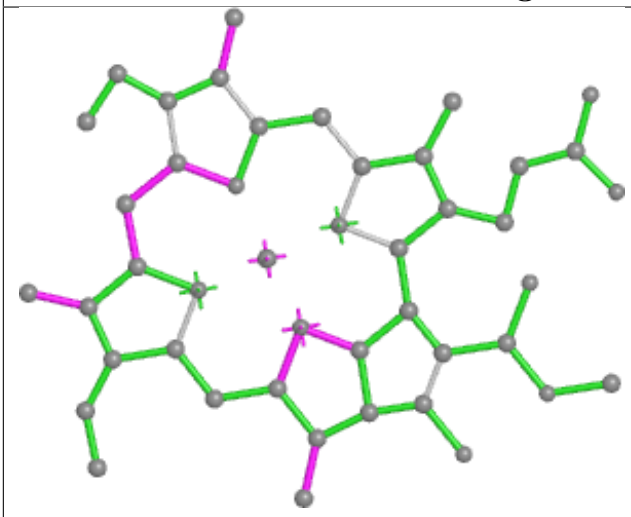


Torsions

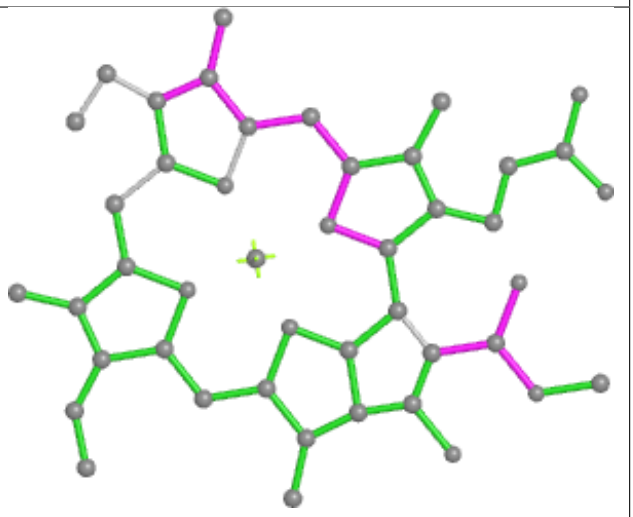


Rings

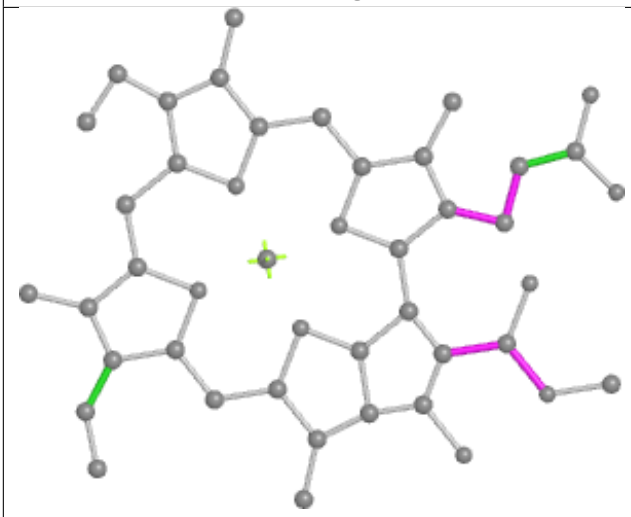
Ligand CLA cB 816



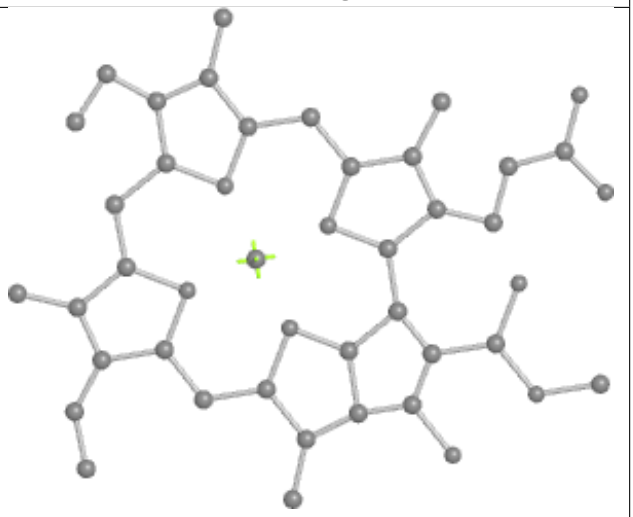
Bond lengths



Bond angles

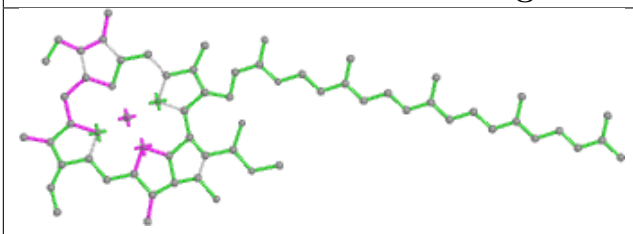


Torsions

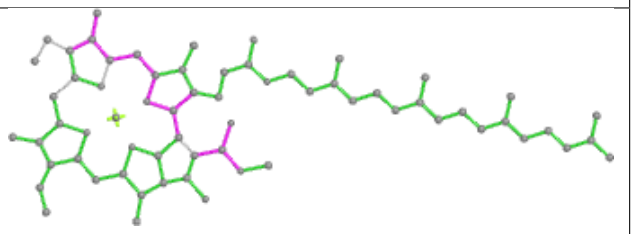


Rings

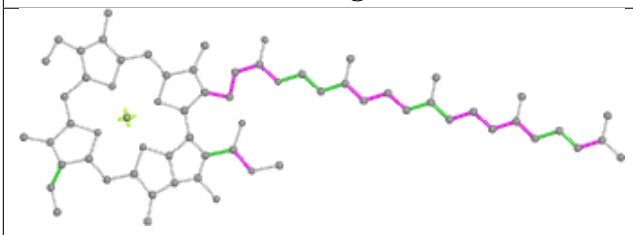
Ligand CLA cB 828



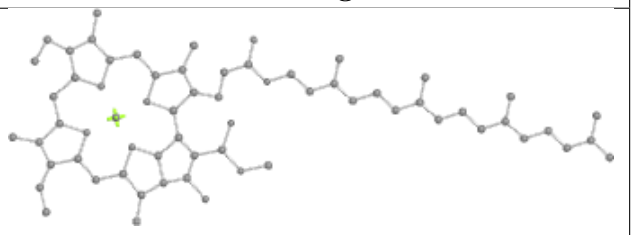
Bond lengths



Bond angles

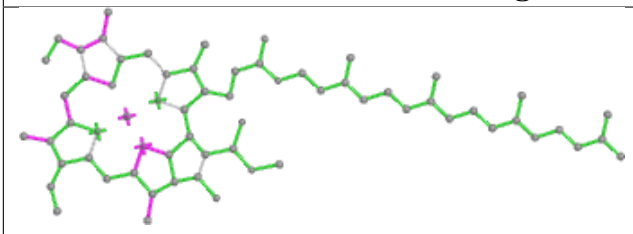


Torsions

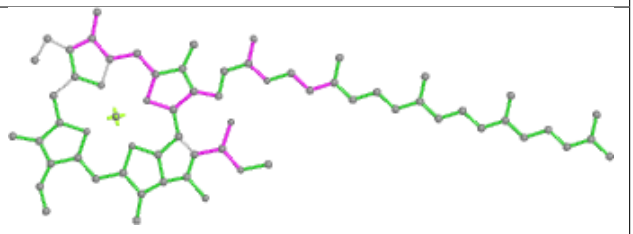


Rings

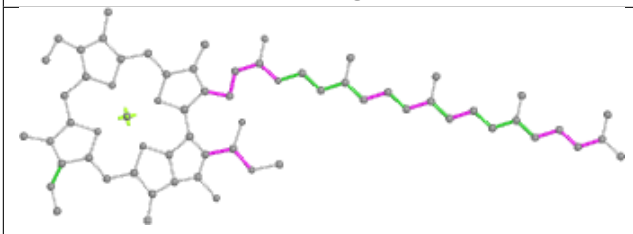
Ligand CLA bA 809



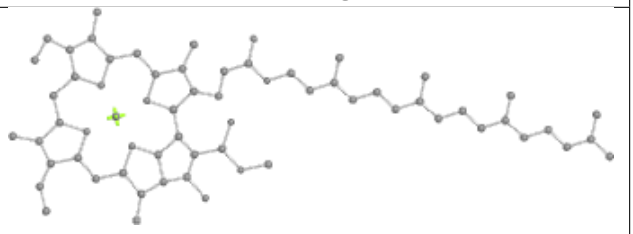
Bond lengths



Bond angles

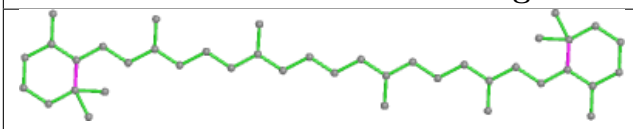


Torsions

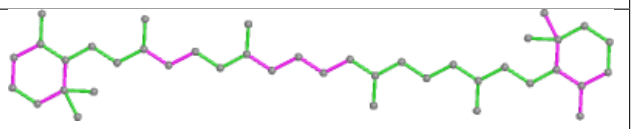


Rings

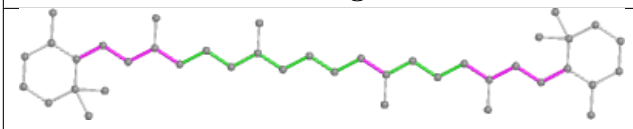
Ligand BCR aA 849



Bond lengths



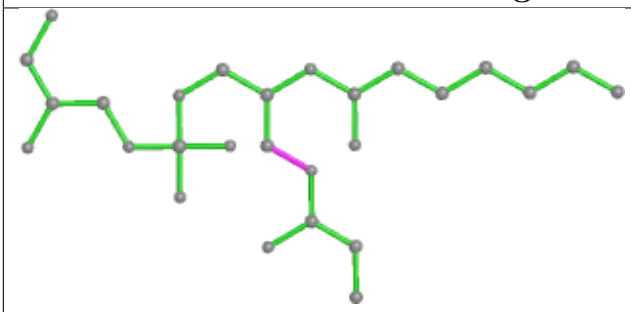
Bond angles



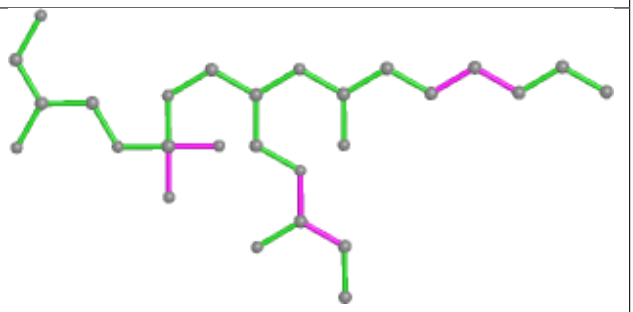
Torsions

Rings

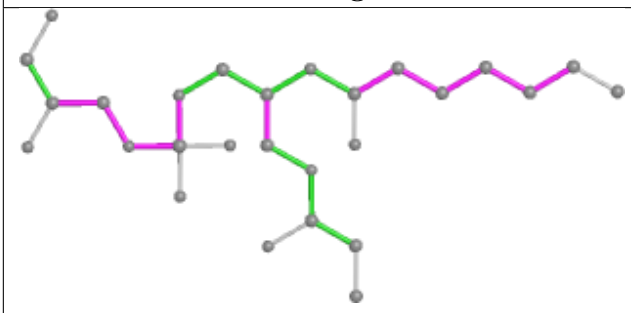
Ligand LHG aA 854



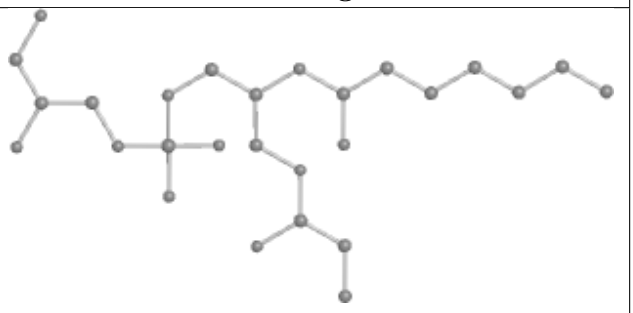
Bond lengths



Bond angles

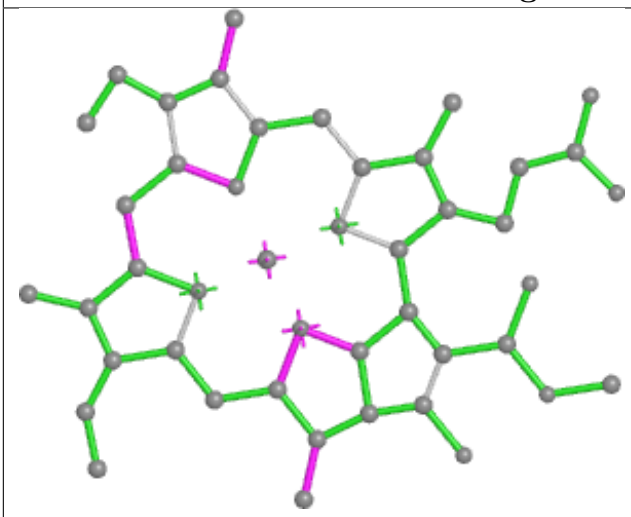


Torsions

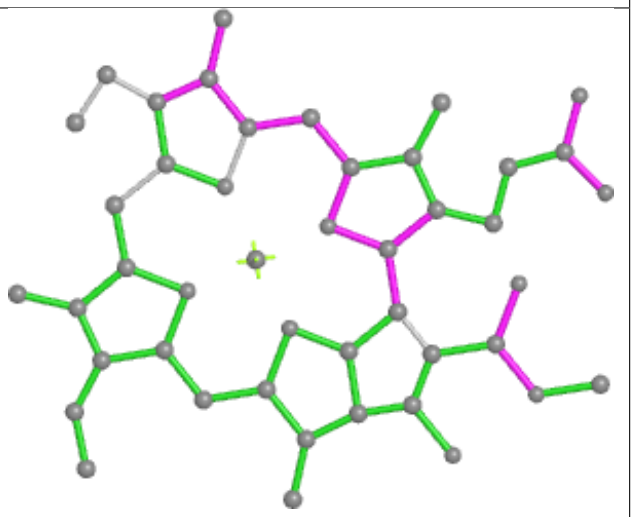


Rings

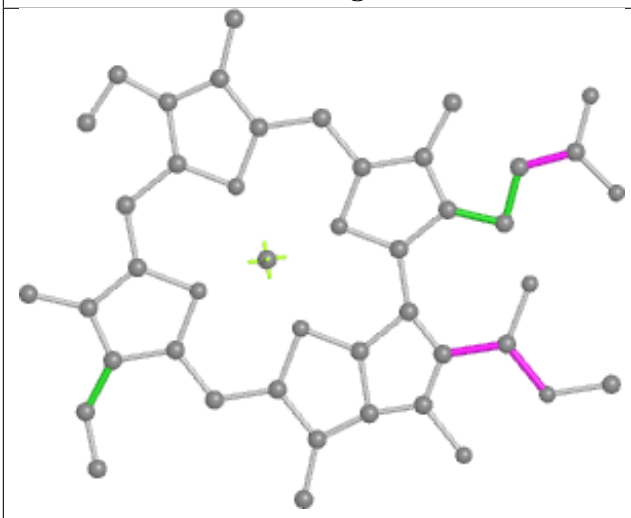
Ligand CLA a5 407



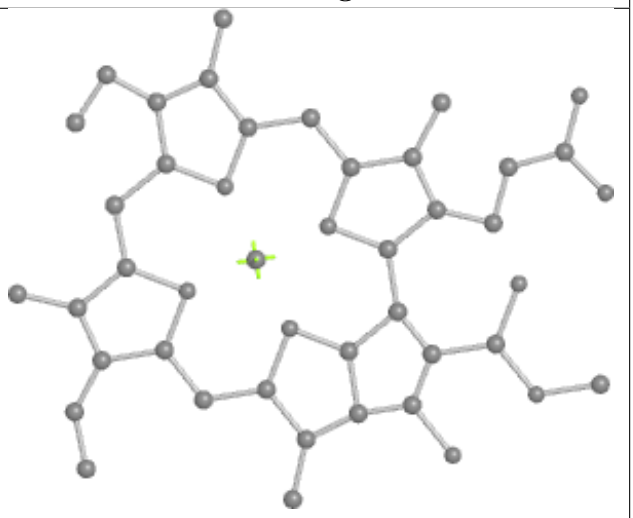
Bond lengths



Bond angles

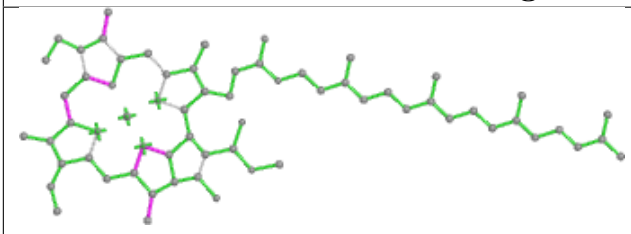


Torsions

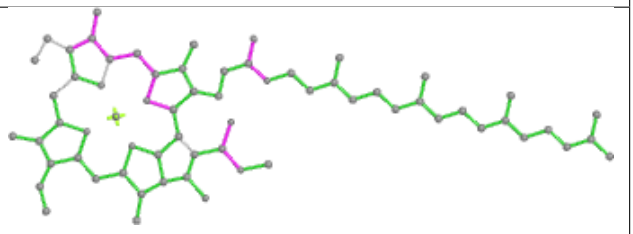


Rings

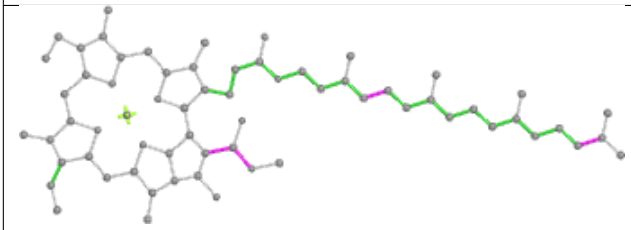
Ligand CLA a1 408



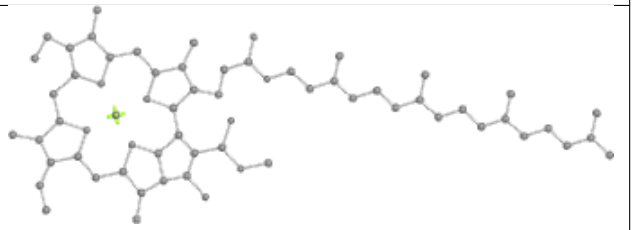
Bond lengths



Bond angles

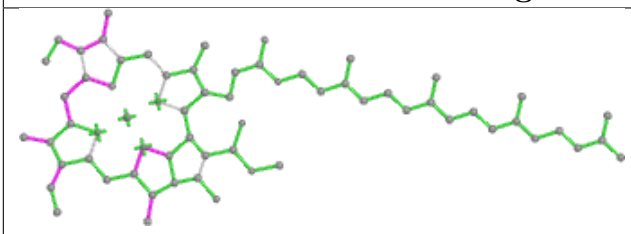


Torsions

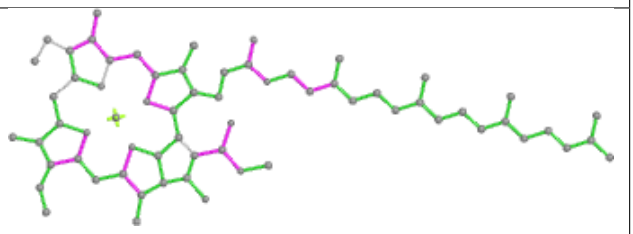


Rings

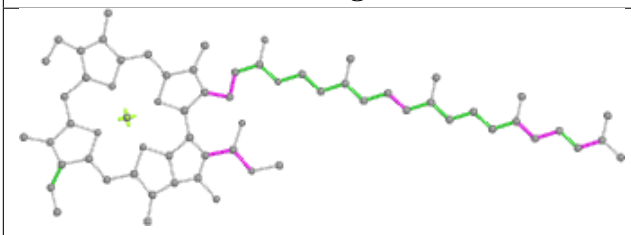
Ligand CLA aA 835



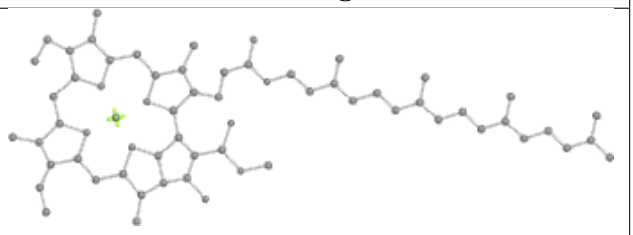
Bond lengths



Bond angles

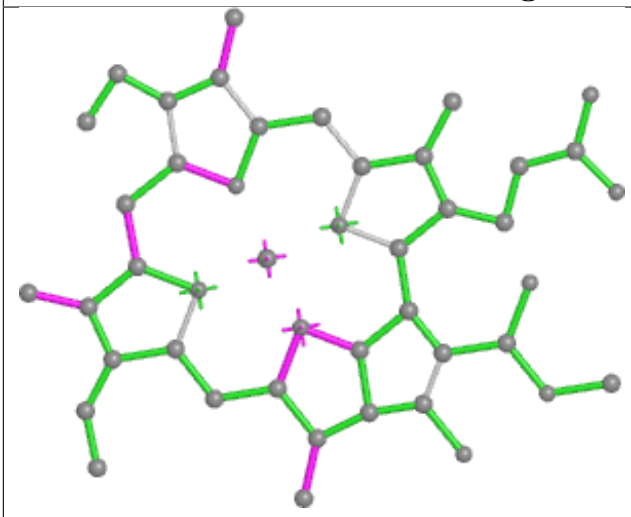


Torsions

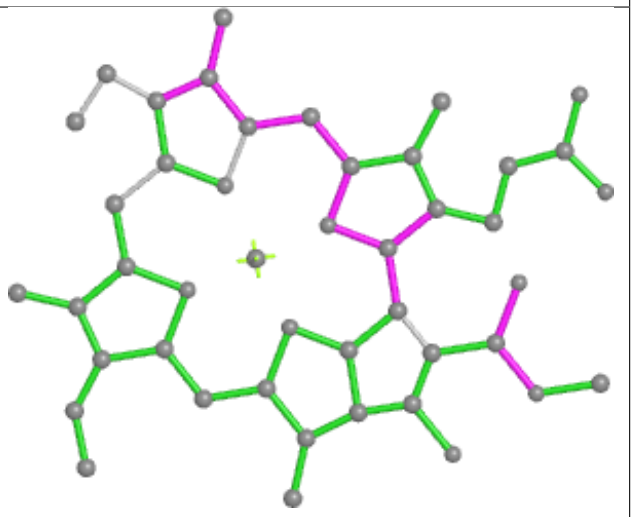


Rings

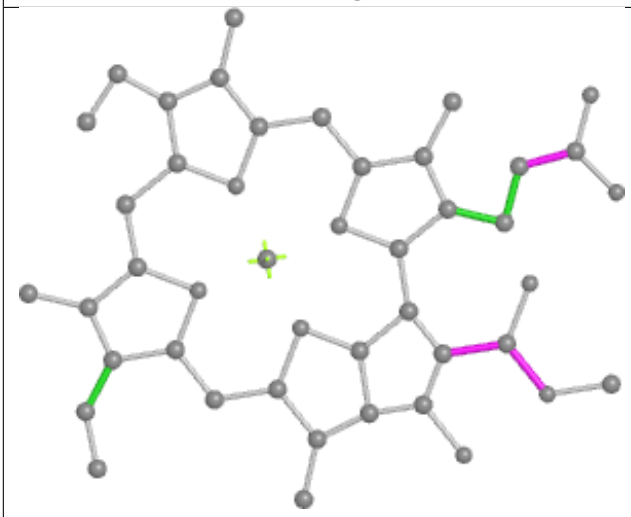
Ligand CLA a4 407



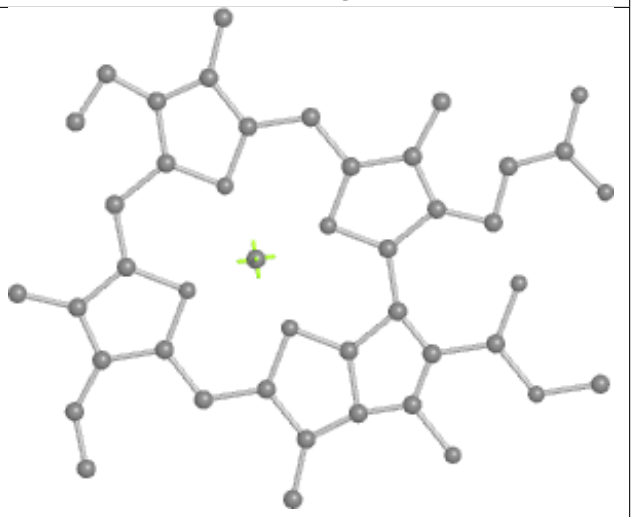
Bond lengths



Bond angles

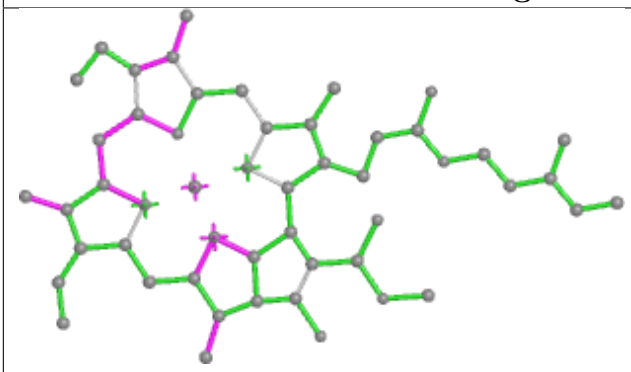


Torsions

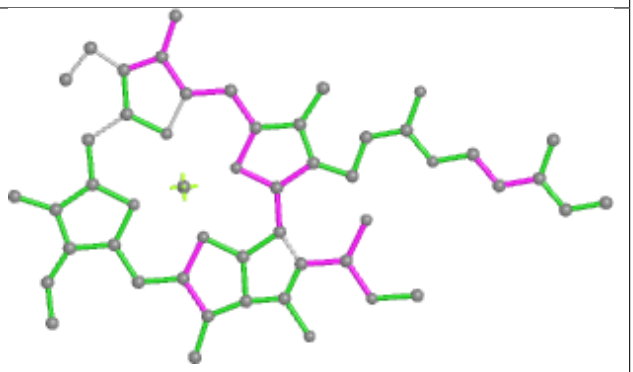


Rings

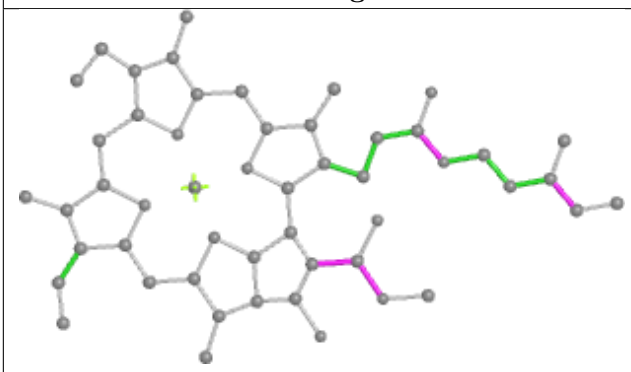
Ligand CLA bA 838



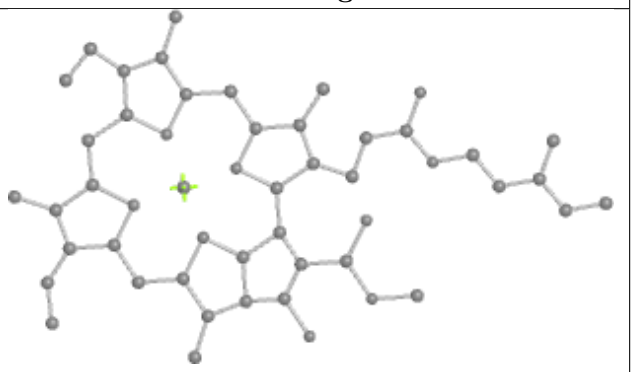
Bond lengths



Bond angles

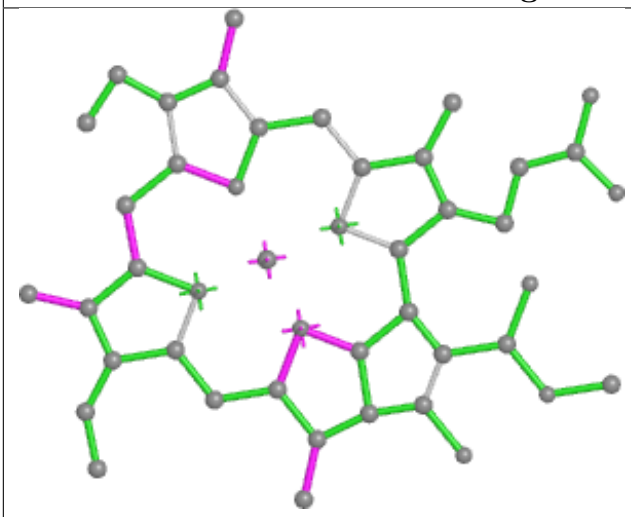


Torsions

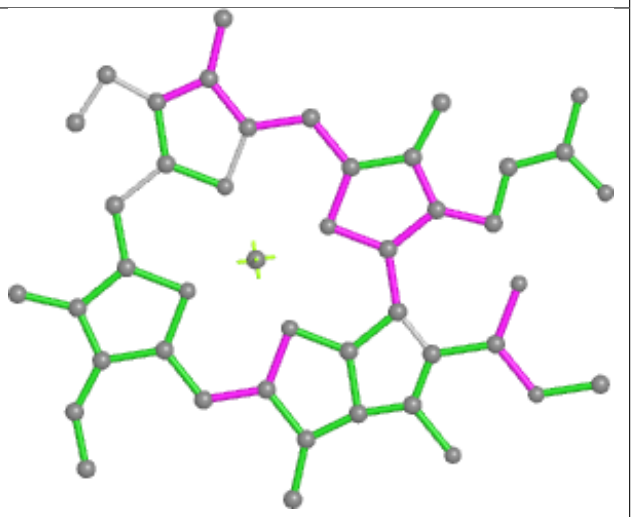


Rings

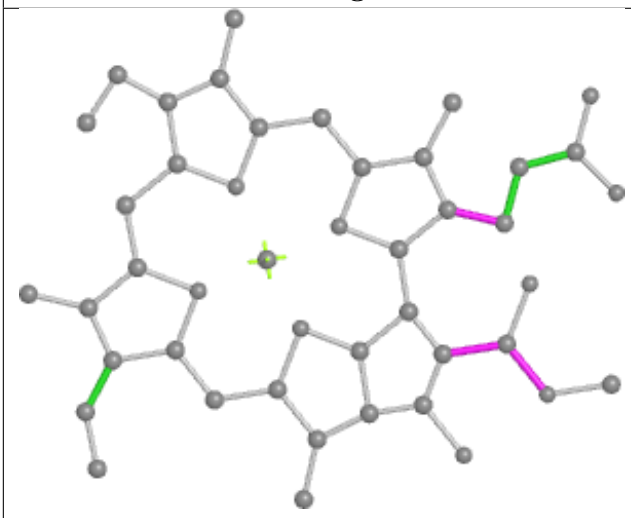
Ligand CLA c3 411



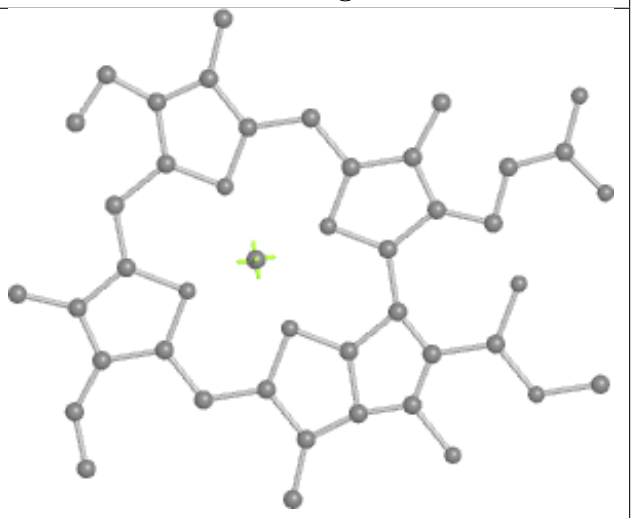
Bond lengths



Bond angles

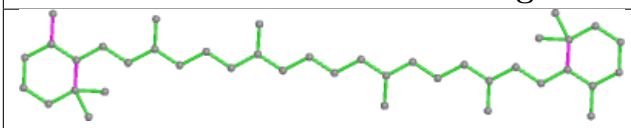


Torsions

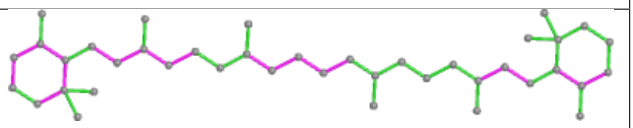


Rings

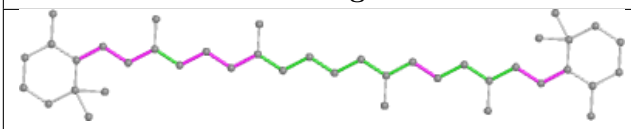
Ligand BCR b4 401



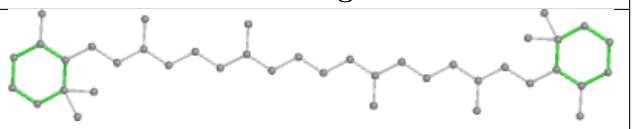
Bond lengths



Bond angles

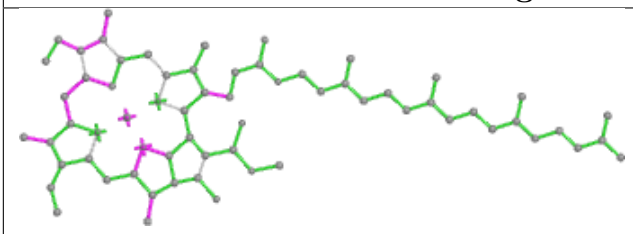


Torsions

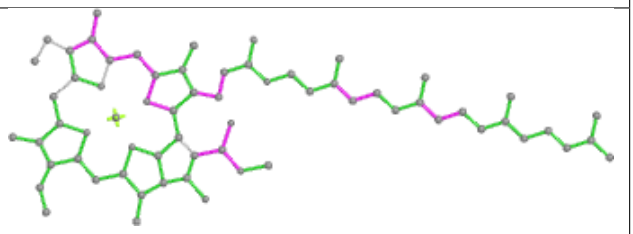


Rings

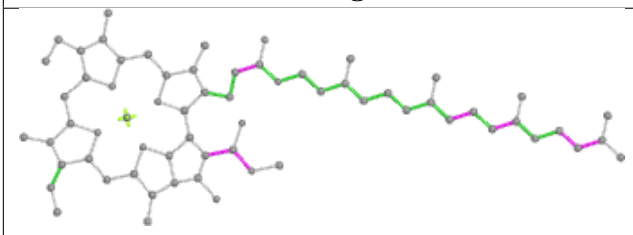
Ligand CLA aB 802



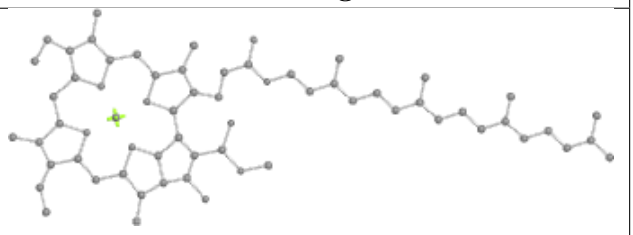
Bond lengths



Bond angles

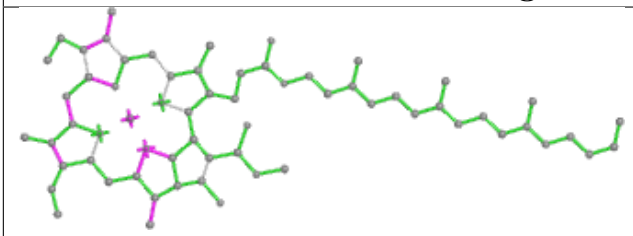


Torsions

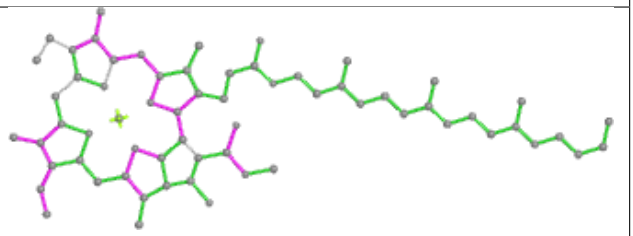


Rings

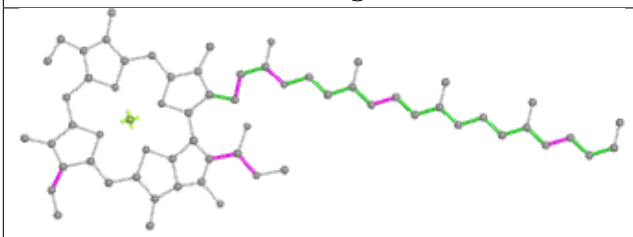
Ligand CLA b3 410



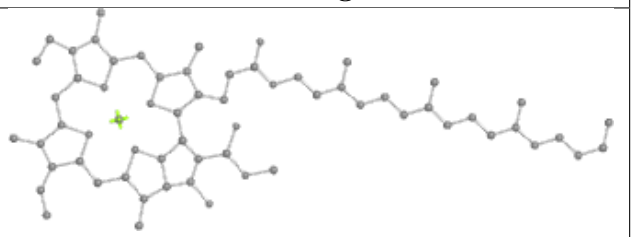
Bond lengths



Bond angles

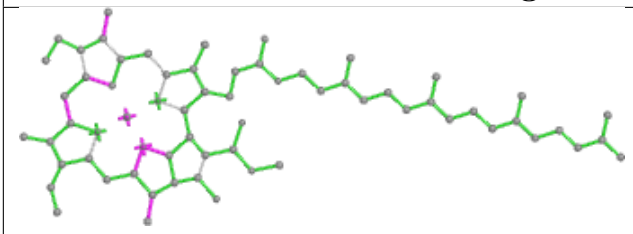


Torsions

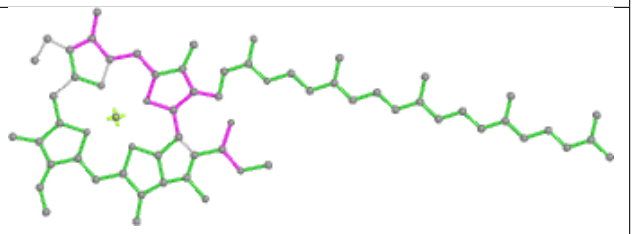


Rings

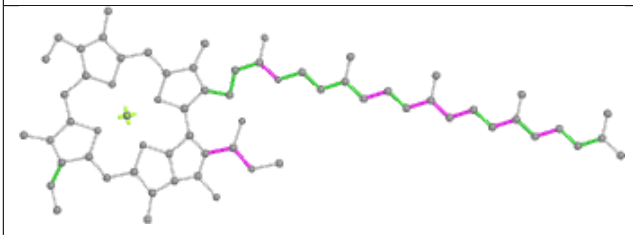
Ligand CLA c6 404



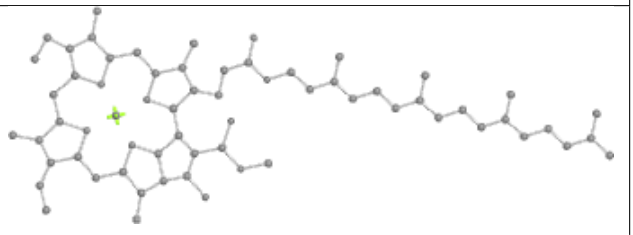
Bond lengths



Bond angles

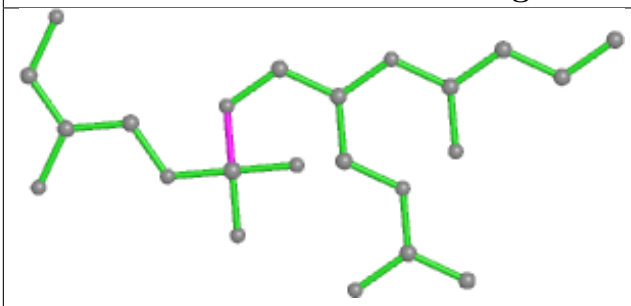


Torsions

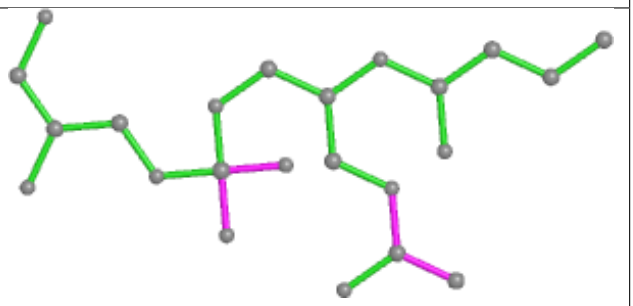


Rings

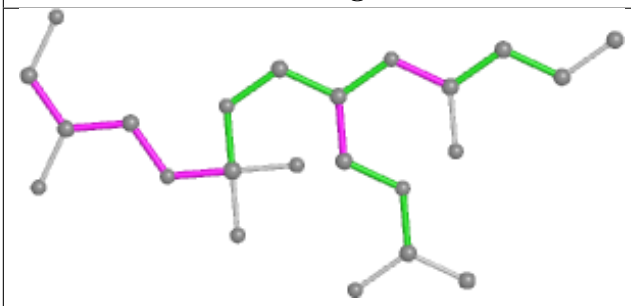
Ligand LHG bX 101



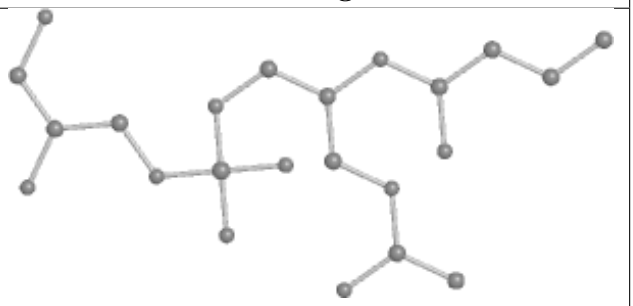
Bond lengths



Bond angles

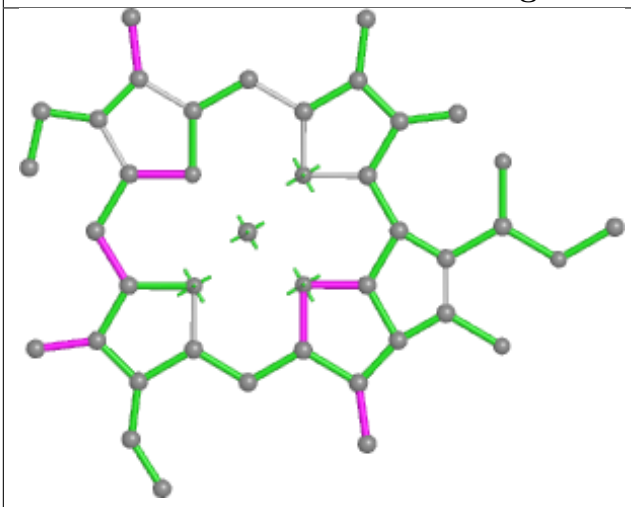


Torsions

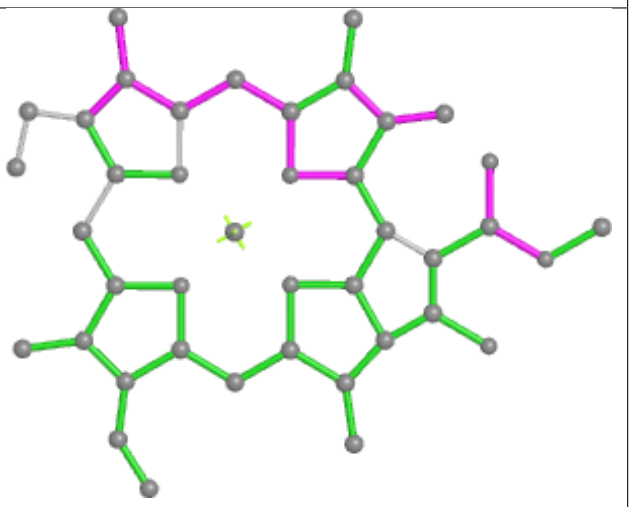


Rings

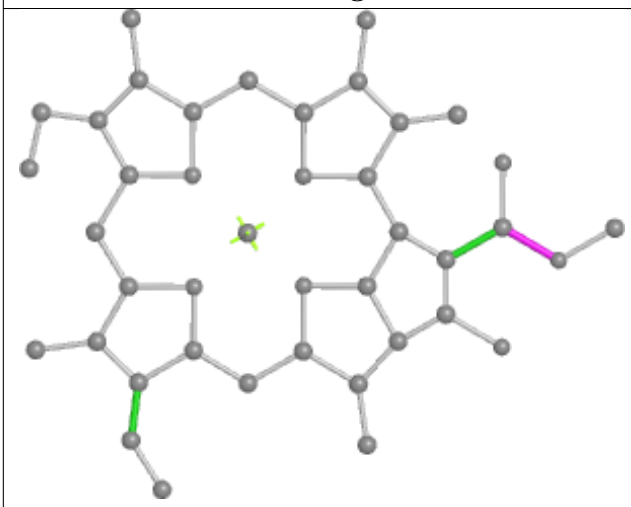
Ligand CLA a6 415



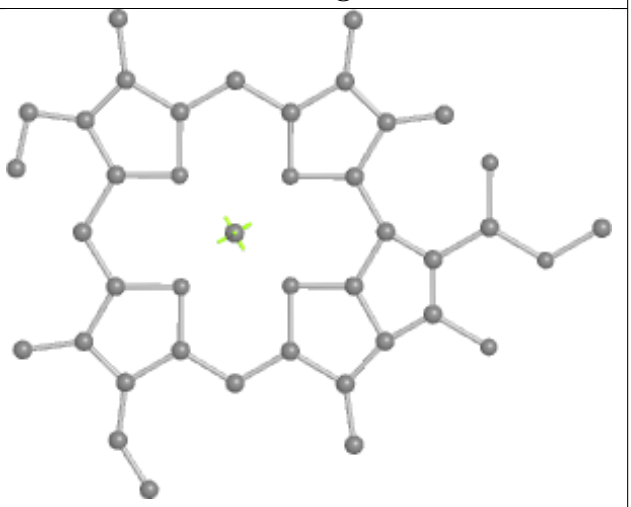
Bond lengths



Bond angles

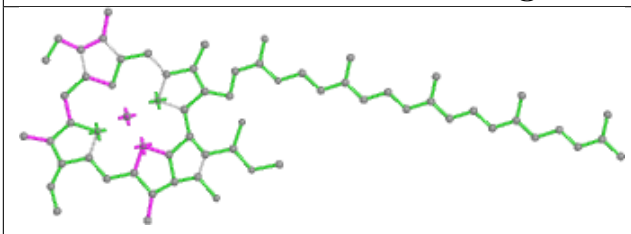


Torsions

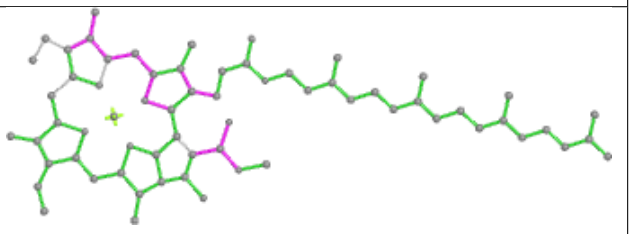


Rings

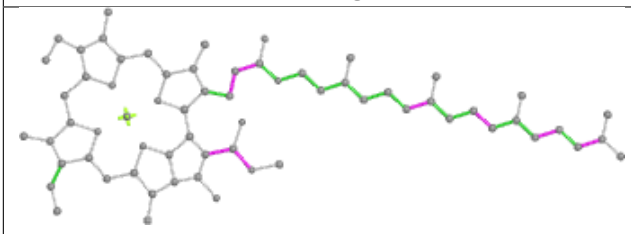
Ligand CLA cL 203



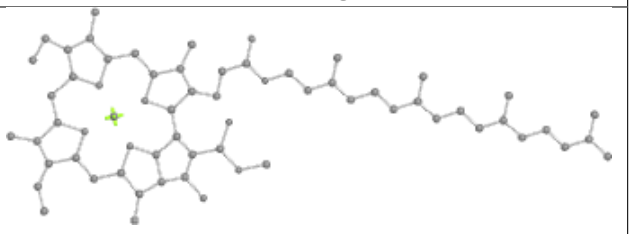
Bond lengths



Bond angles

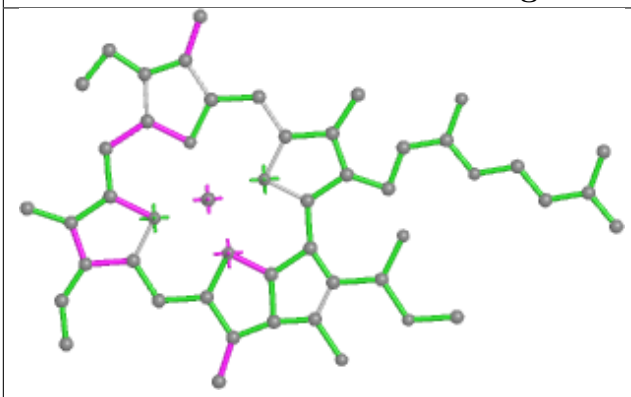


Torsions

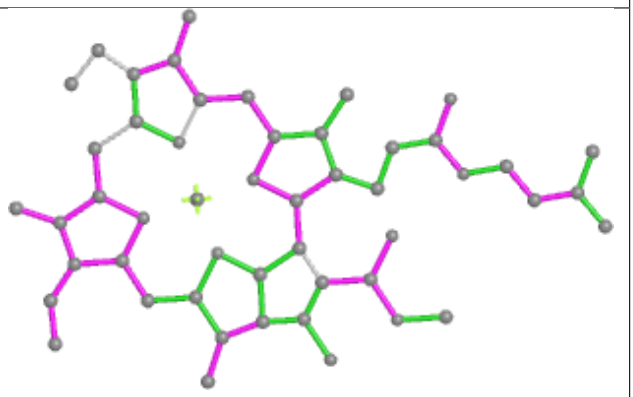


Rings

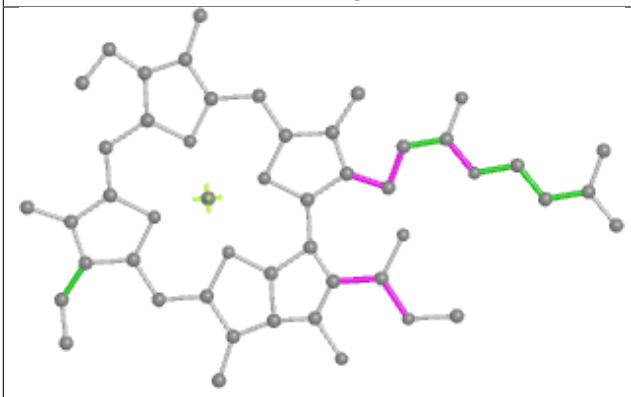
Ligand CLA c2 417



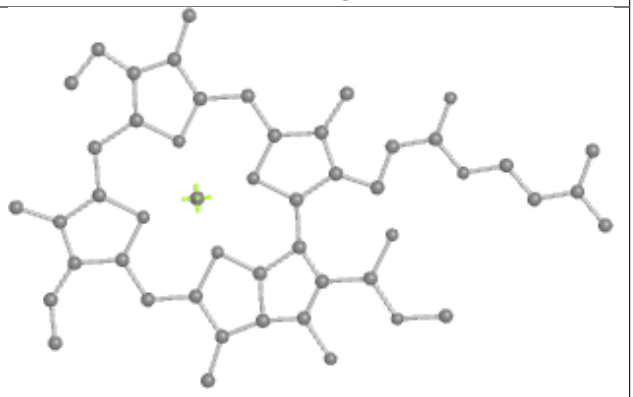
Bond lengths



Bond angles

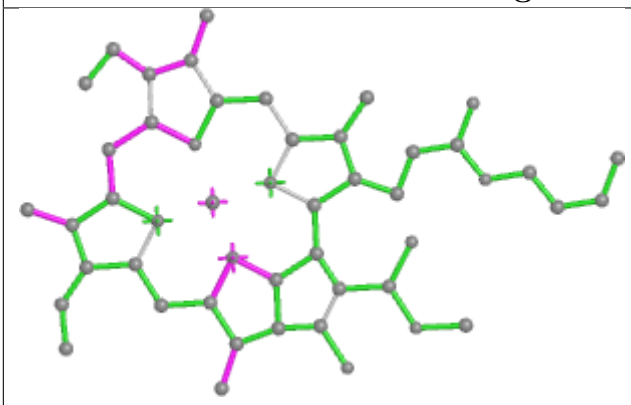


Torsions

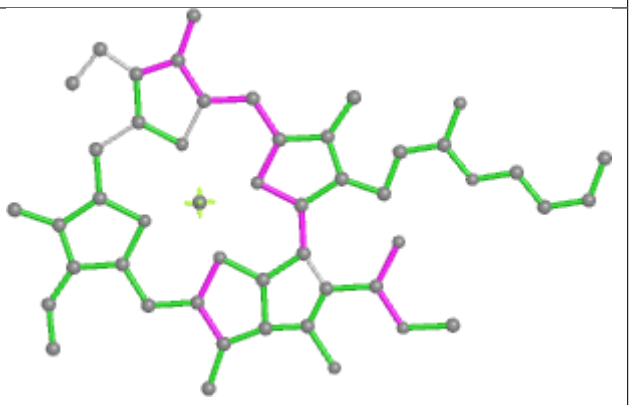


Rings

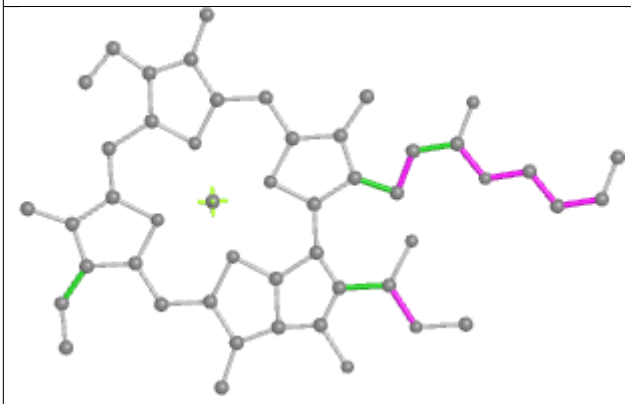
Ligand CLA bB 832



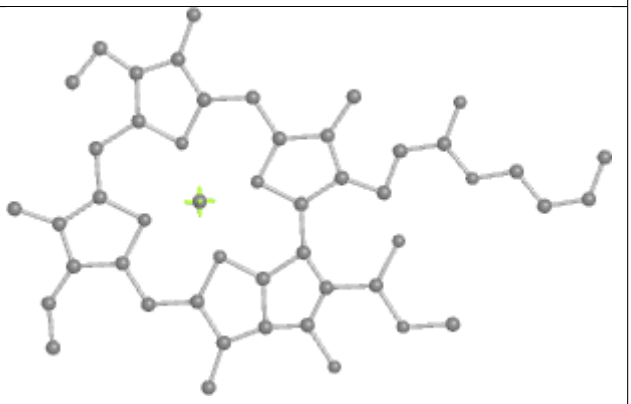
Bond lengths



Bond angles

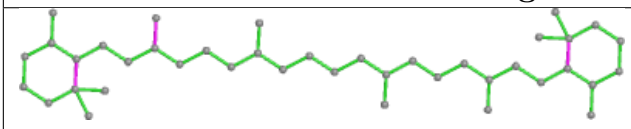


Torsions

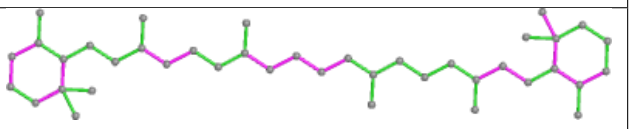


Rings

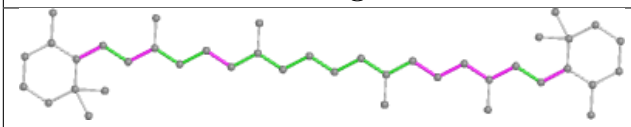
Ligand BCR c2 420



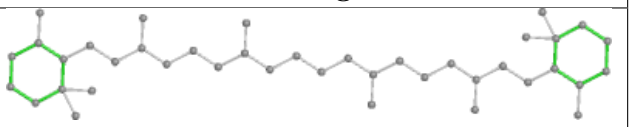
Bond lengths



Bond angles

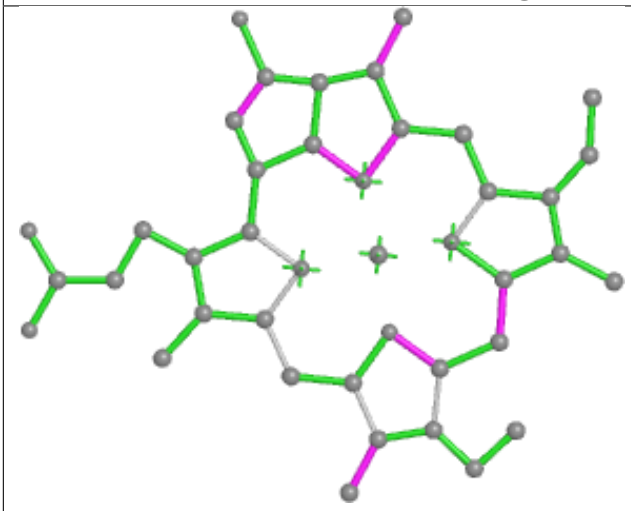


Torsions

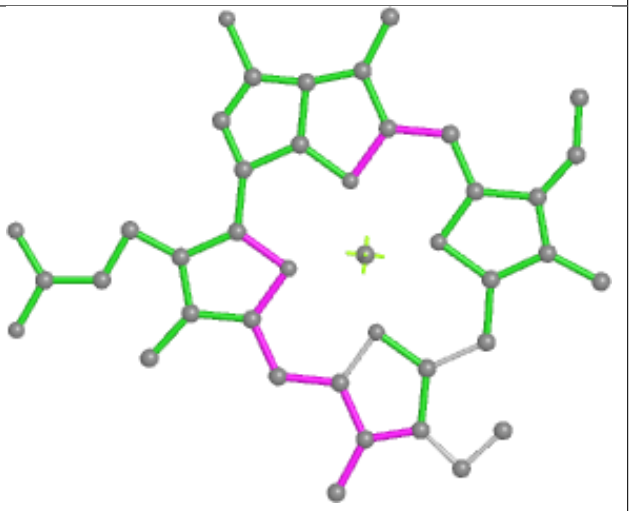


Rings

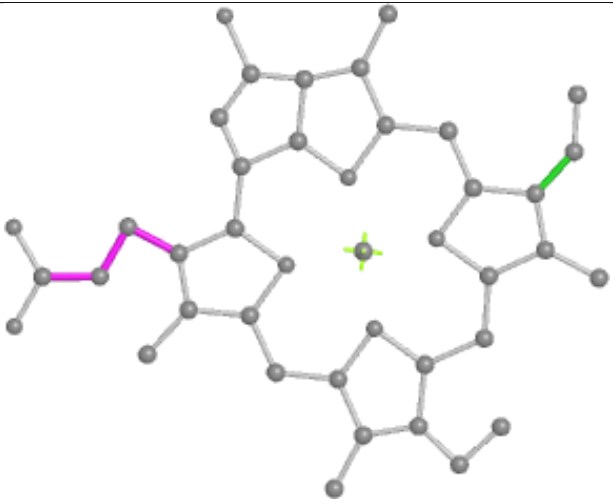
Ligand CLA cA 843



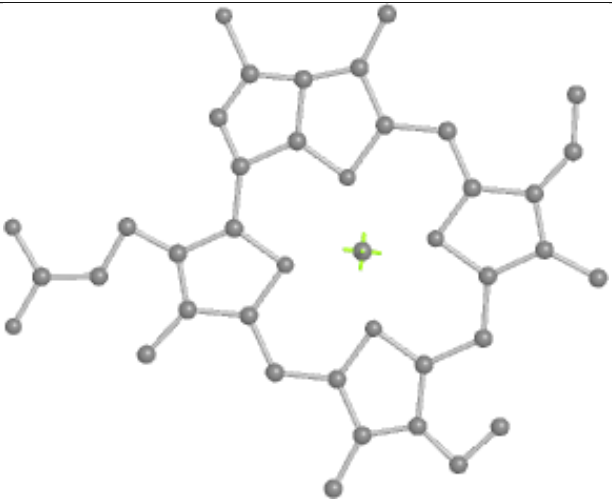
Bond lengths



Bond angles

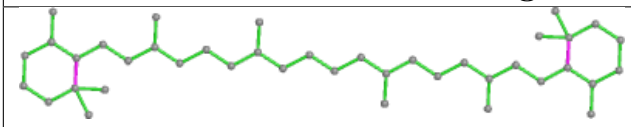


Torsions

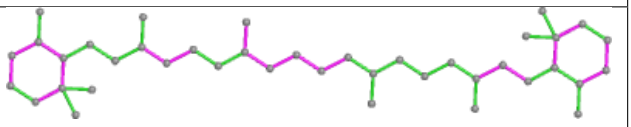


Rings

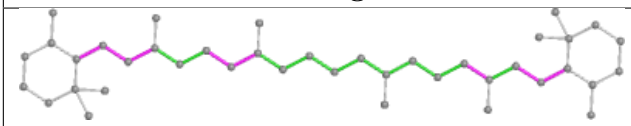
Ligand BCR c4 420



Bond lengths



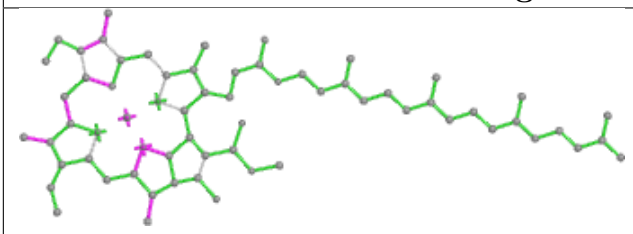
Bond angles



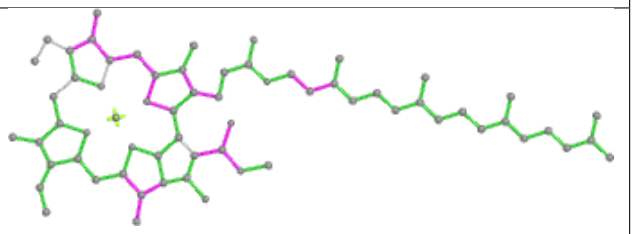
Torsions

Rings

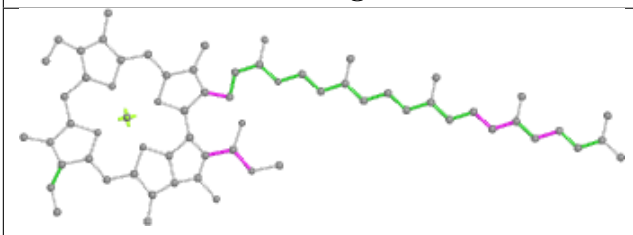
Ligand CLA cA 804



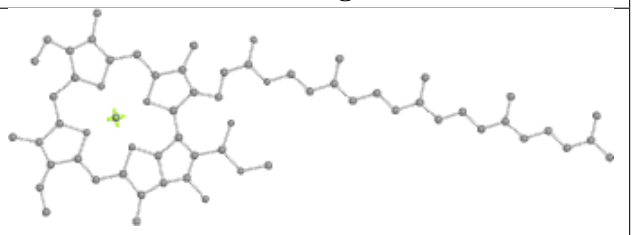
Bond lengths



Bond angles

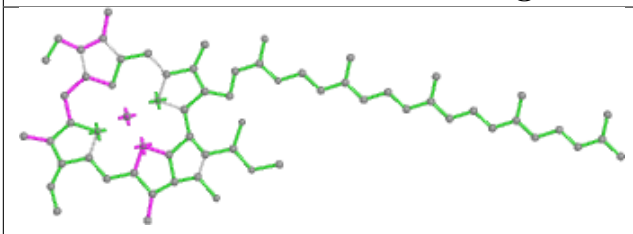


Torsions

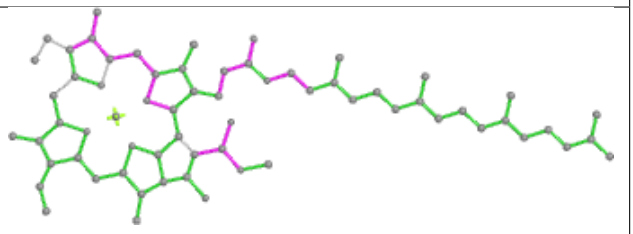


Rings

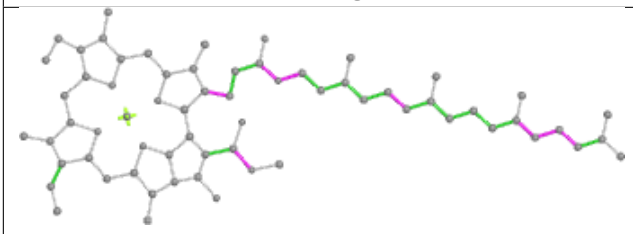
Ligand CLA cA 812



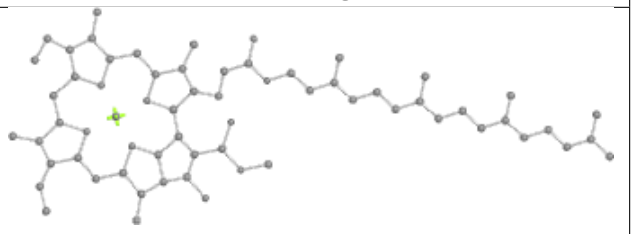
Bond lengths



Bond angles

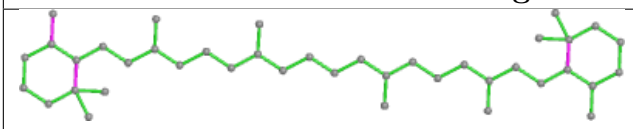


Torsions

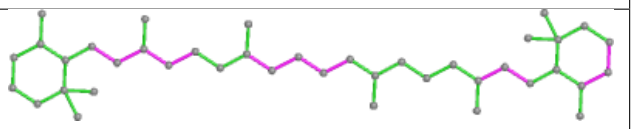


Rings

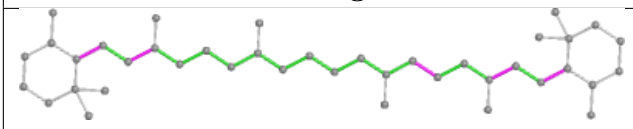
Ligand BCR bB 844



Bond lengths



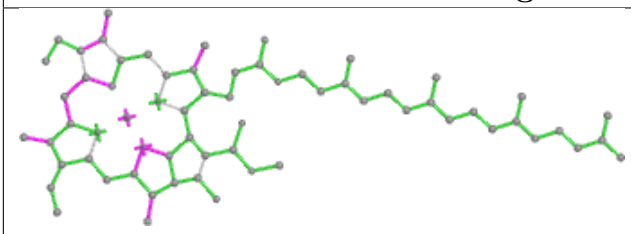
Bond angles



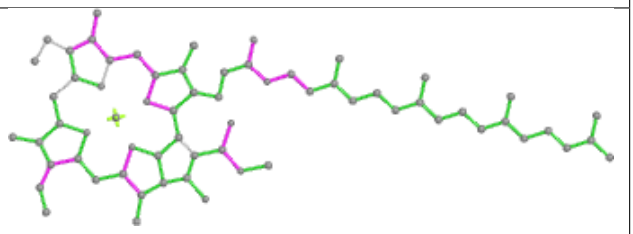
Torsions

Rings

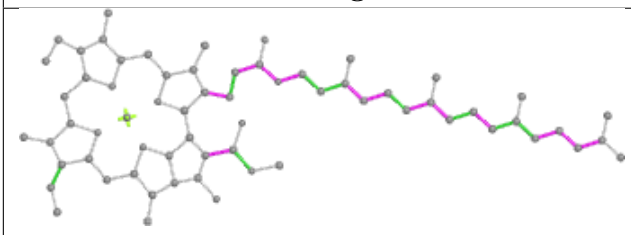
Ligand CLA cB 806



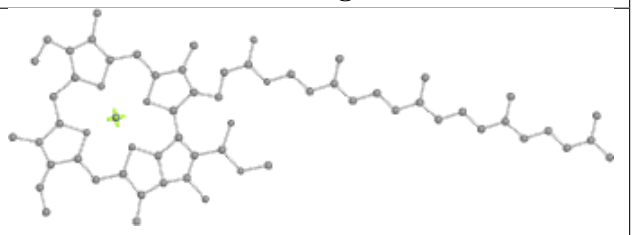
Bond lengths



Bond angles

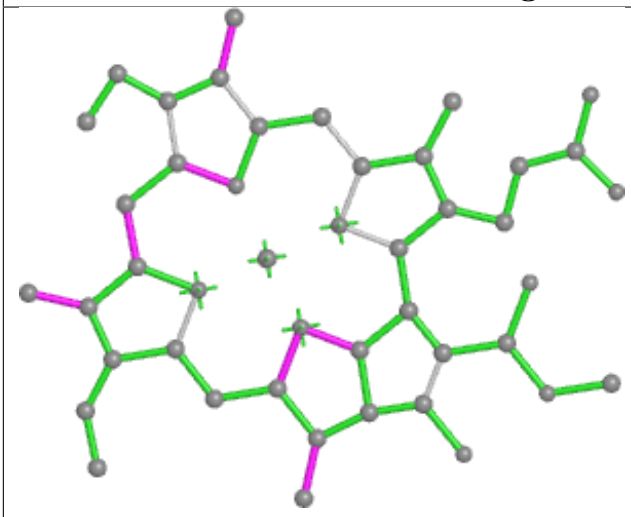


Torsions

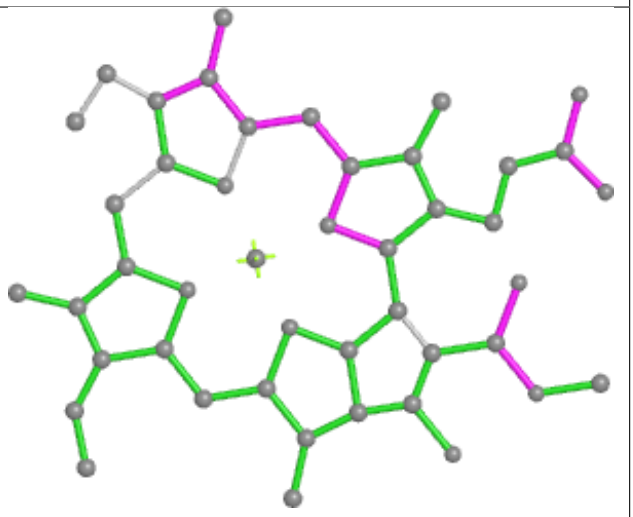


Rings

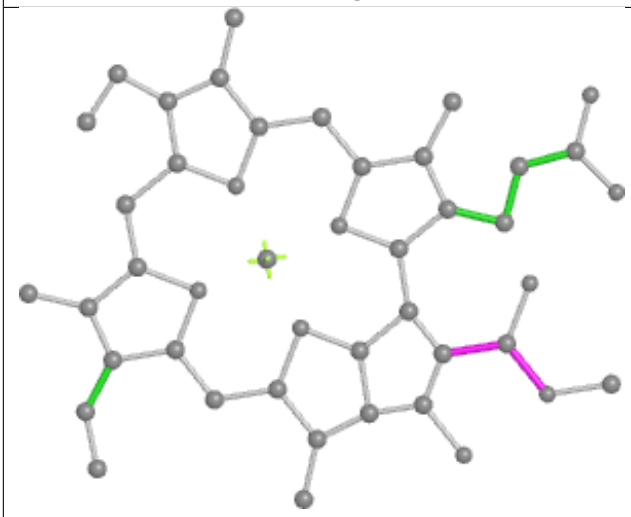
Ligand CLA a1 405



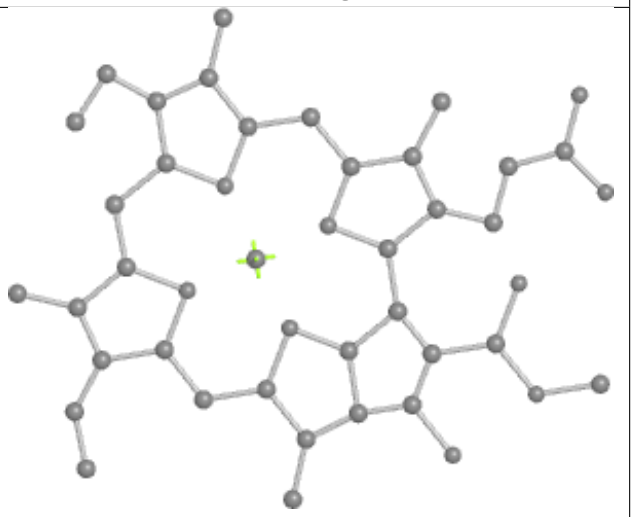
Bond lengths



Bond angles

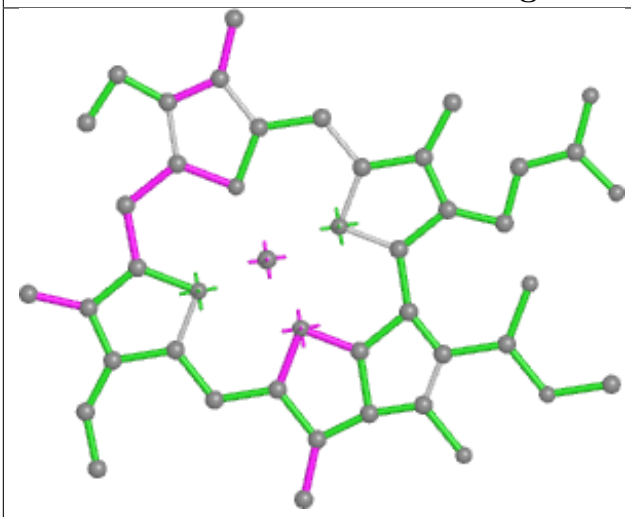


Torsions

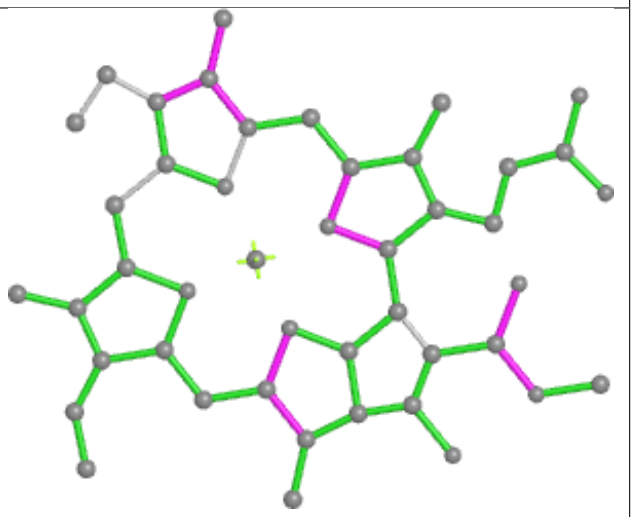


Rings

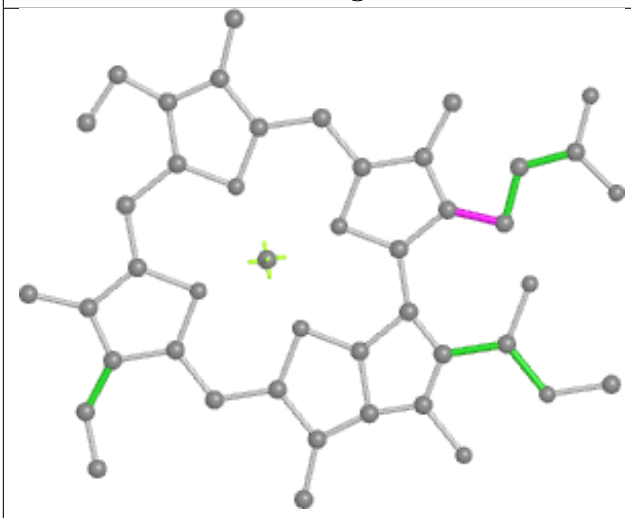
Ligand CLA a3 413



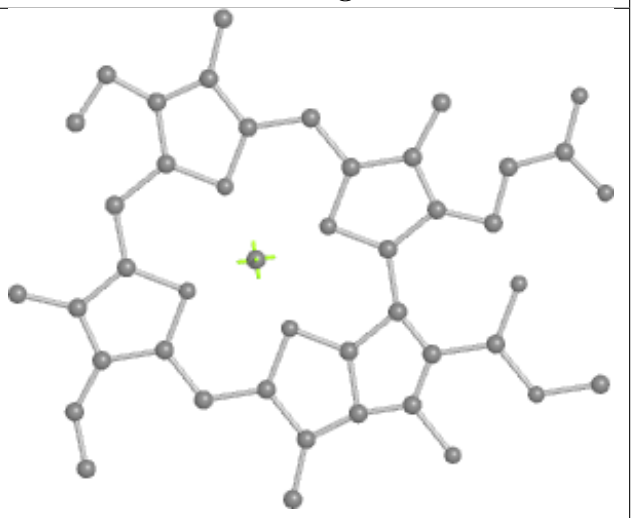
Bond lengths



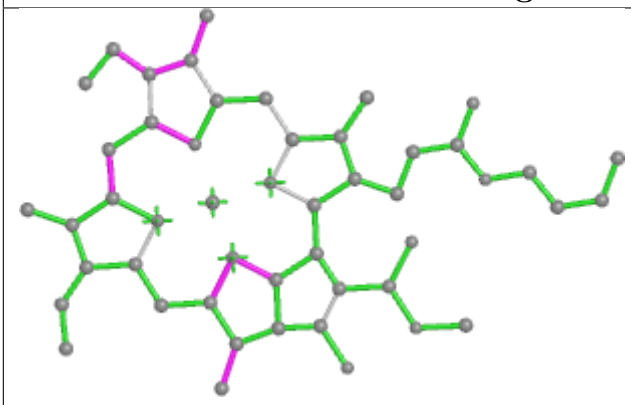
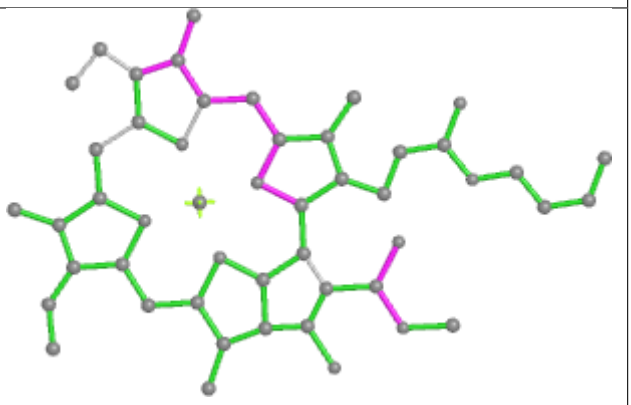
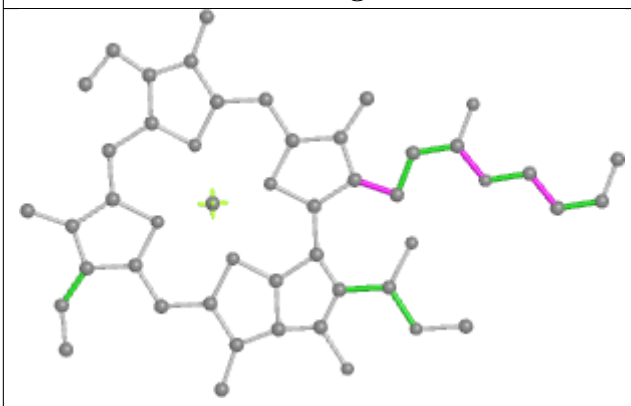
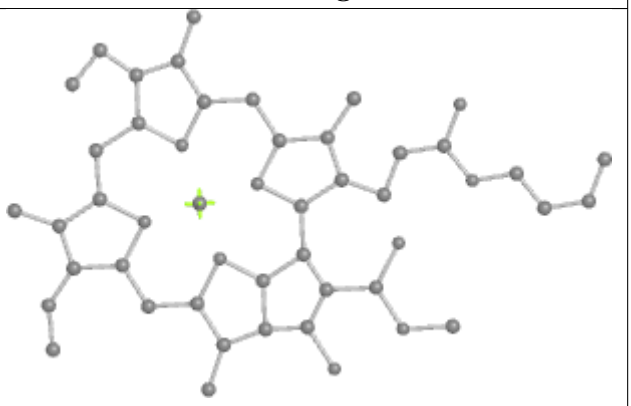
Bond angles



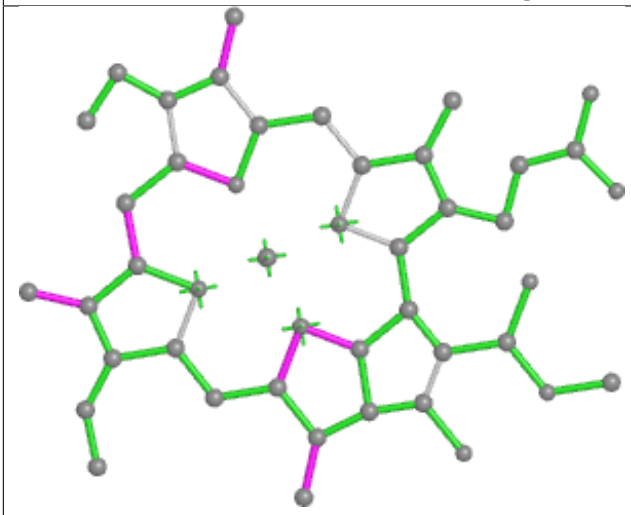
Torsions



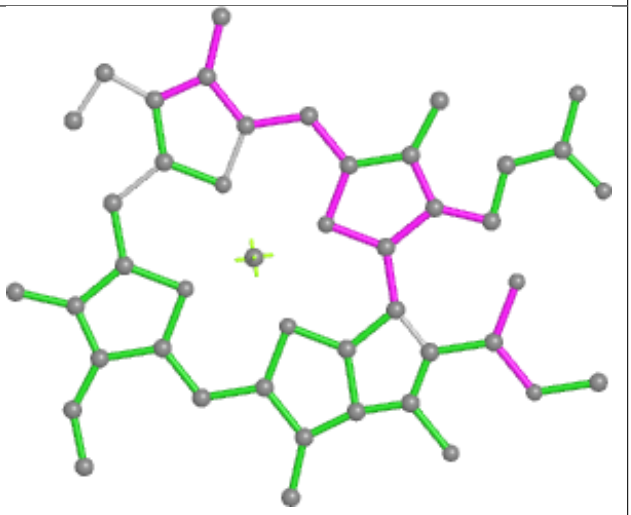
Rings

Ligand CLA cA 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

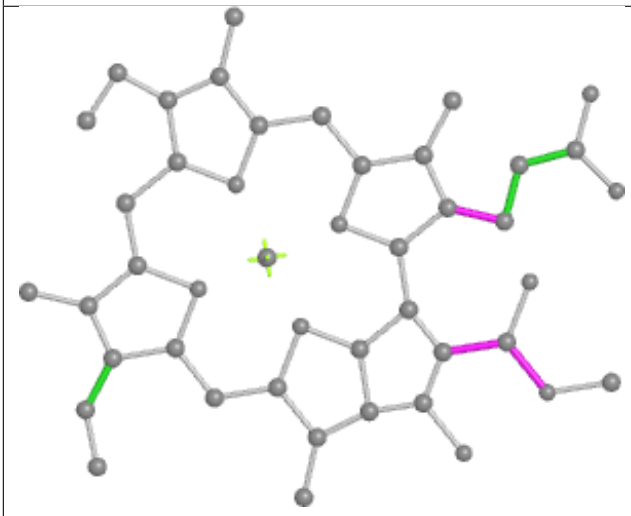
Ligand CLA b1 411



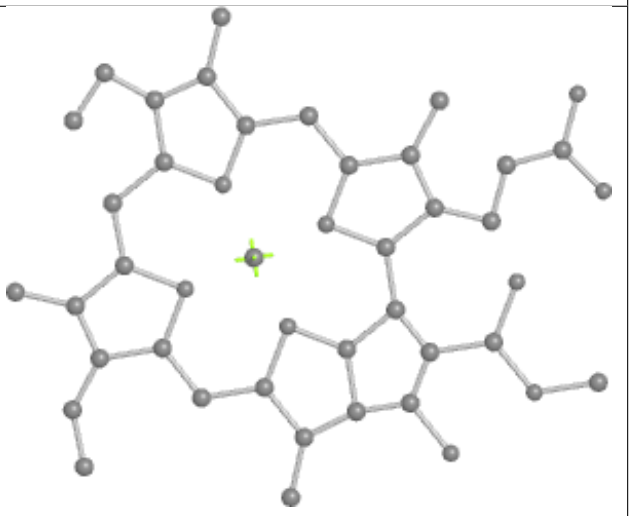
Bond lengths



Bond angles

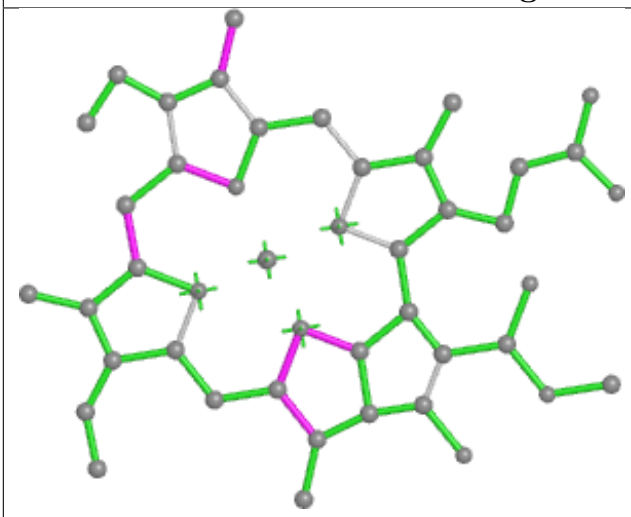


Torsions

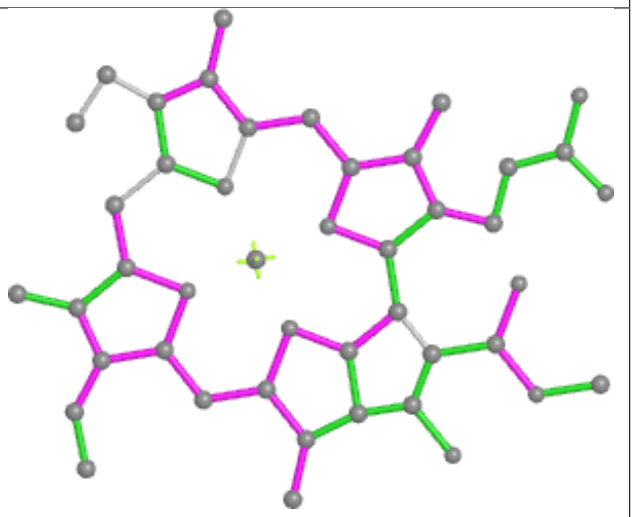


Rings

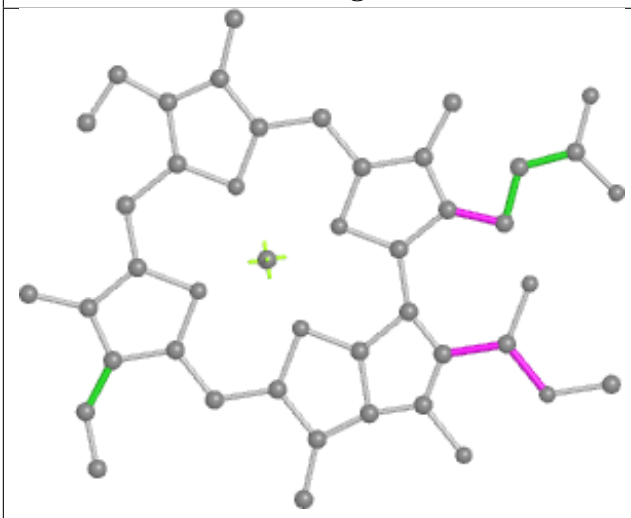
Ligand CLA a2 405



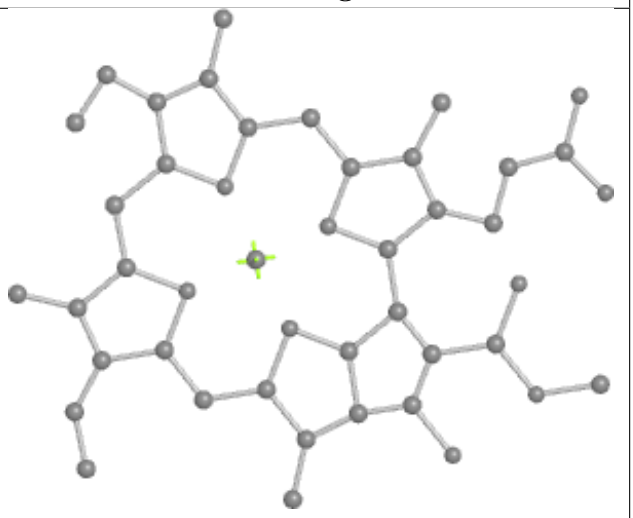
Bond lengths



Bond angles

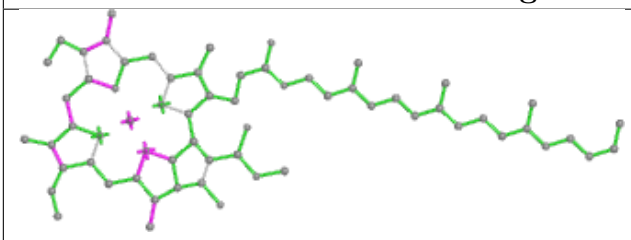


Torsions

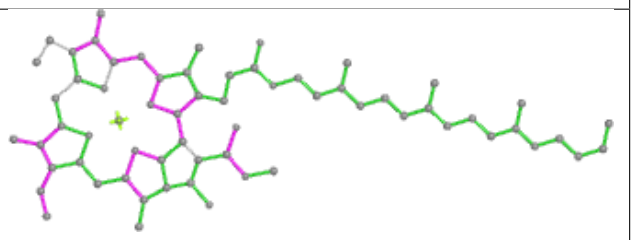


Rings

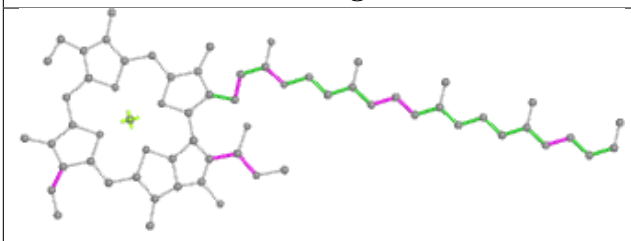
Ligand CLA a4 410



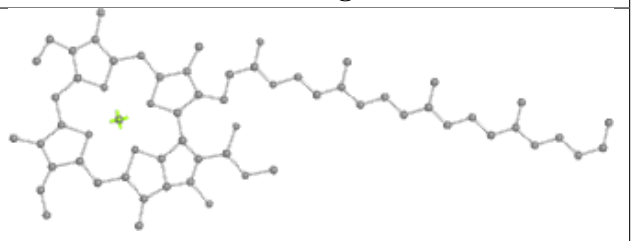
Bond lengths



Bond angles

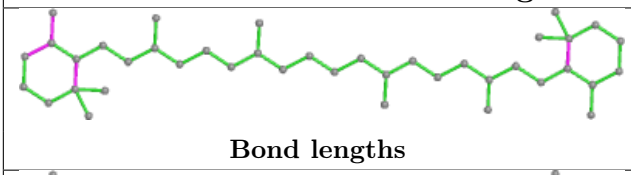


Torsions

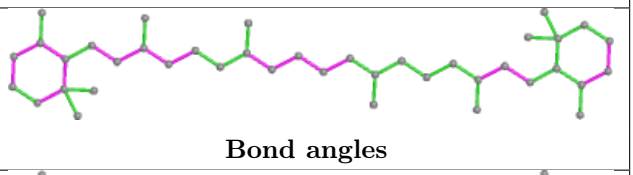


Rings

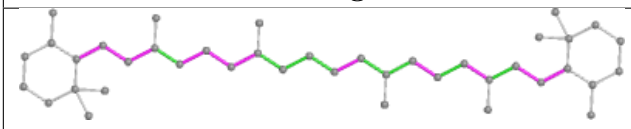
Ligand BCR b6 402



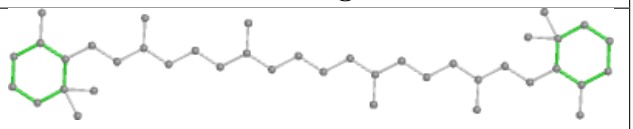
Bond lengths



Bond angles

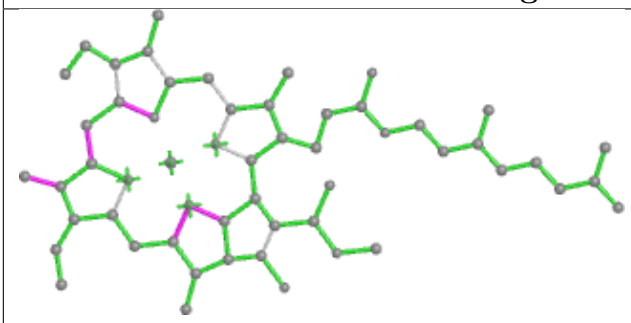


Torsions

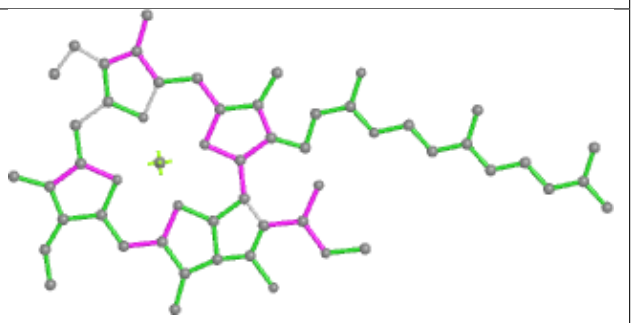


Rings

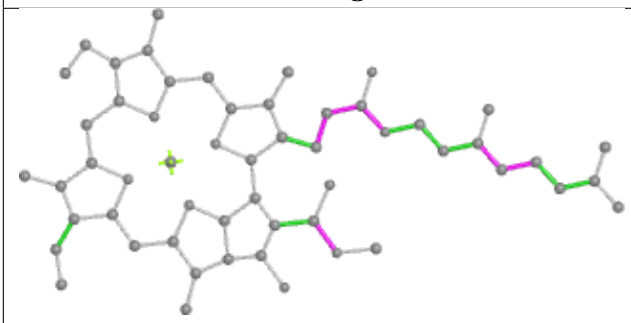
Ligand CLA c6 418



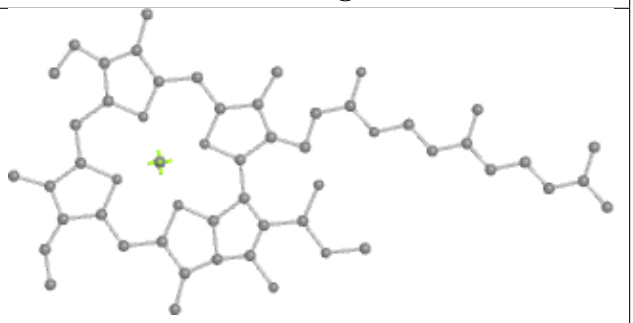
Bond lengths



Bond angles

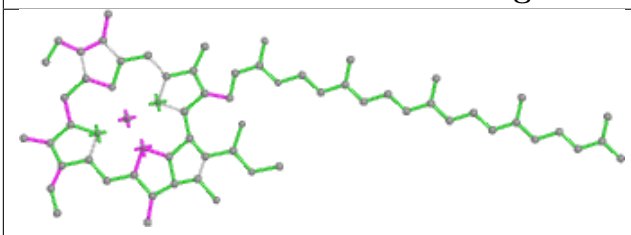


Torsions

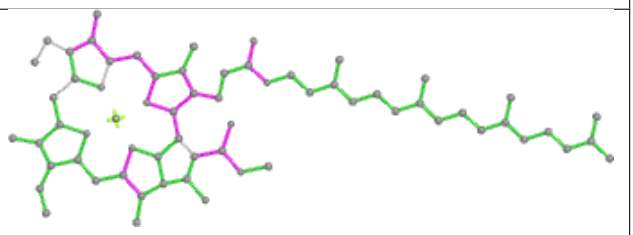


Rings

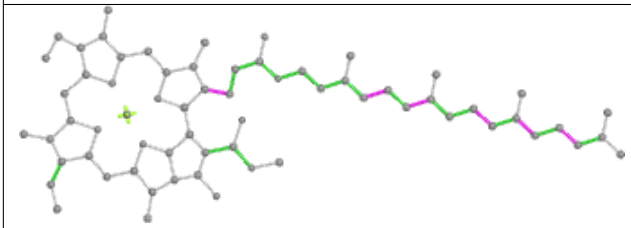
Ligand CLA bA 807



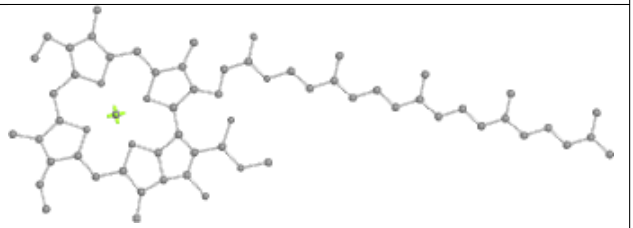
Bond lengths



Bond angles

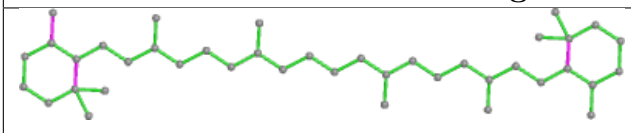


Torsions

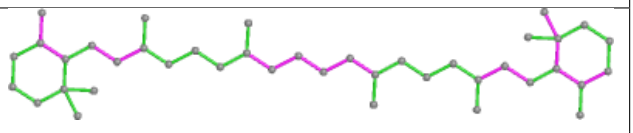


Rings

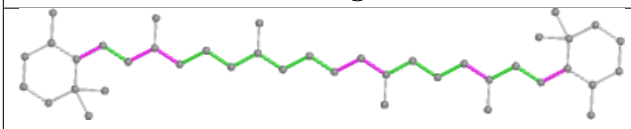
Ligand BCR aM 101



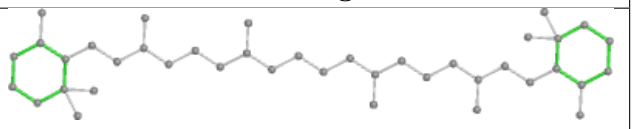
Bond lengths



Bond angles

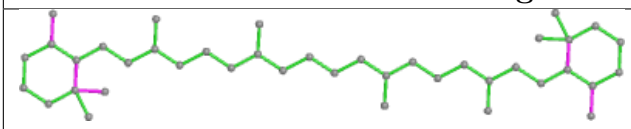


Torsions

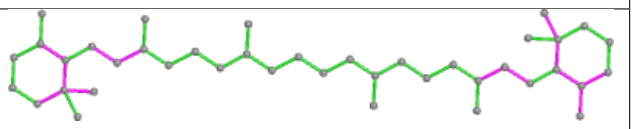


Rings

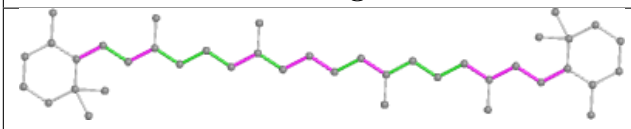
Ligand BCR cF 202



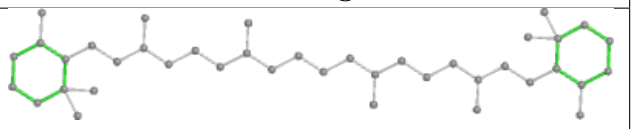
Bond lengths



Bond angles

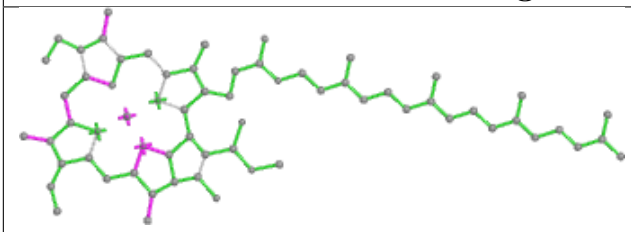


Torsions

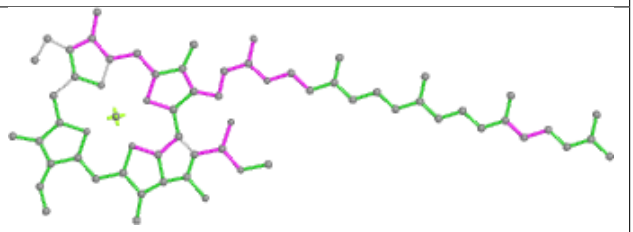


Rings

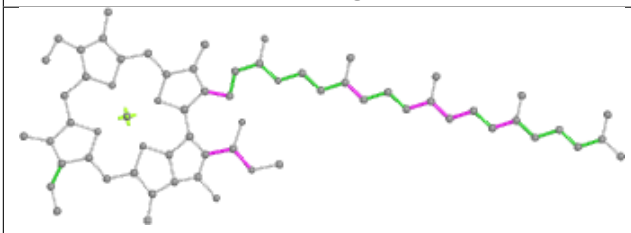
Ligand CLA cB 827



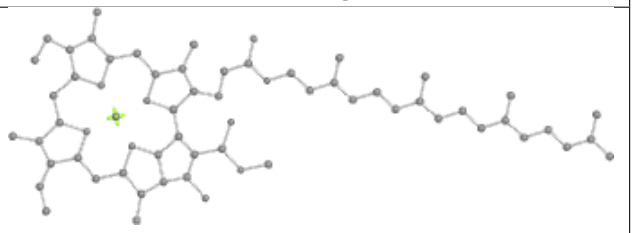
Bond lengths



Bond angles

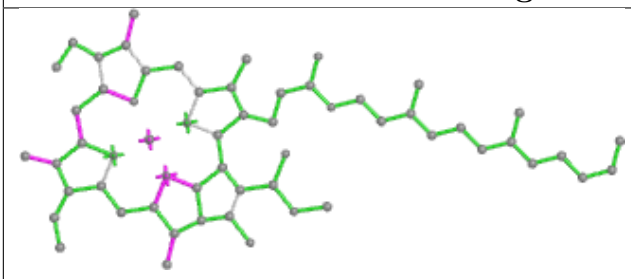


Torsions

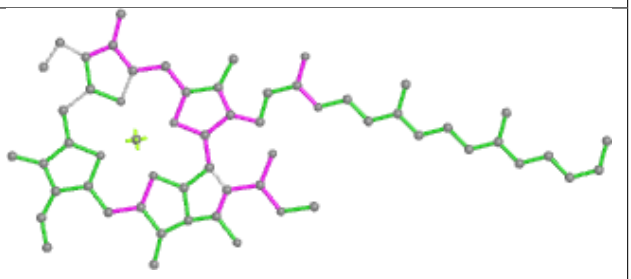


Rings

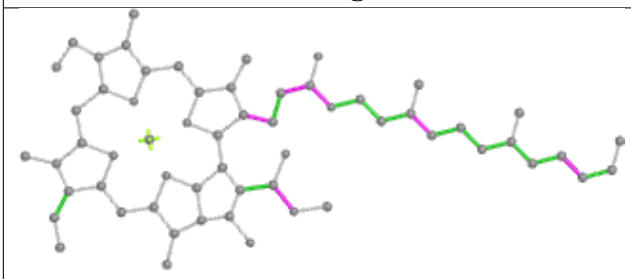
Ligand CLA aB 818



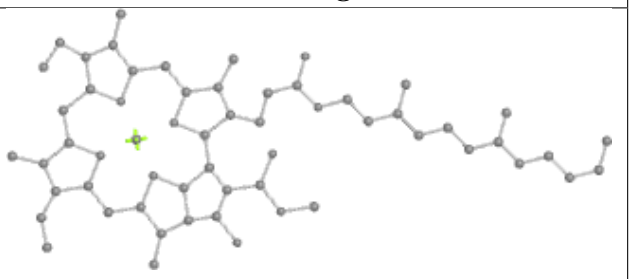
Bond lengths



Bond angles

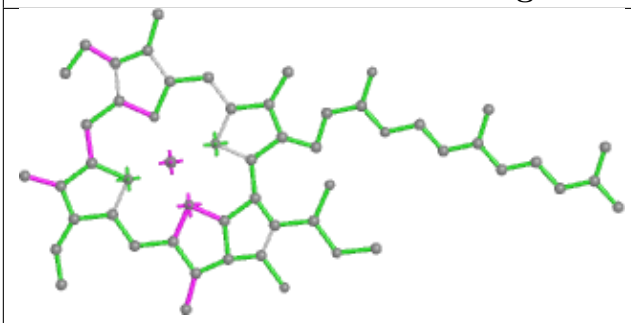


Torsions

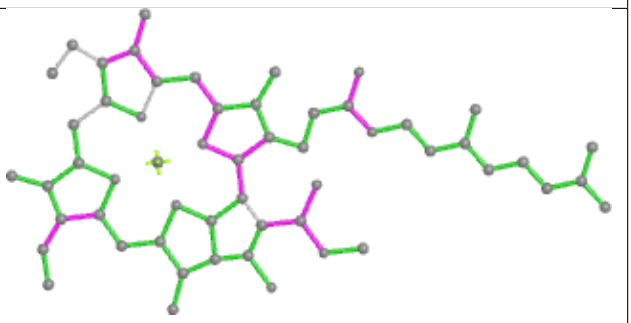


Rings

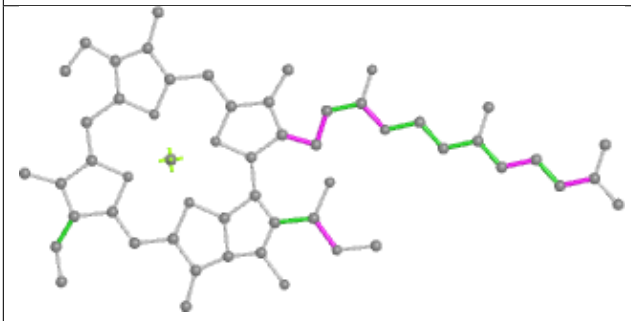
Ligand CLA cB 817



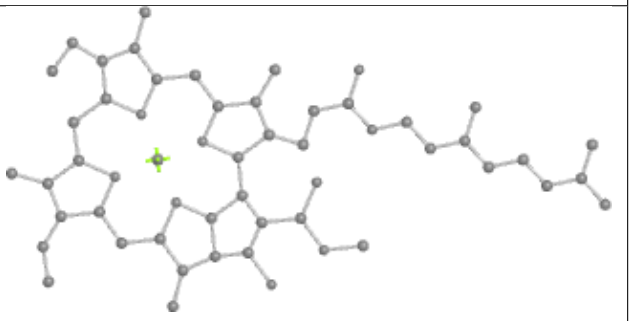
Bond lengths



Bond angles

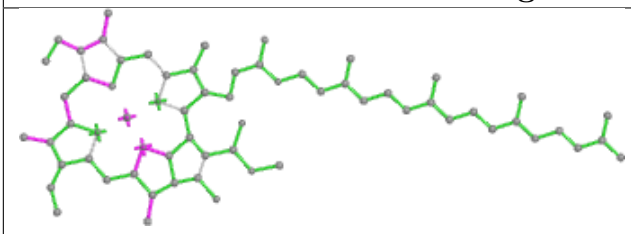


Torsions

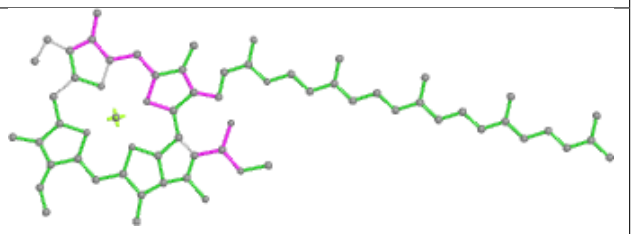


Rings

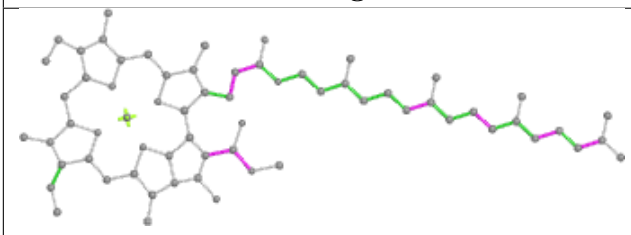
Ligand CLA aL 203



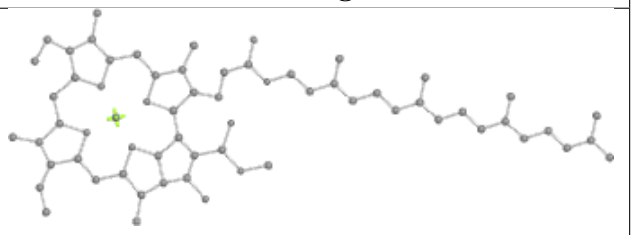
Bond lengths



Bond angles

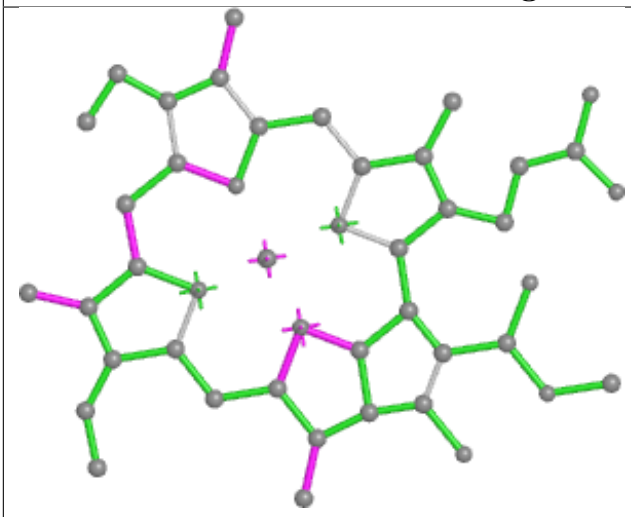


Torsions

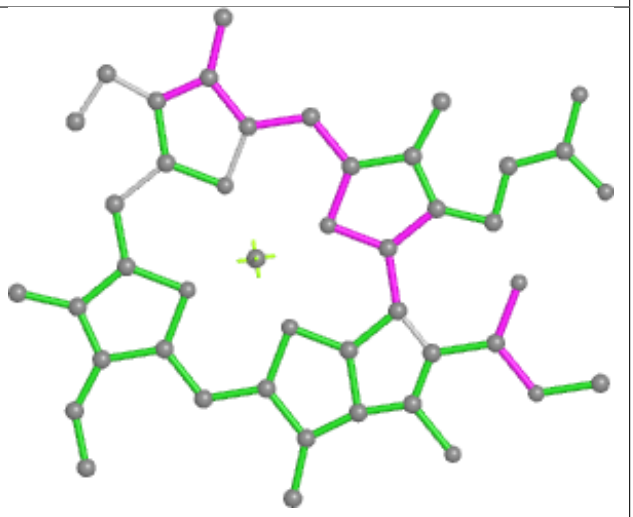


Rings

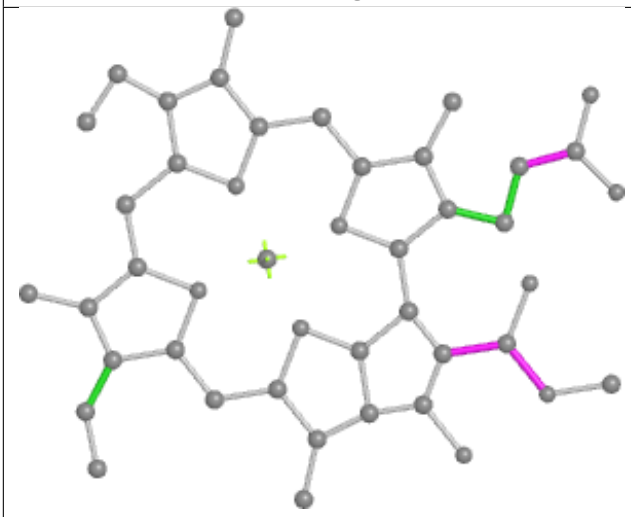
Ligand CLA c4 407



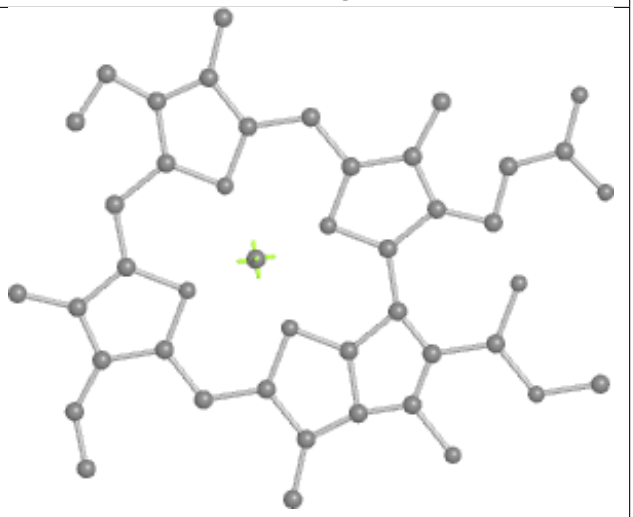
Bond lengths



Bond angles

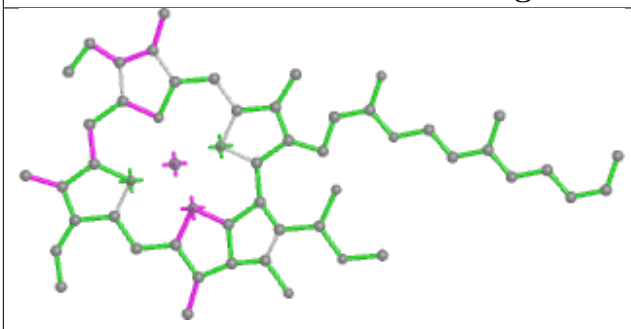


Torsions

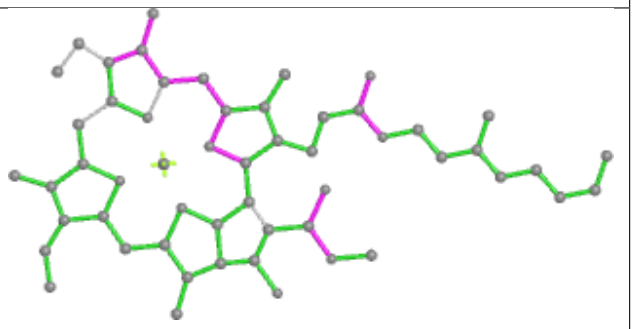


Rings

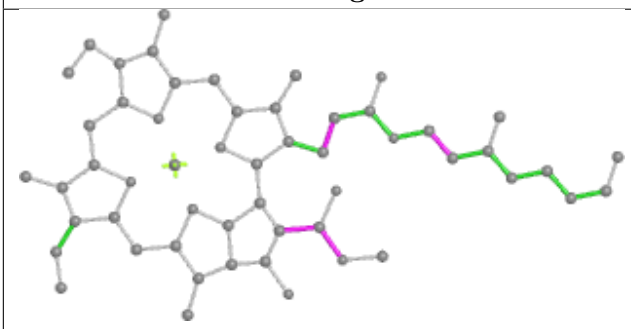
Ligand CLA bB 805



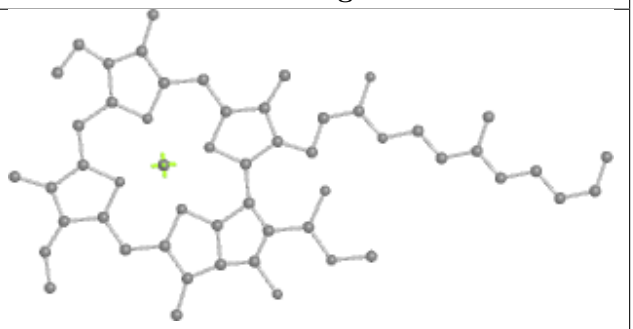
Bond lengths



Bond angles

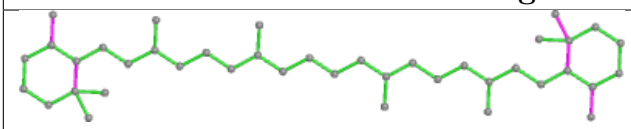


Torsions

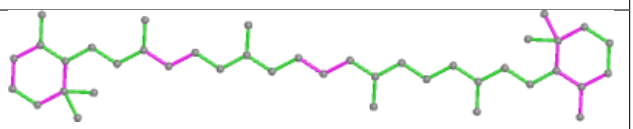


Rings

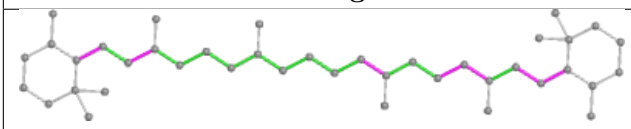
Ligand BCR c2 419



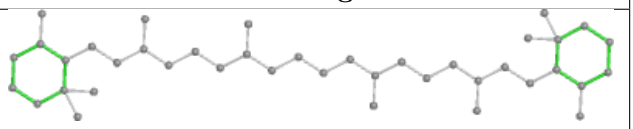
Bond lengths



Bond angles

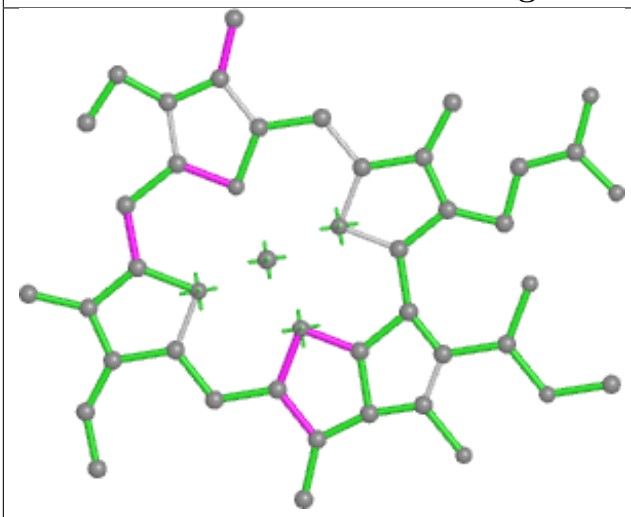


Torsions

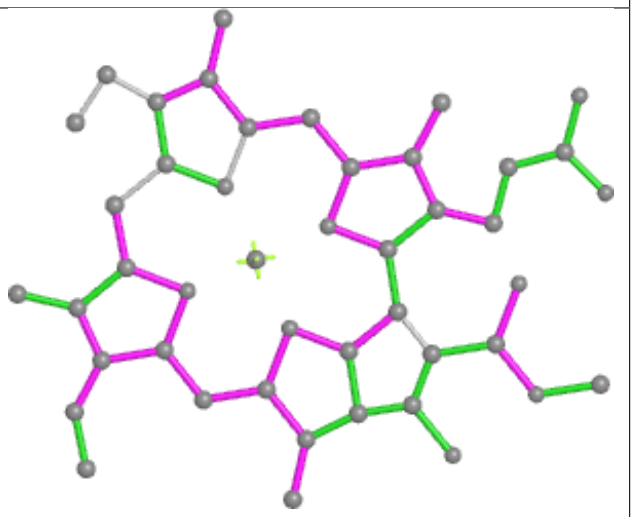


Rings

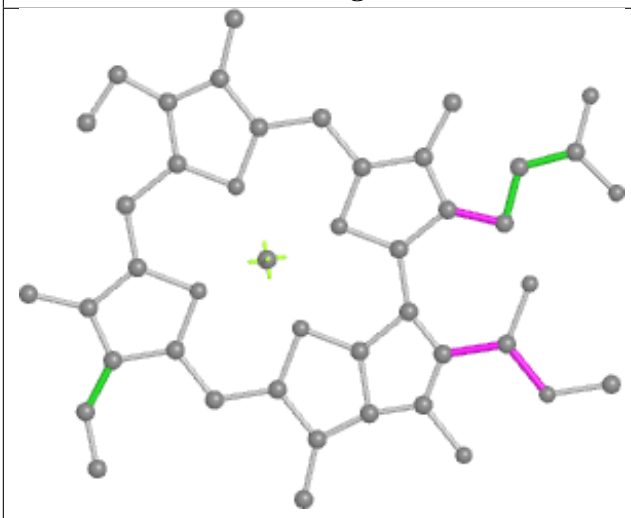
Ligand CLA b2 405



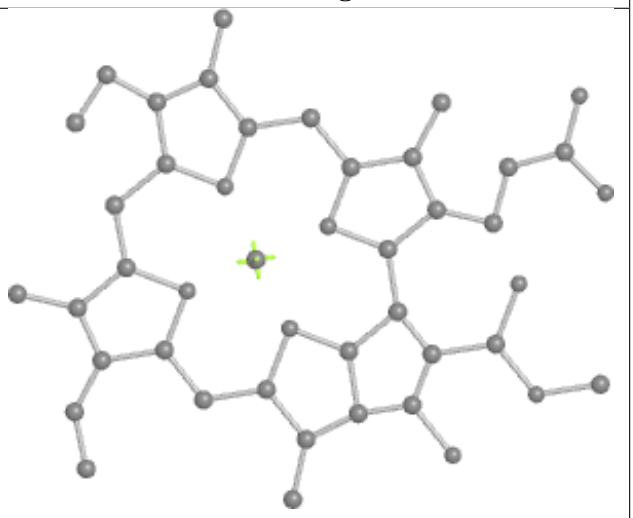
Bond lengths



Bond angles

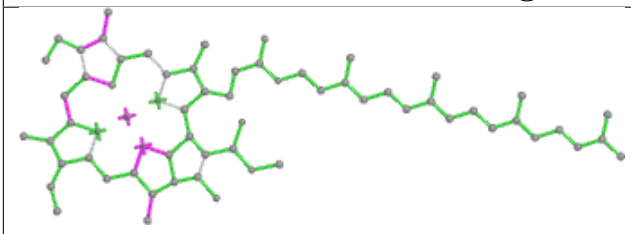


Torsions

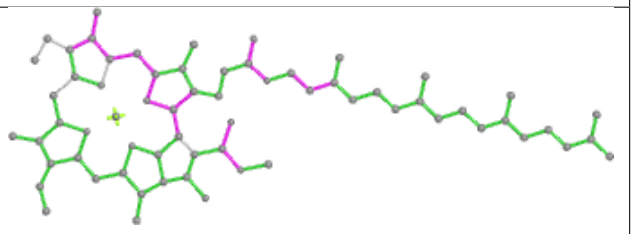


Rings

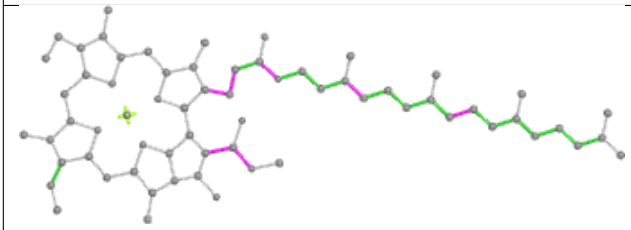
Ligand CLA b3 404



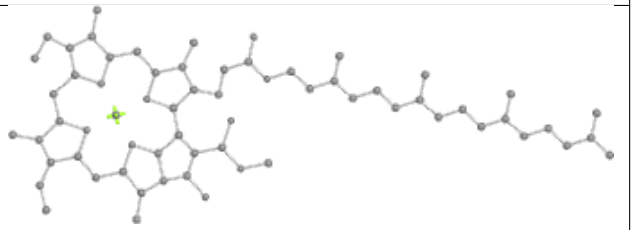
Bond lengths



Bond angles

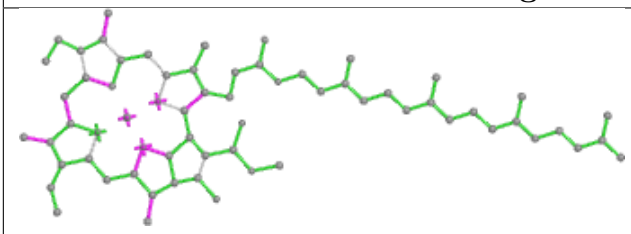


Torsions

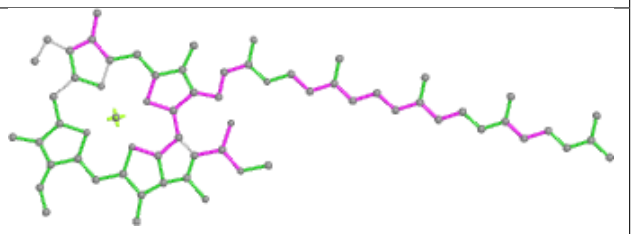


Rings

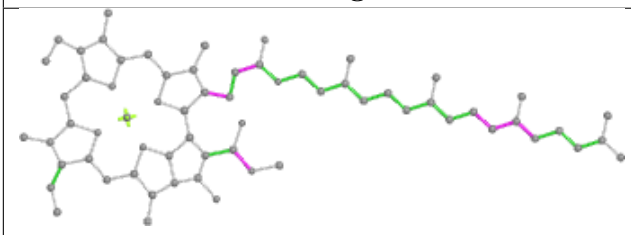
Ligand CLA a3 421



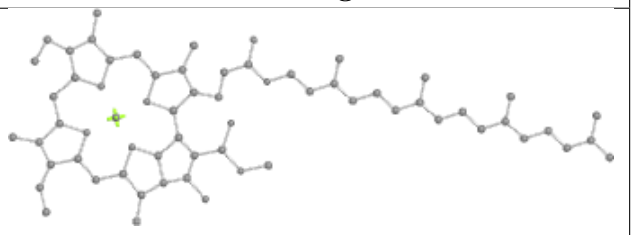
Bond lengths



Bond angles

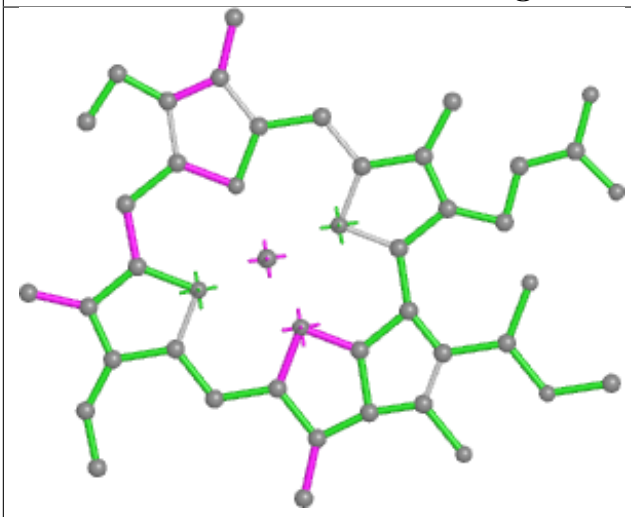


Torsions

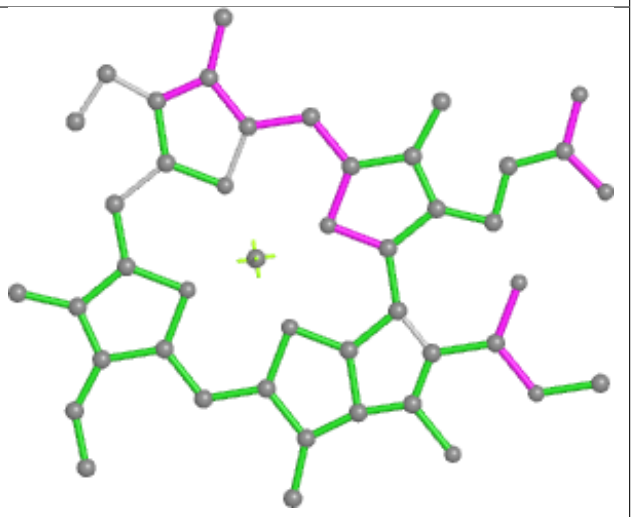


Rings

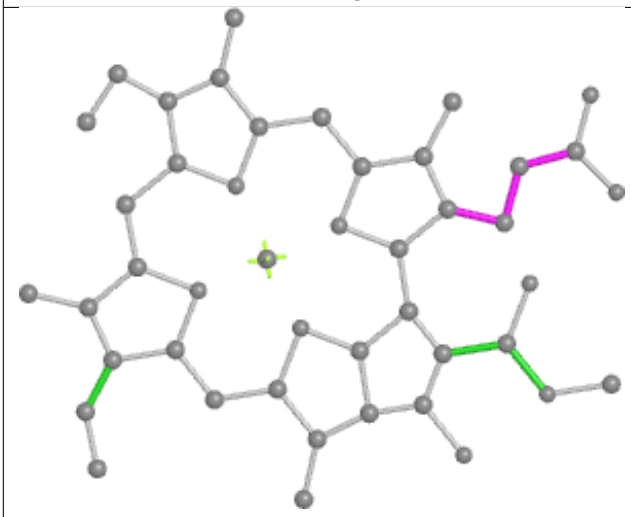
Ligand CLA bB 813



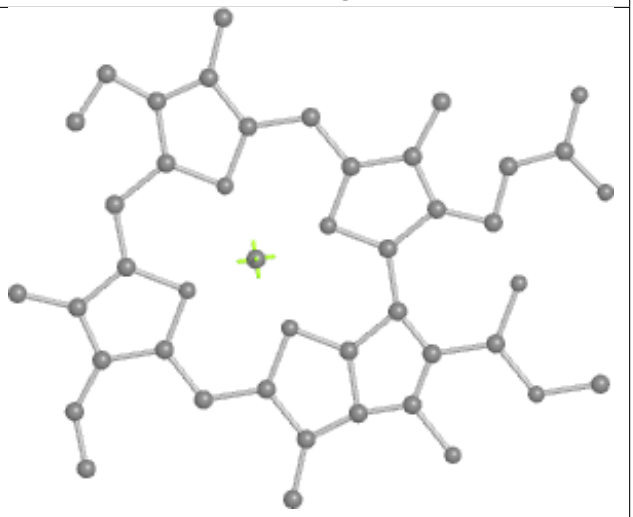
Bond lengths



Bond angles

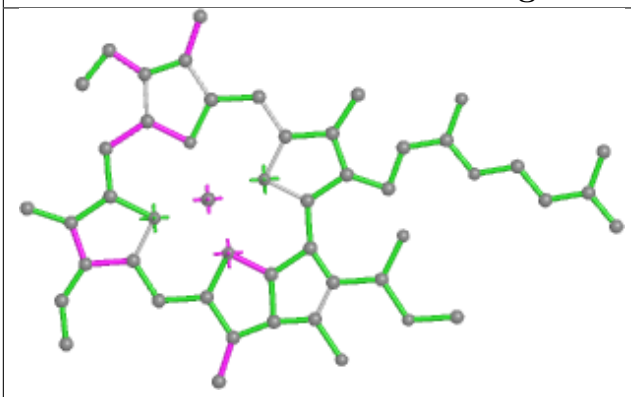


Torsions

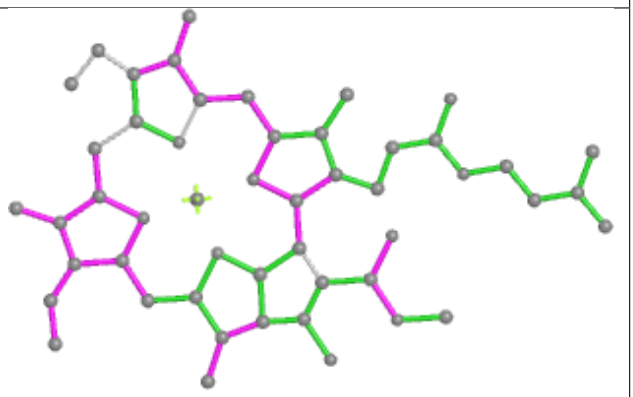


Rings

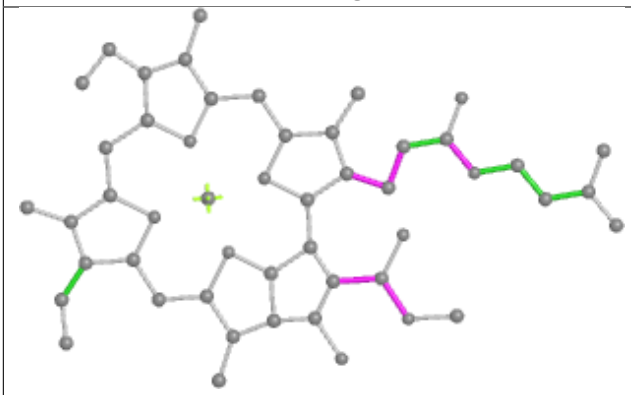
Ligand CLA b4 416



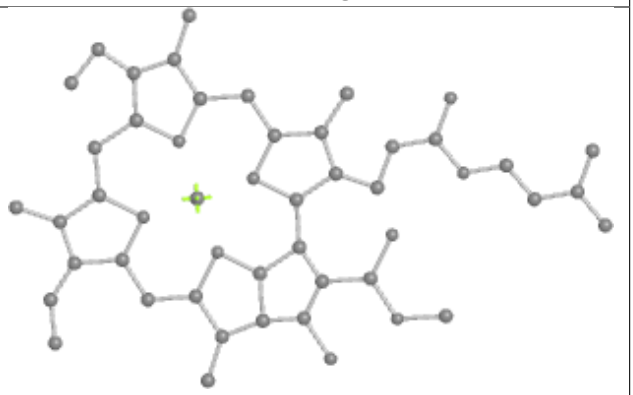
Bond lengths



Bond angles

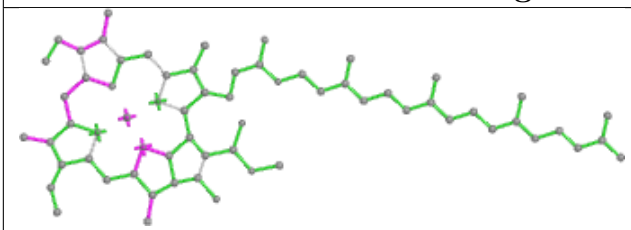


Torsions

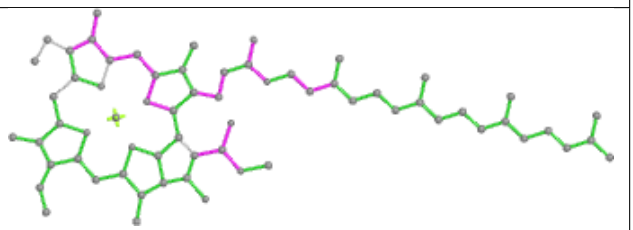


Rings

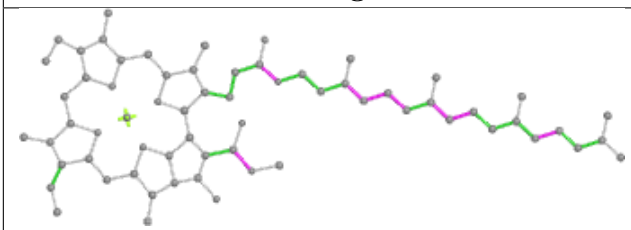
Ligand CLA bB 809



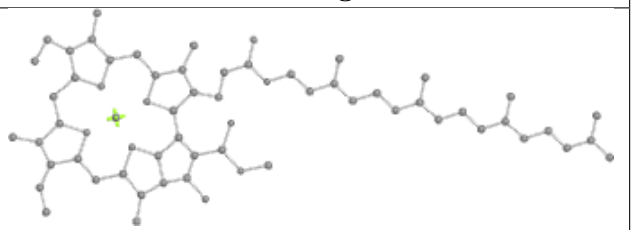
Bond lengths



Bond angles

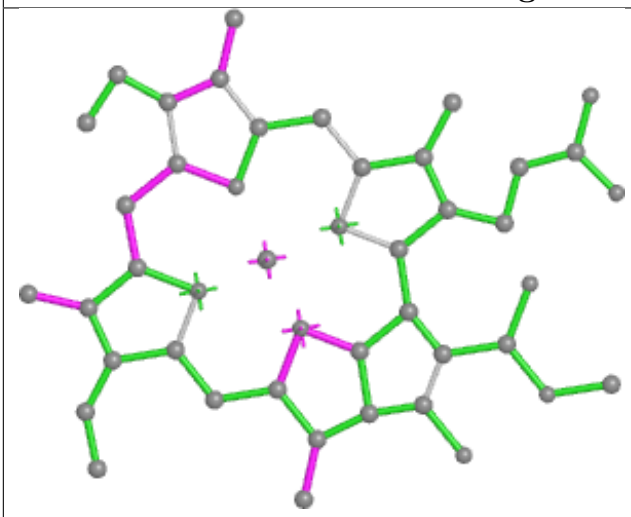


Torsions

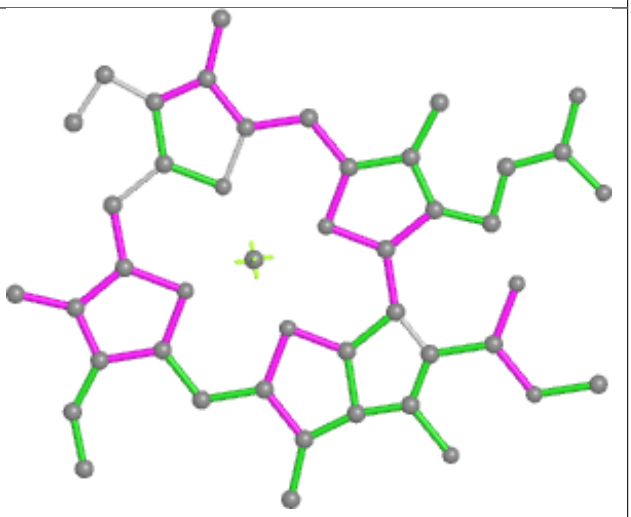


Rings

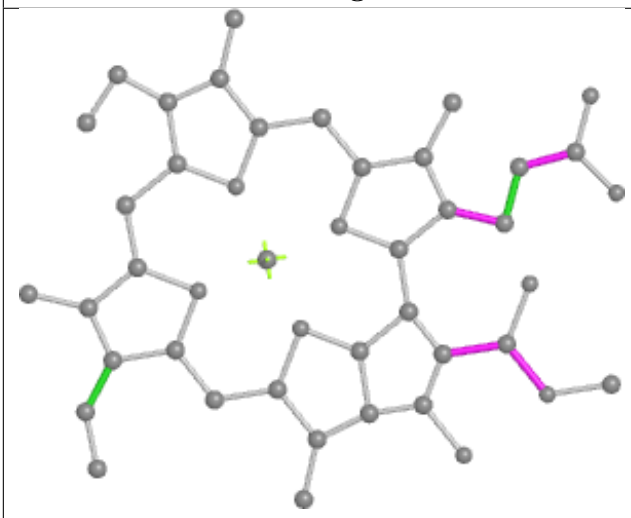
Ligand CLA b1 412



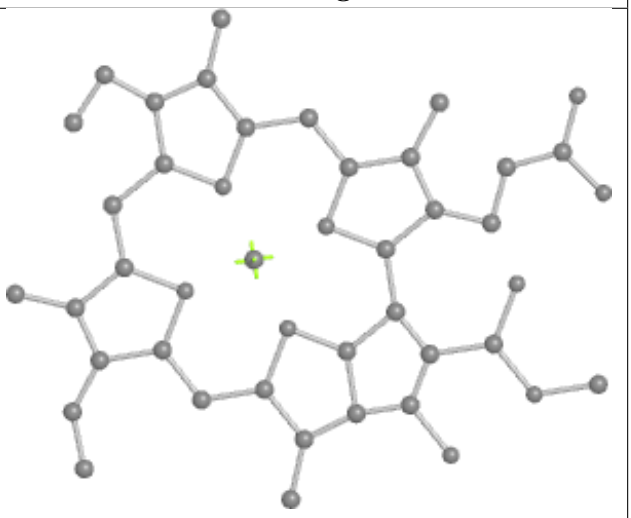
Bond lengths



Bond angles

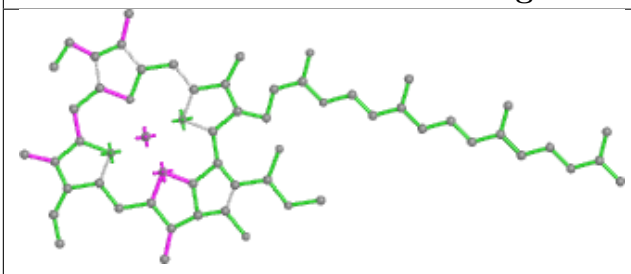


Torsions

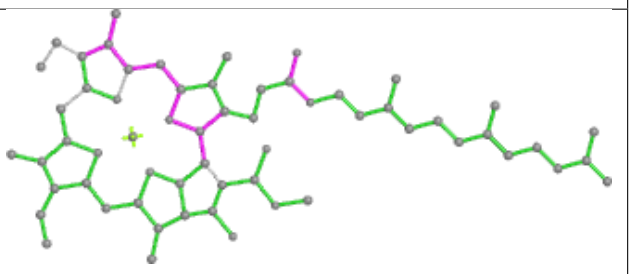


Rings

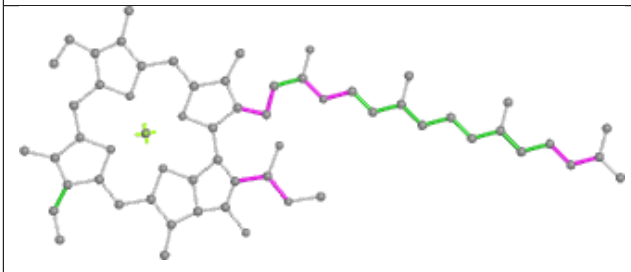
Ligand CLA cA 814



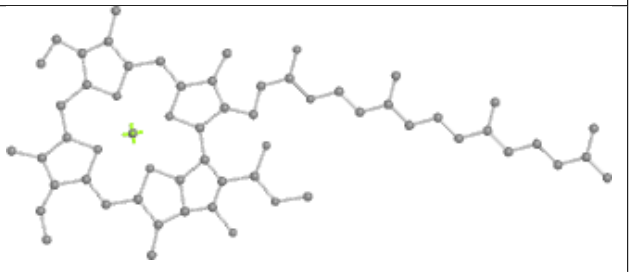
Bond lengths



Bond angles

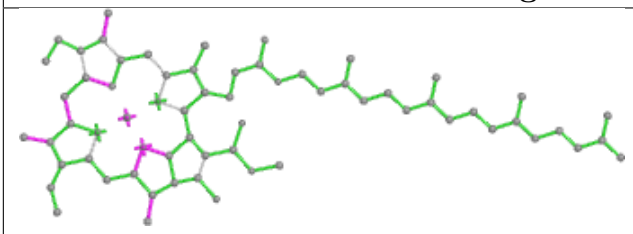


Torsions

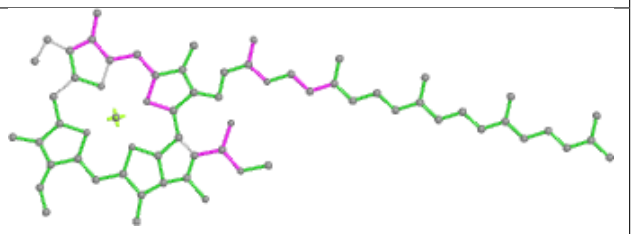


Rings

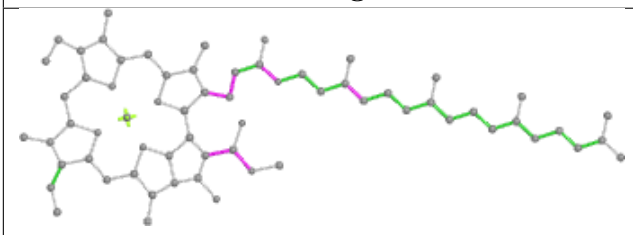
Ligand CLA a2 404



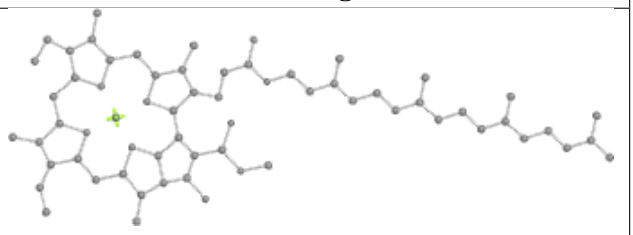
Bond lengths



Bond angles

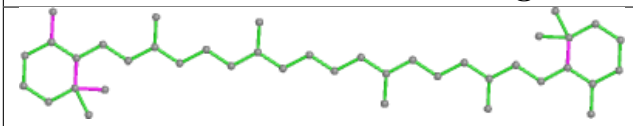


Torsions

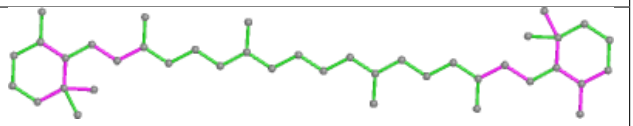


Rings

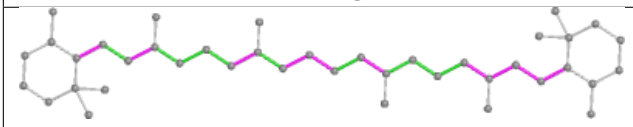
Ligand BCR aF 201



Bond lengths



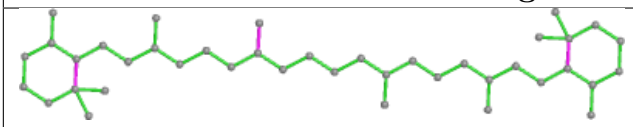
Bond angles



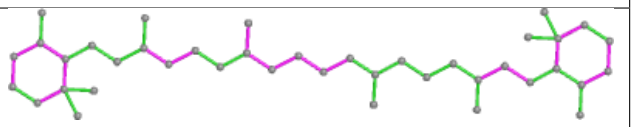
Torsions

Rings

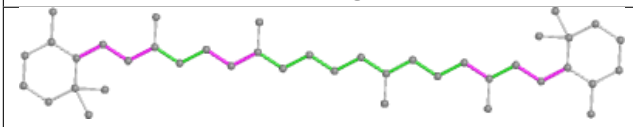
Ligand BCR c1 420



Bond lengths



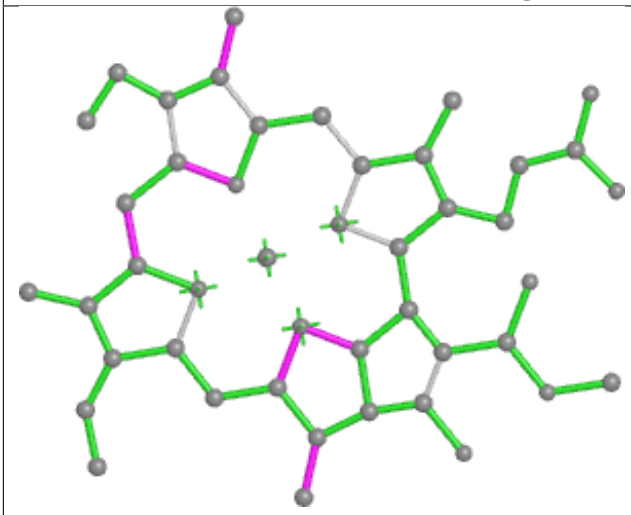
Bond angles



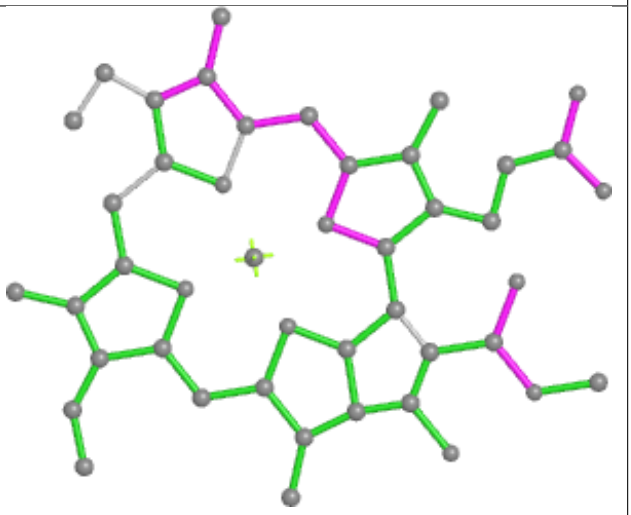
Torsions

Rings

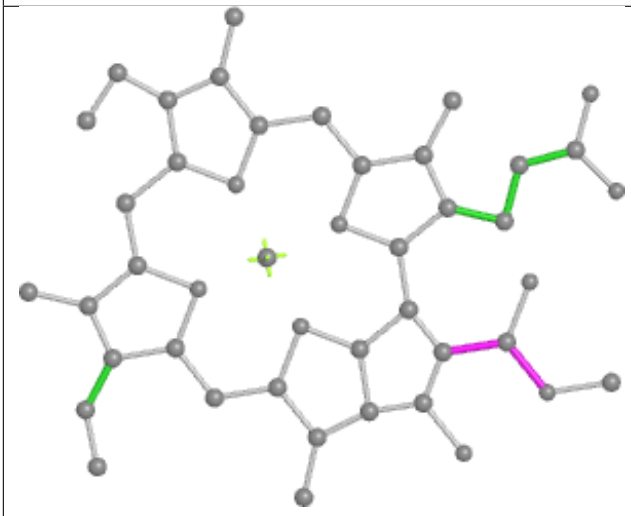
Ligand CLA b2 407



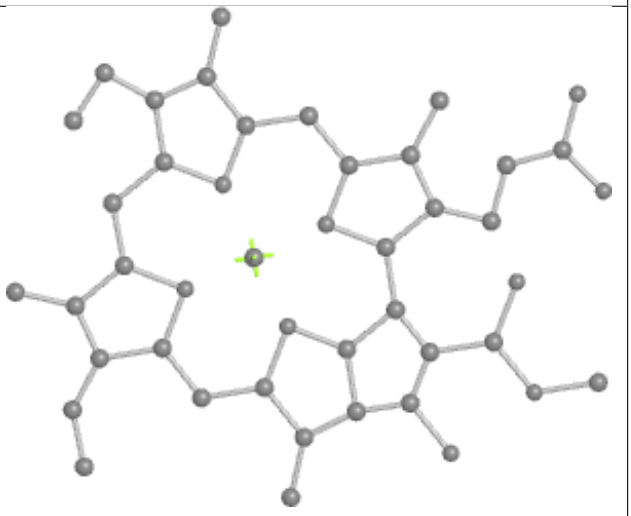
Bond lengths



Bond angles

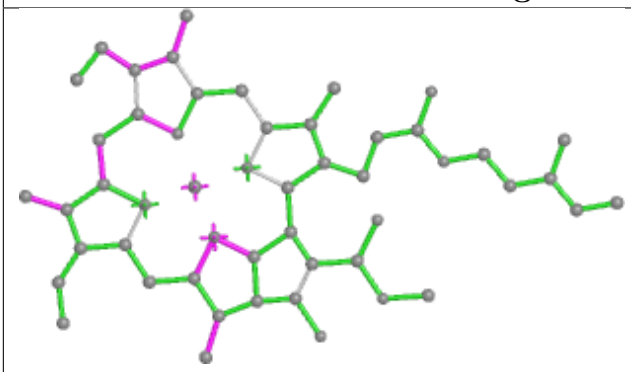


Torsions

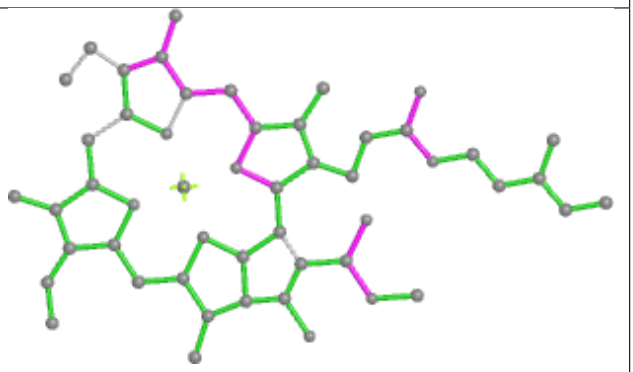


Rings

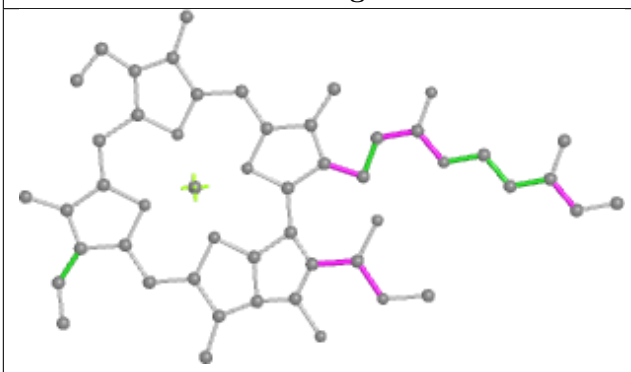
Ligand CLA bA 824



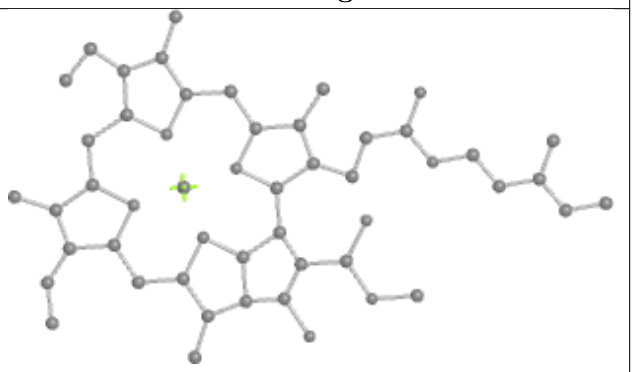
Bond lengths



Bond angles

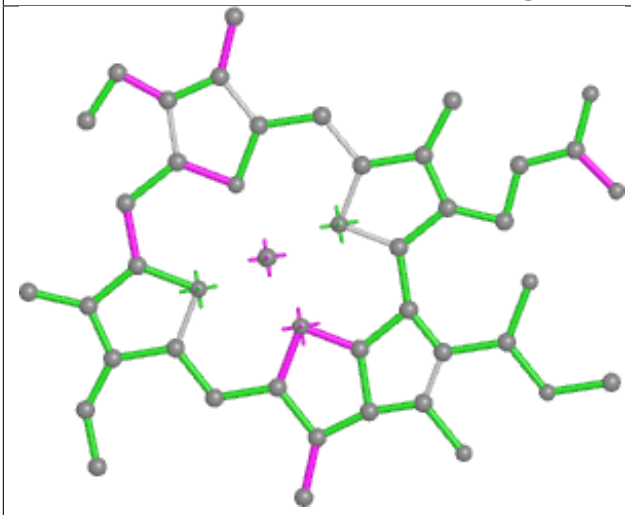


Torsions

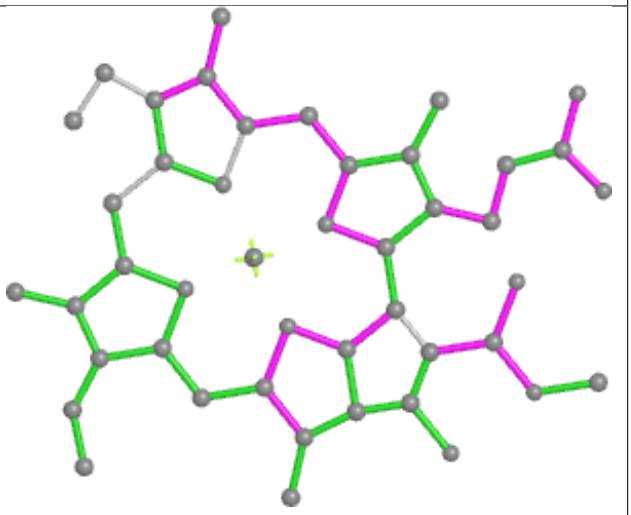


Rings

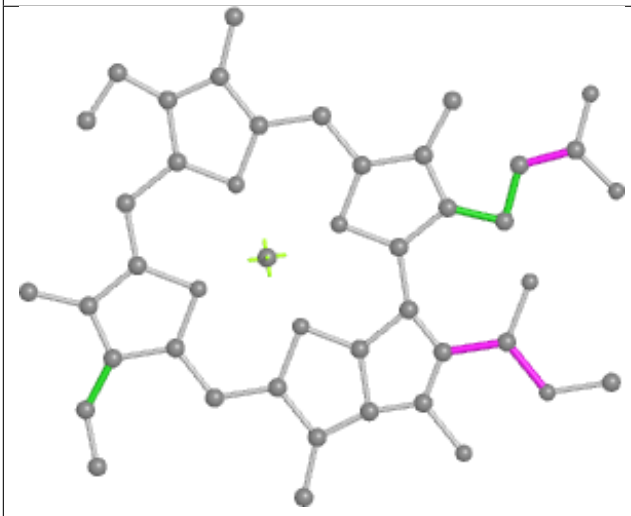
Ligand CLA a5 415



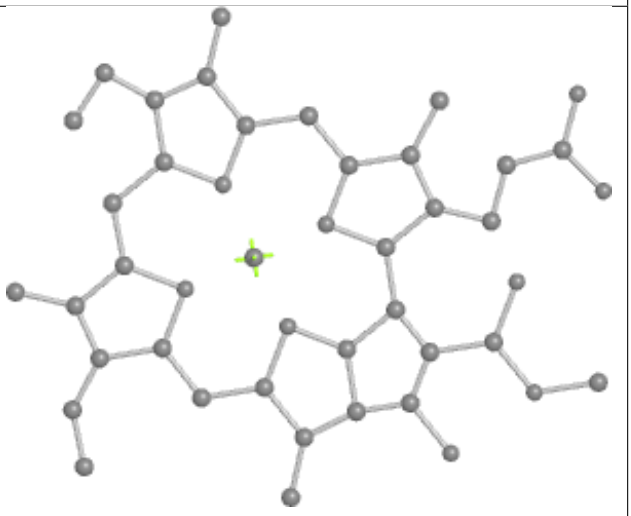
Bond lengths



Bond angles

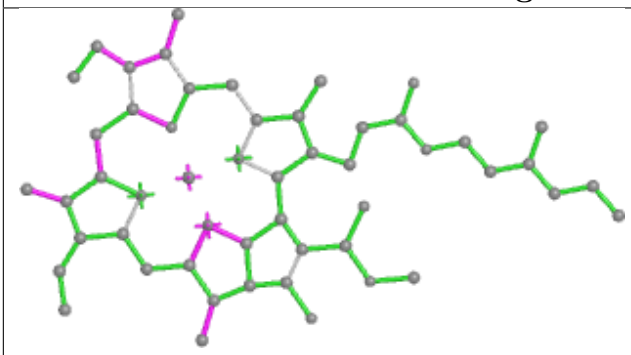


Torsions

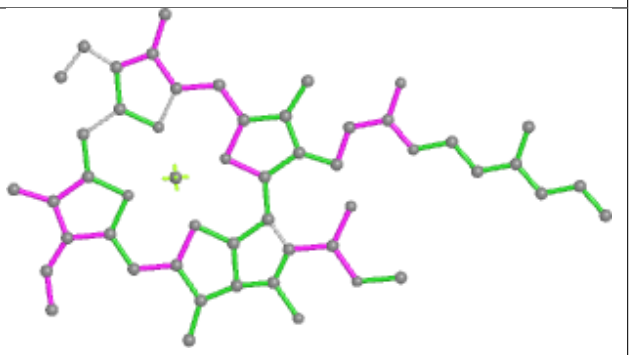


Rings

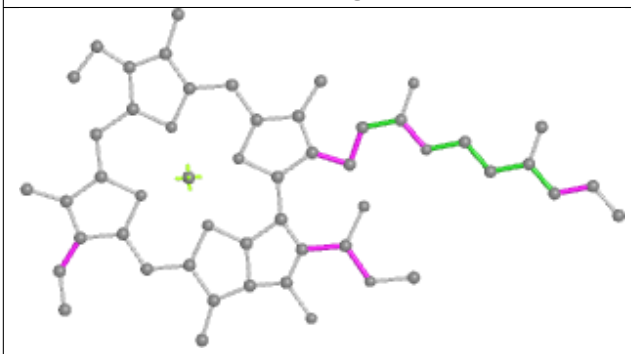
Ligand CLA cA 844



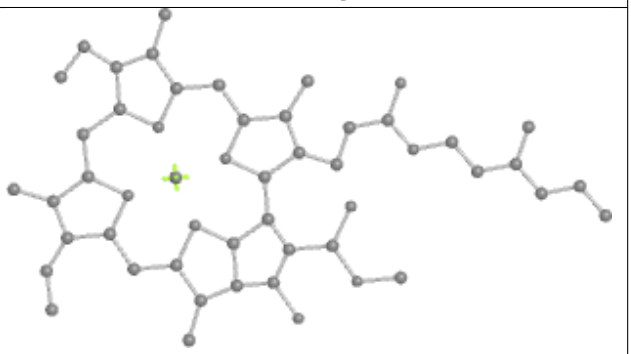
Bond lengths



Bond angles

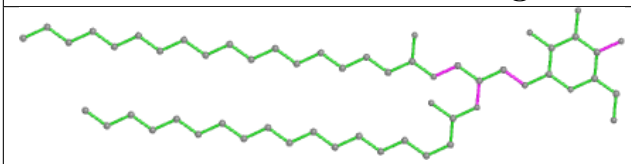


Torsions

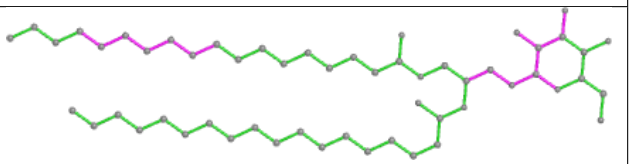


Rings

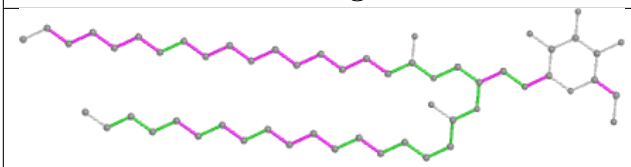
Ligand LMG aB 850



Bond lengths



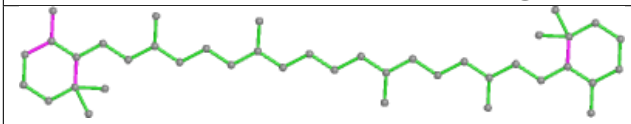
Bond angles



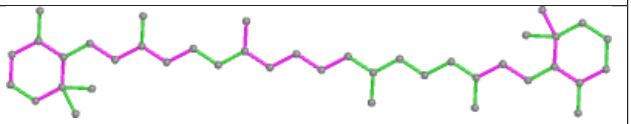
Torsions

Rings

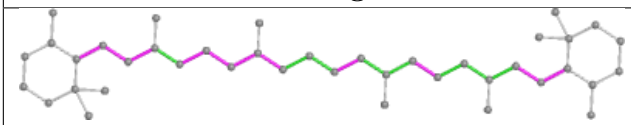
Ligand BCR b5 401



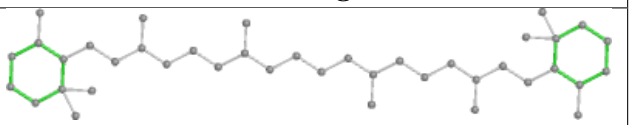
Bond lengths



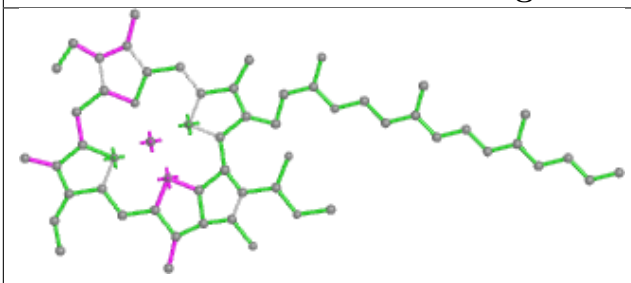
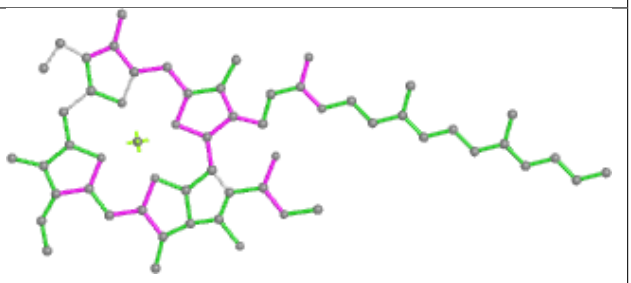
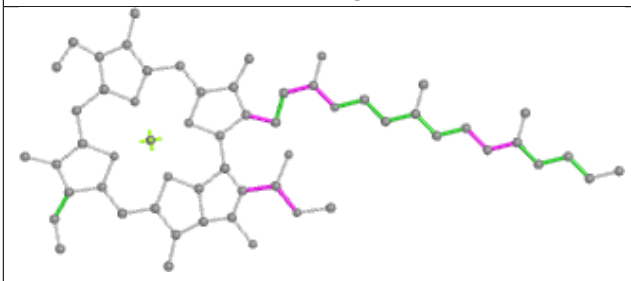
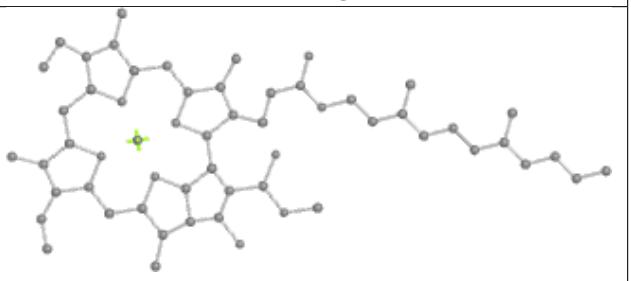
Bond angles



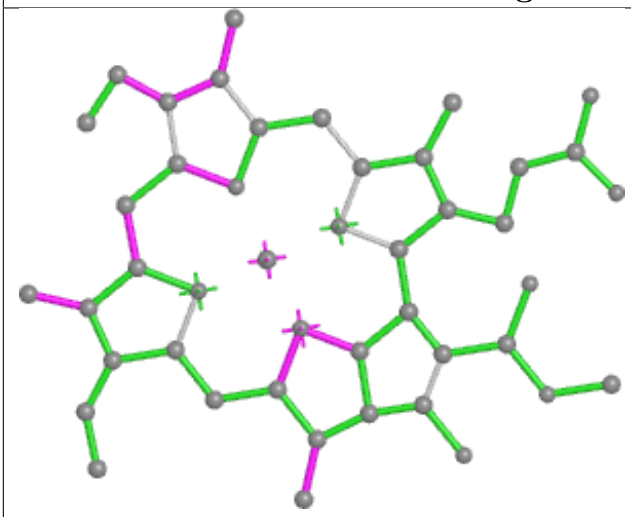
Torsions



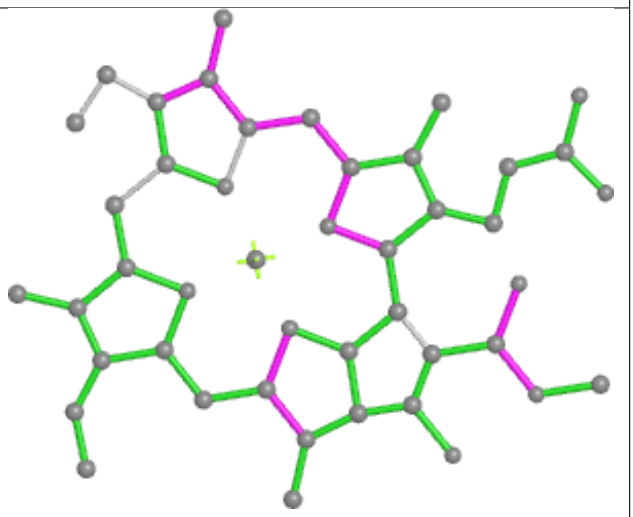
Rings

Ligand CLA aB 834	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

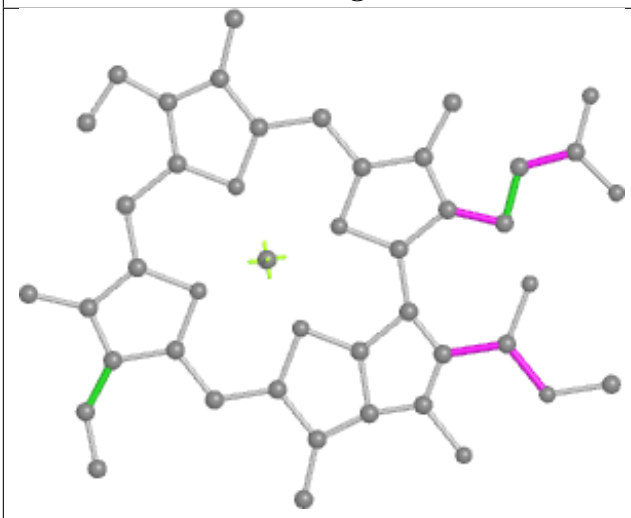
Ligand CLA cA 811



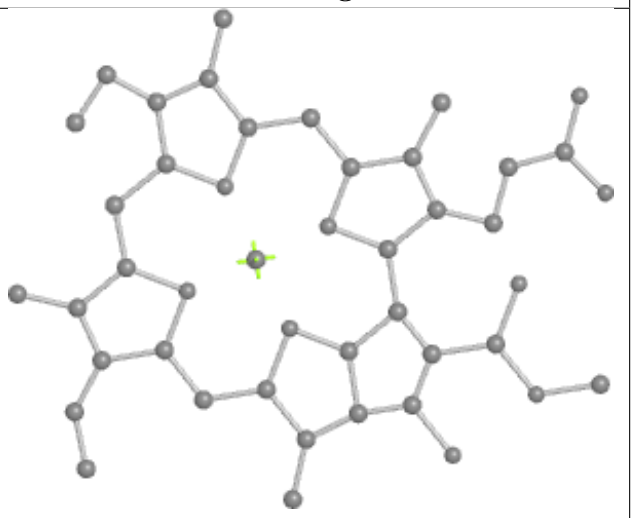
Bond lengths



Bond angles

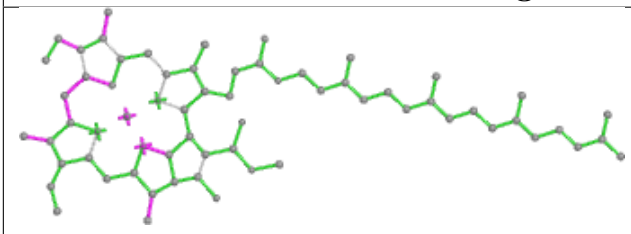


Torsions

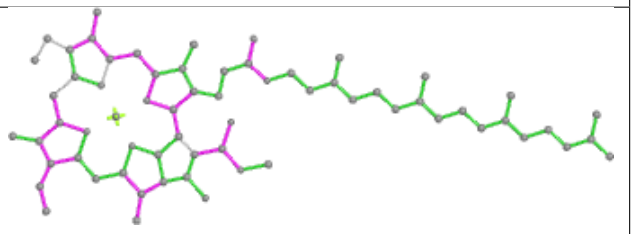


Rings

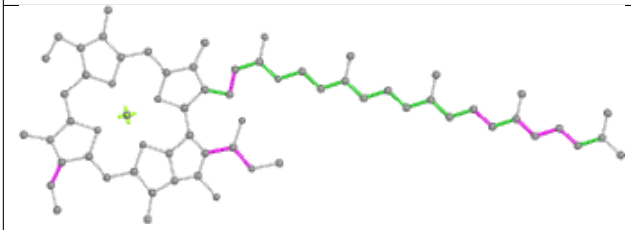
Ligand CLA aB 804



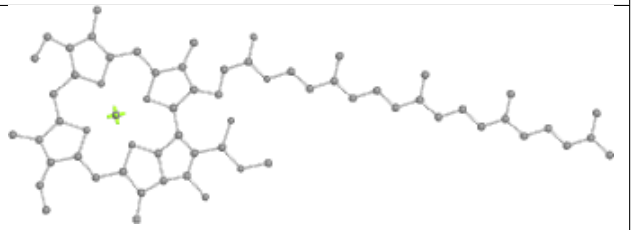
Bond lengths



Bond angles

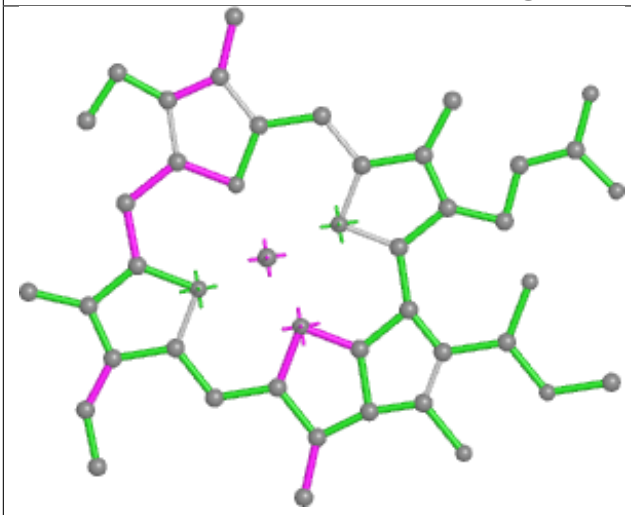


Torsions

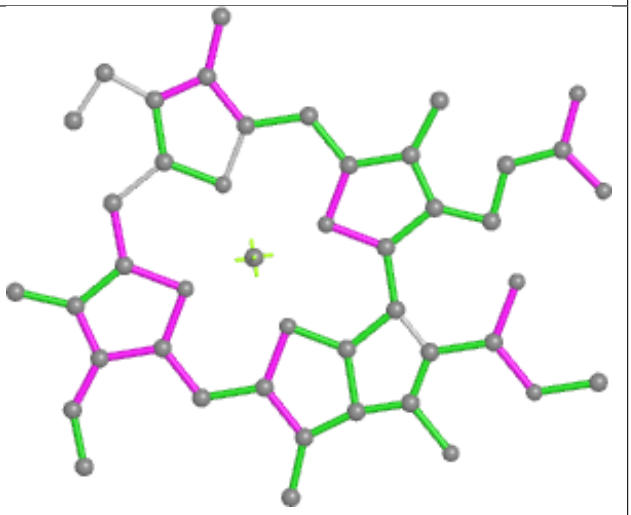


Rings

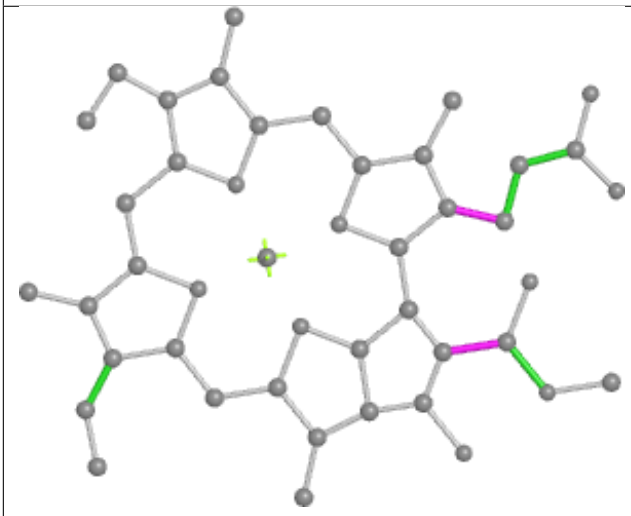
Ligand CLA a6 414



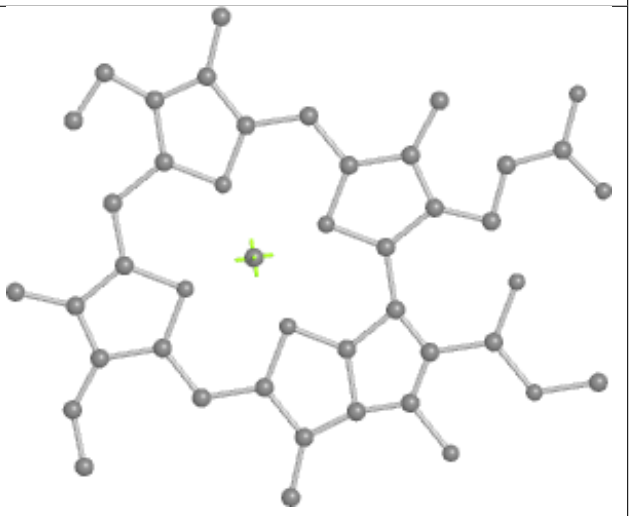
Bond lengths



Bond angles

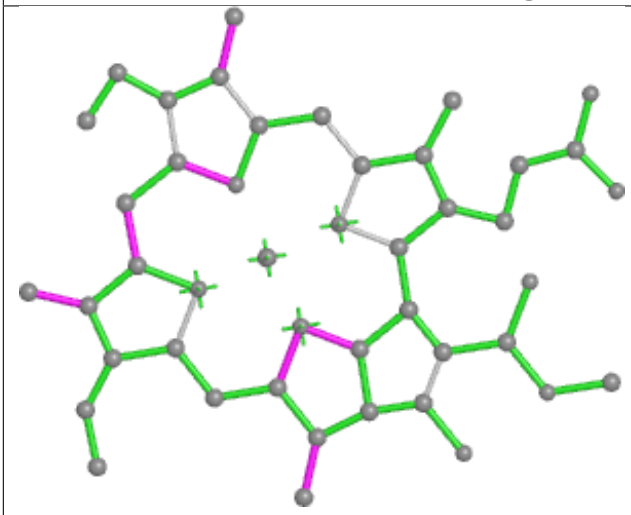


Torsions

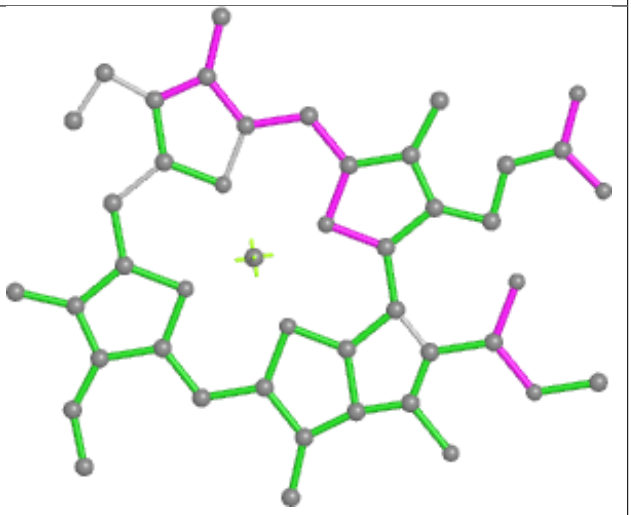


Rings

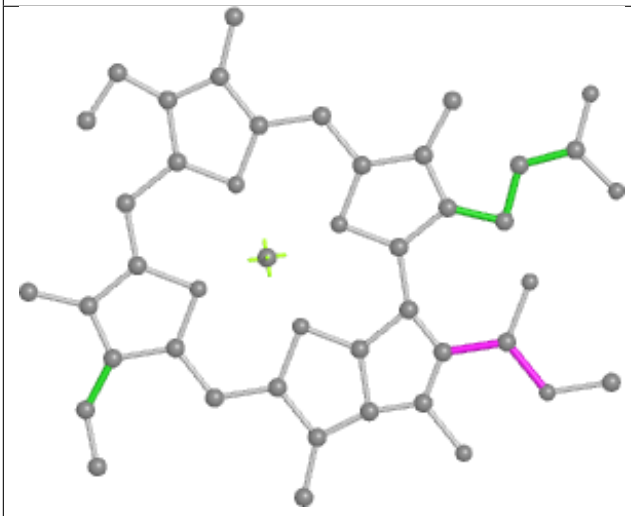
Ligand CLA c1 406



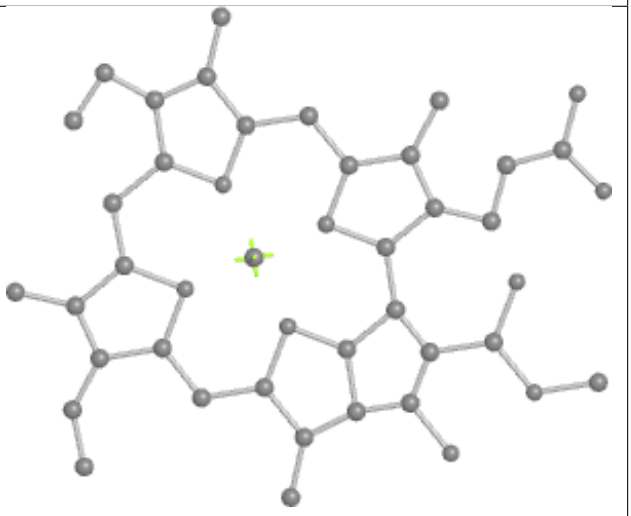
Bond lengths



Bond angles

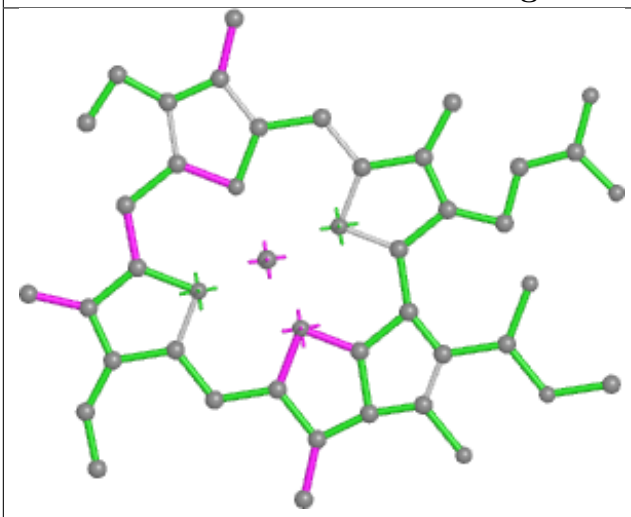


Torsions

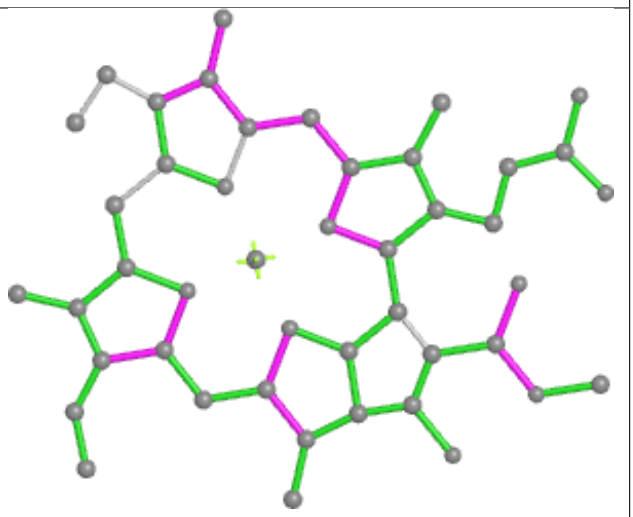


Rings

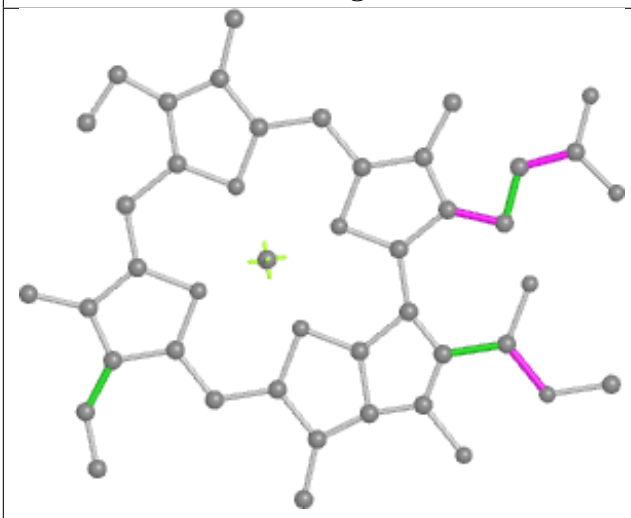
Ligand CLA c1 408



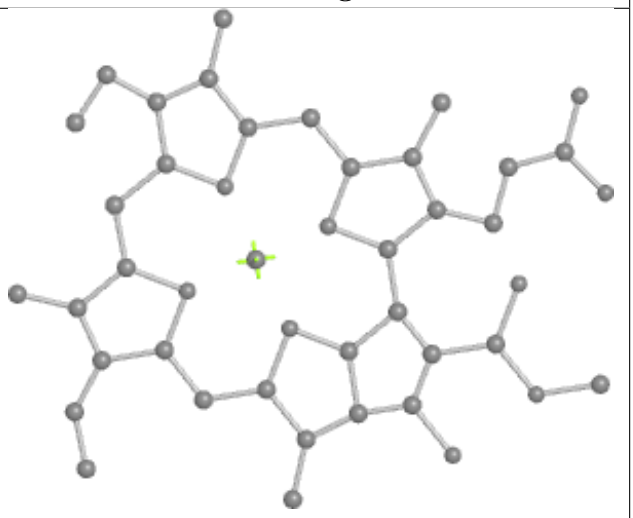
Bond lengths



Bond angles

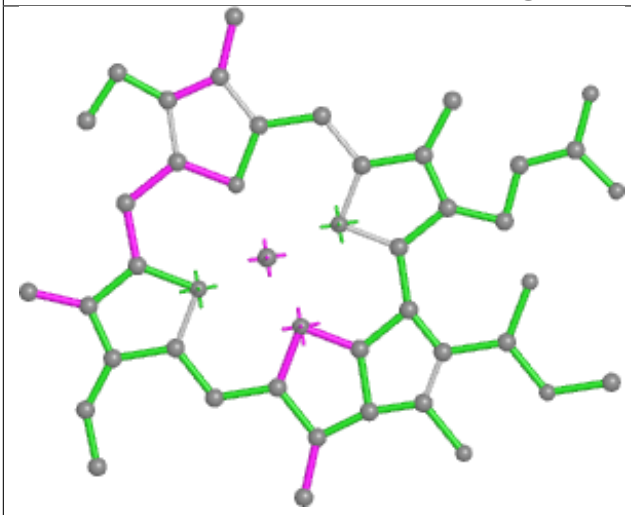


Torsions

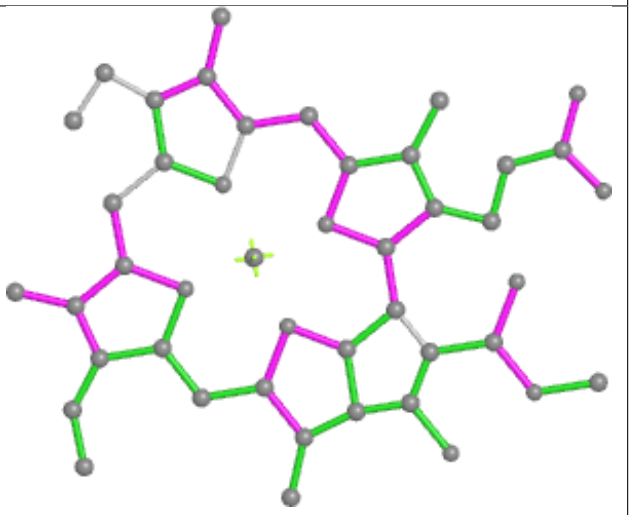


Rings

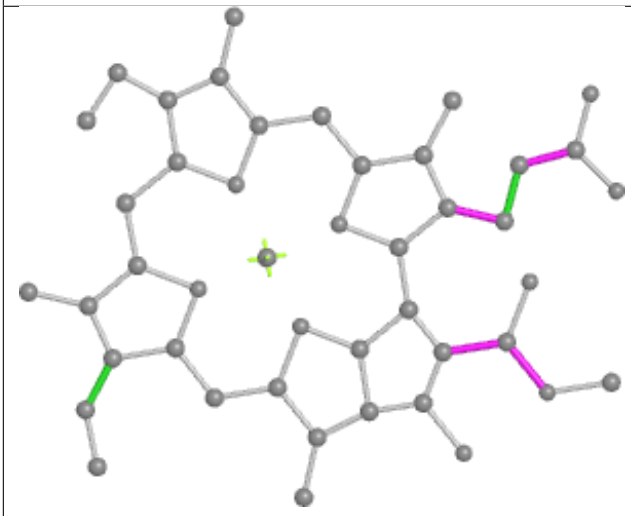
Ligand CLA a6 413



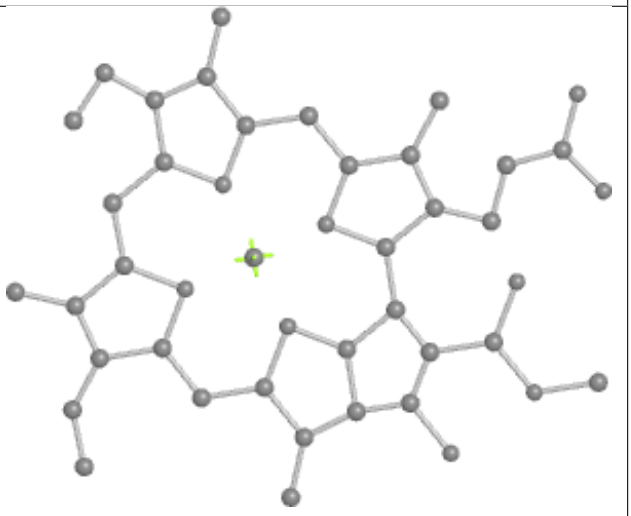
Bond lengths



Bond angles

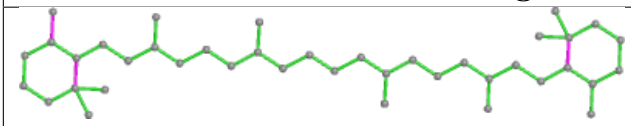


Torsions

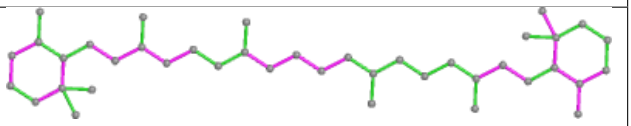


Rings

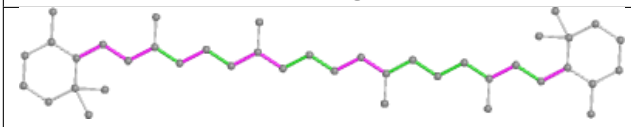
Ligand BCR bL 201



Bond lengths



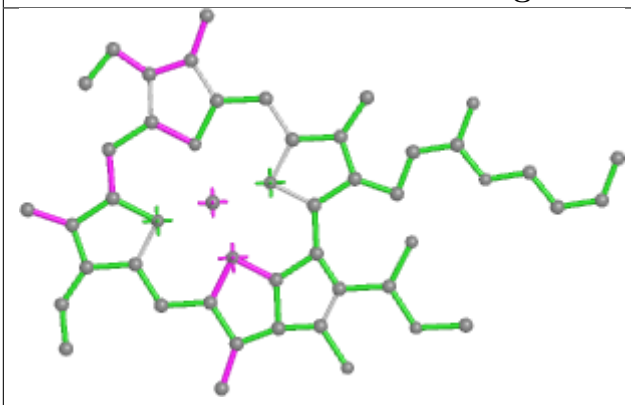
Bond angles



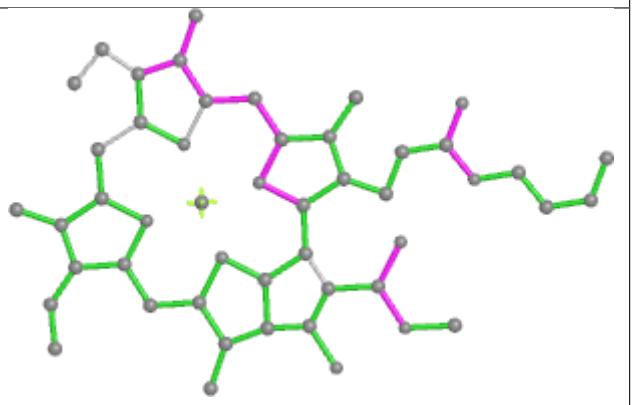
Torsions

Rings

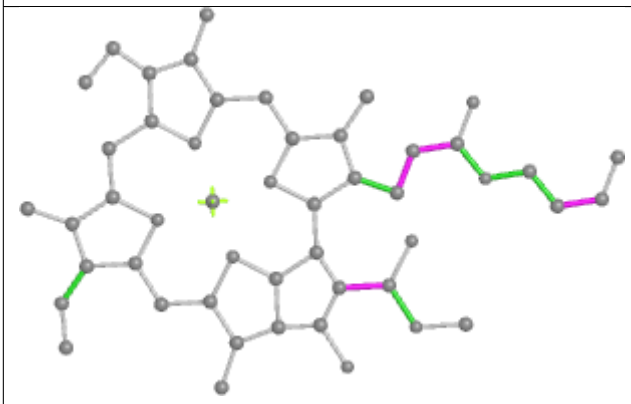
Ligand CLA bA 823



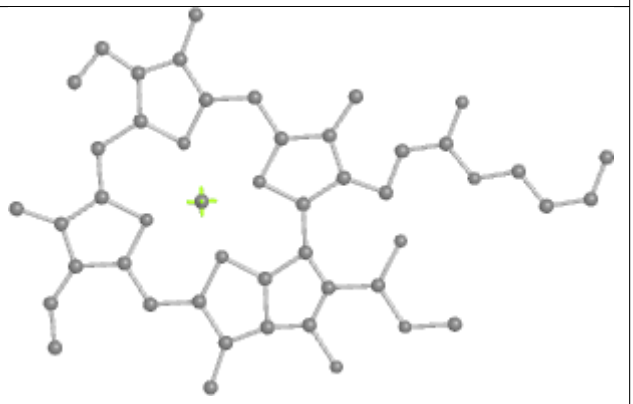
Bond lengths



Bond angles

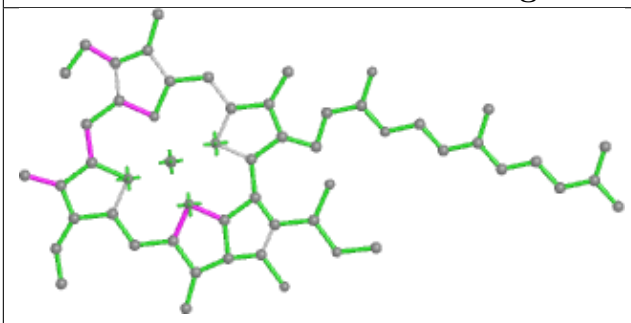


Torsions

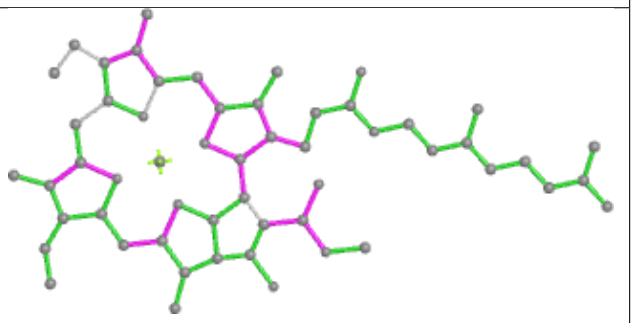


Rings

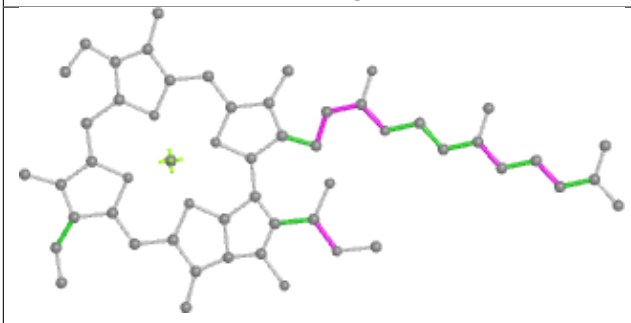
Ligand CLA a2 418



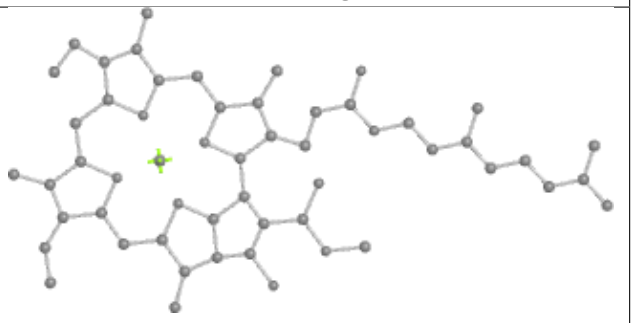
Bond lengths



Bond angles

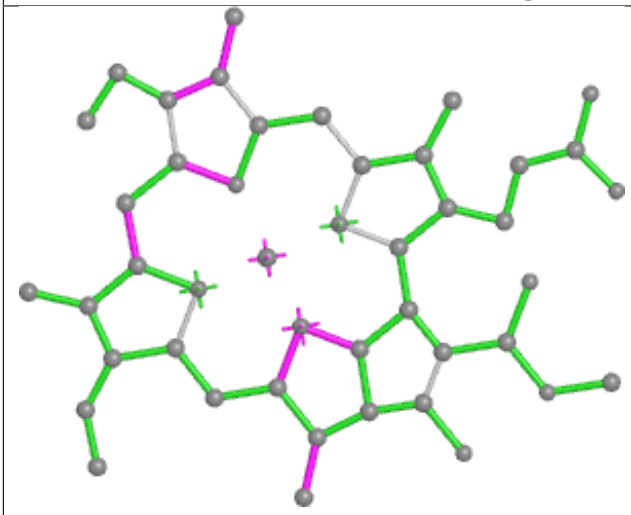


Torsions

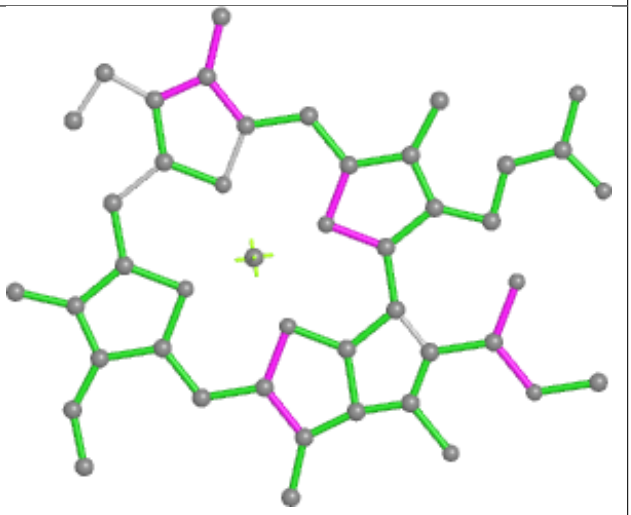


Rings

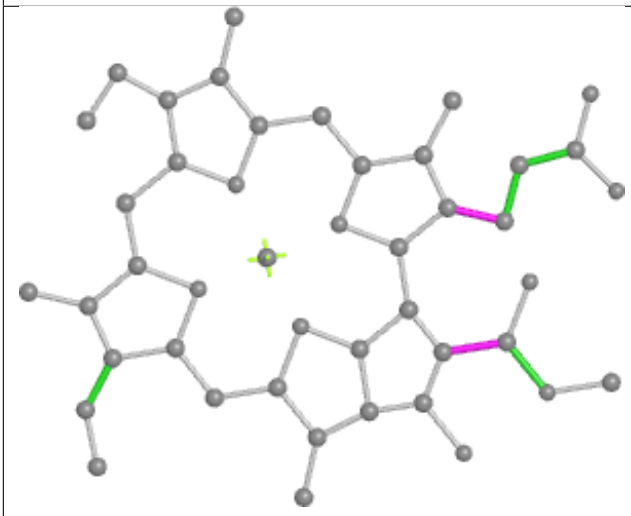
Ligand CLA a4 413



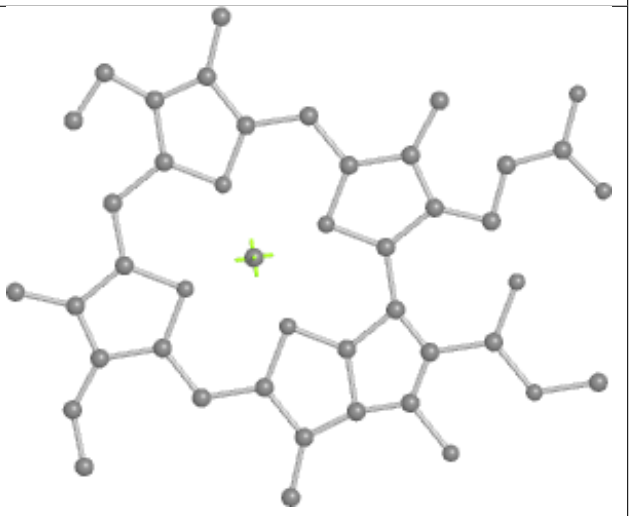
Bond lengths



Bond angles

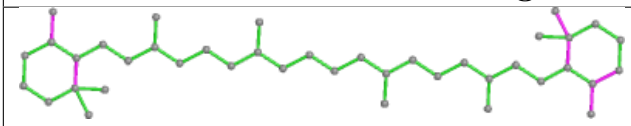


Torsions

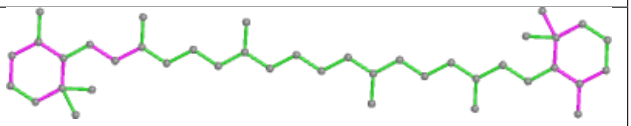


Rings

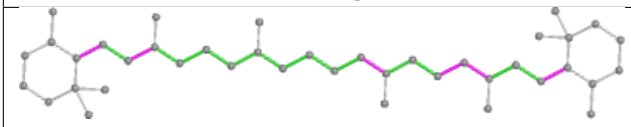
Ligand BCR b4 418



Bond lengths



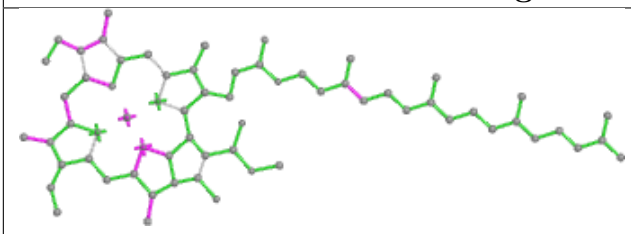
Bond angles



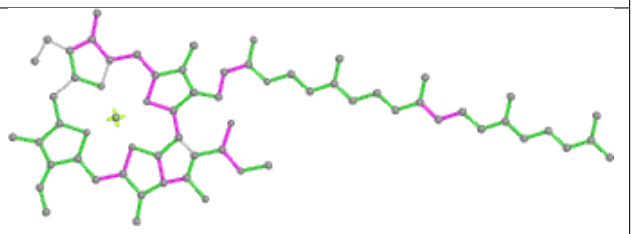
Torsions

Rings

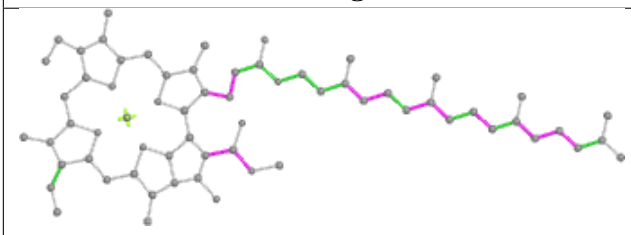
Ligand CLA aA 802



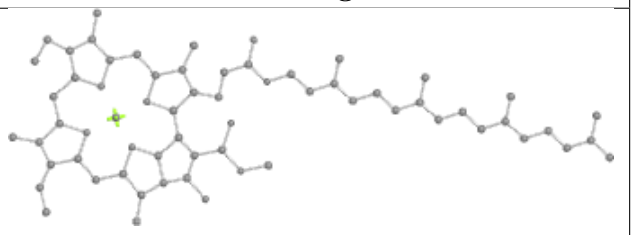
Bond lengths



Bond angles

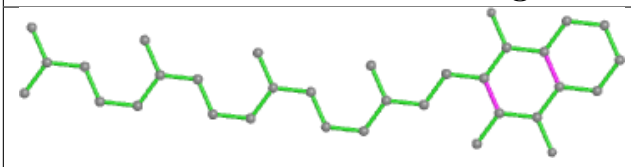


Torsions

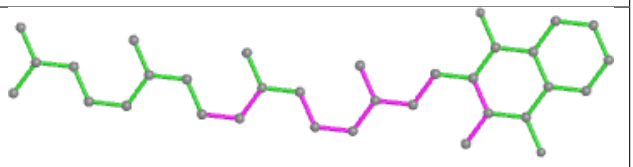


Rings

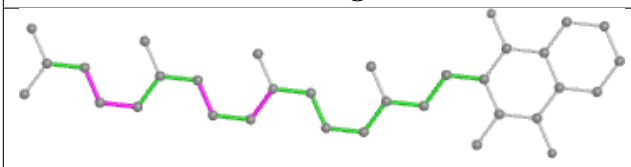
Ligand PQN bA 846



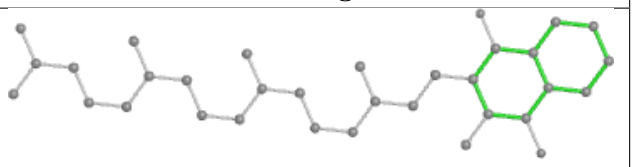
Bond lengths



Bond angles

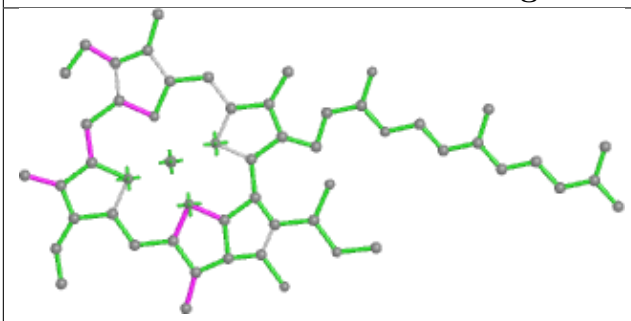


Torsions

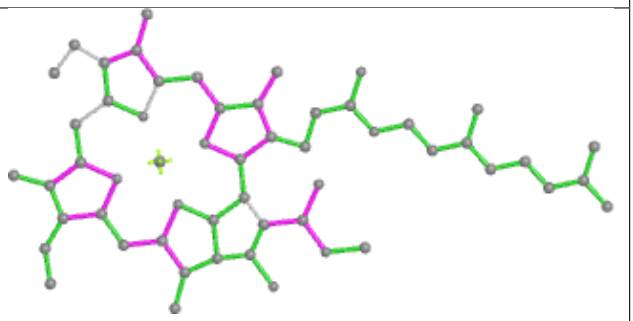


Rings

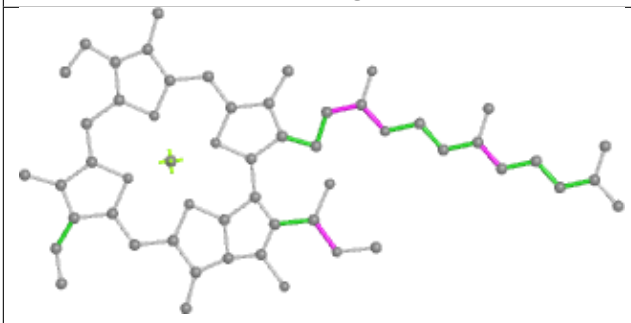
Ligand CLA c4 417



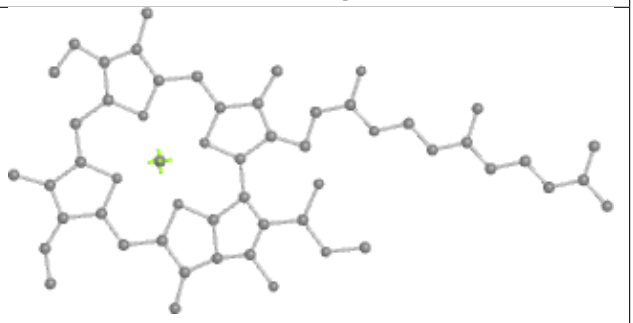
Bond lengths



Bond angles

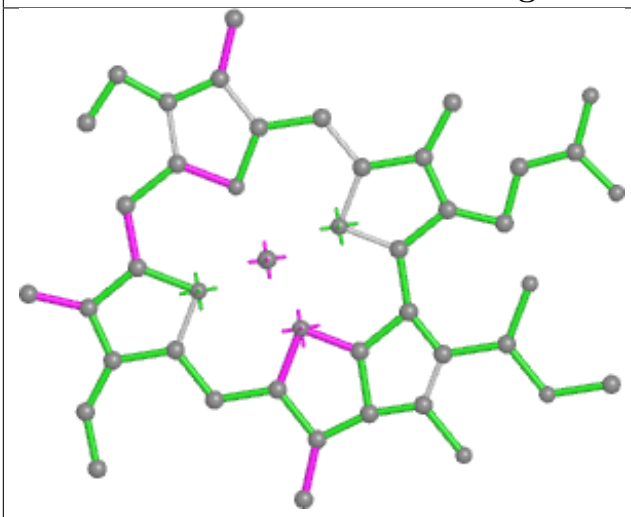


Torsions

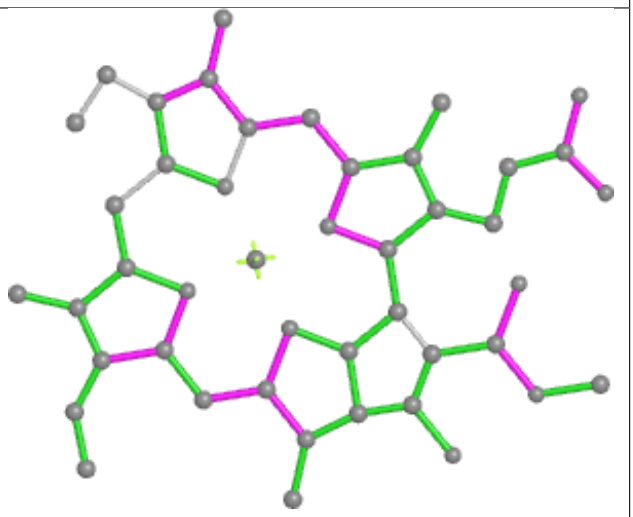


Rings

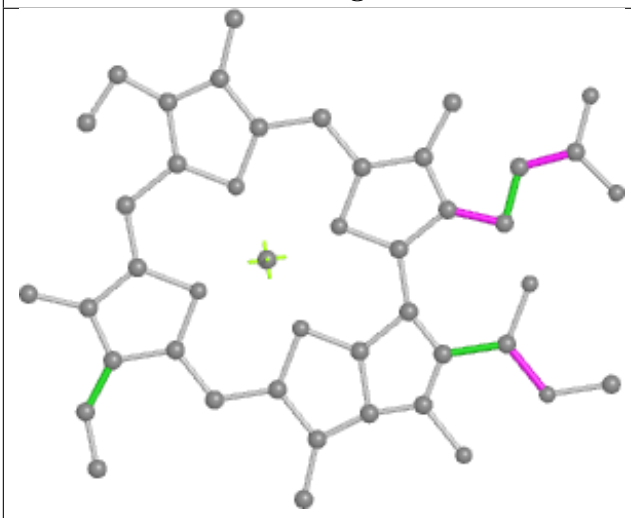
Ligand CLA b2 409



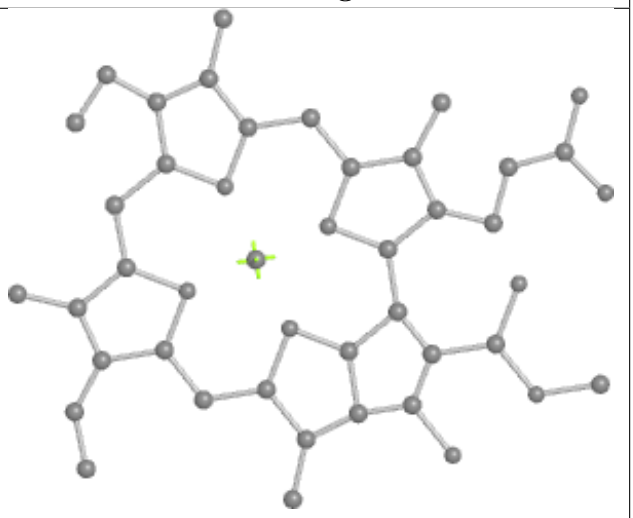
Bond lengths



Bond angles

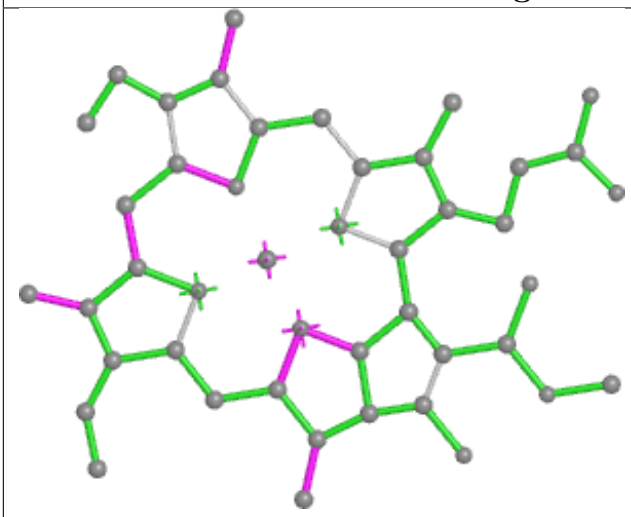


Torsions

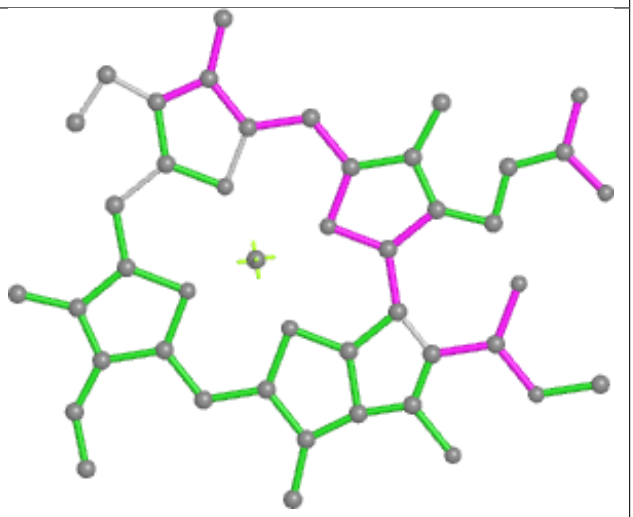


Rings

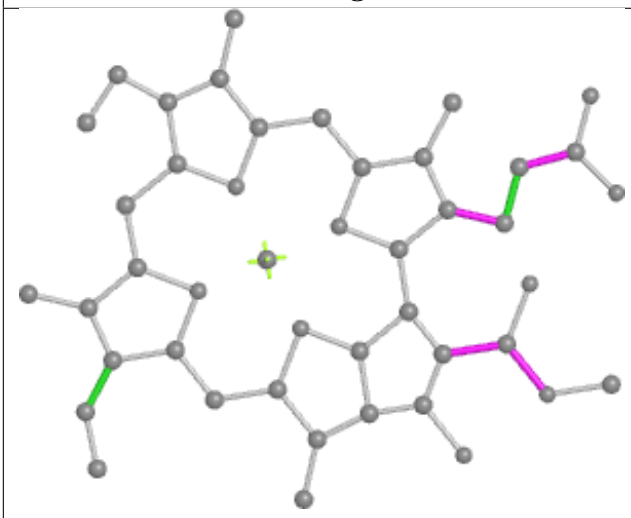
Ligand CLA bK 101



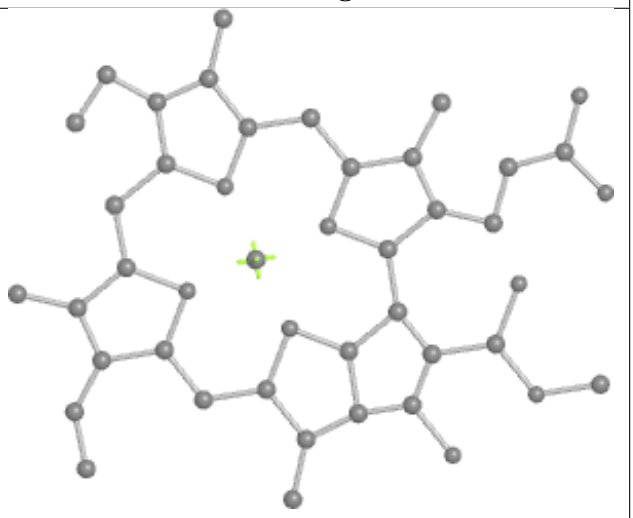
Bond lengths



Bond angles

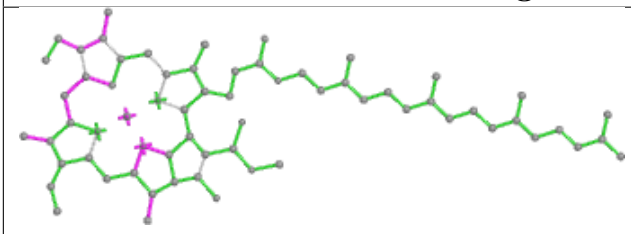


Torsions

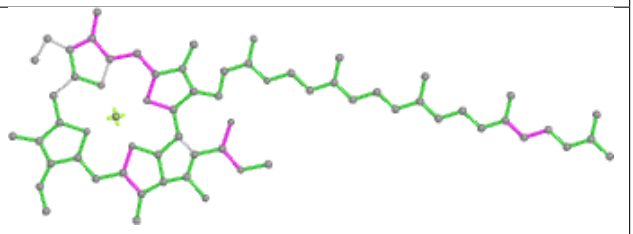


Rings

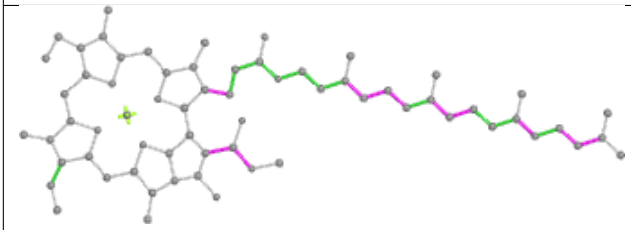
Ligand CLA cA 822



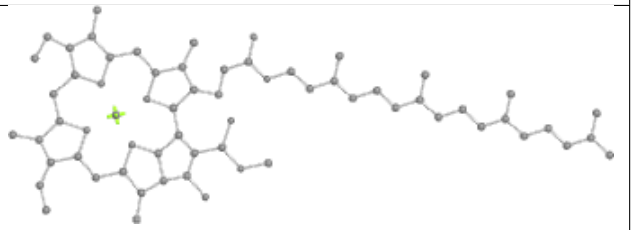
Bond lengths



Bond angles

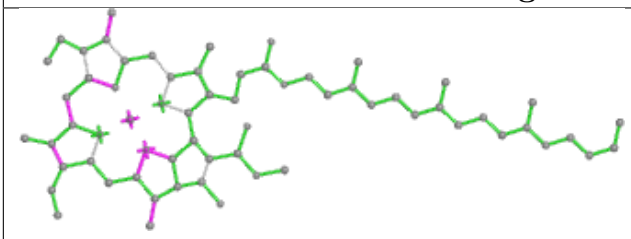


Torsions

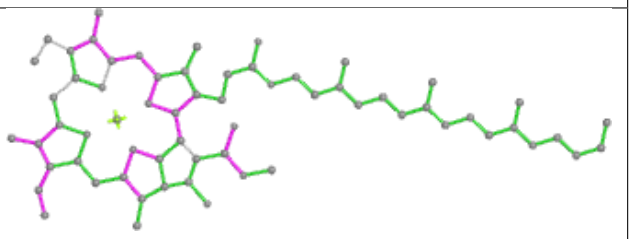


Rings

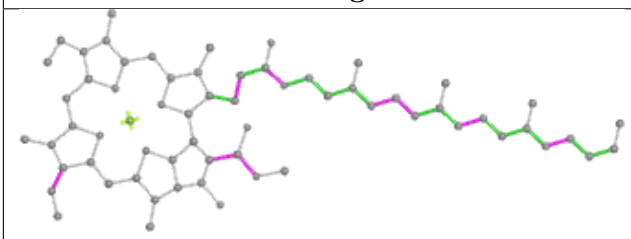
Ligand CLA b5 410



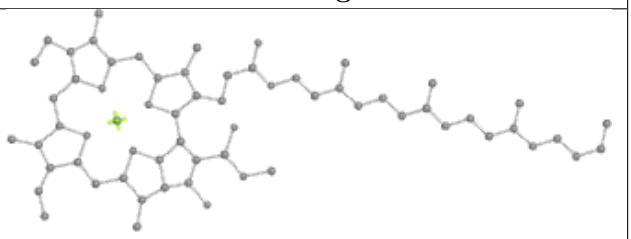
Bond lengths



Bond angles

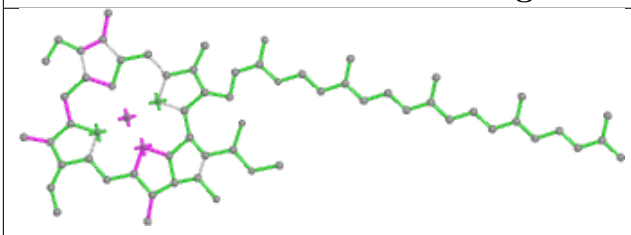


Torsions

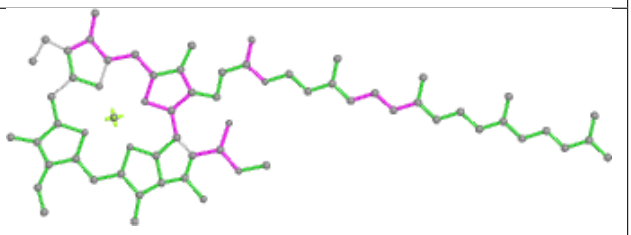


Rings

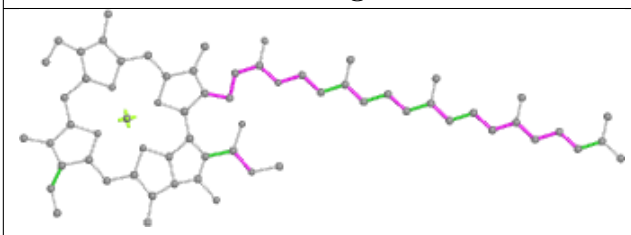
Ligand CLA cA 829



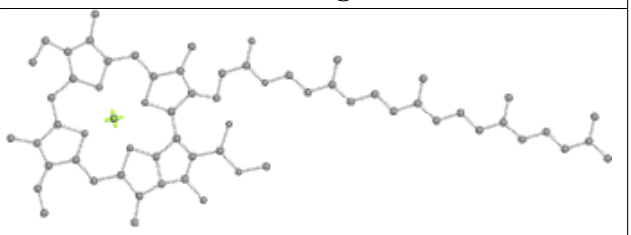
Bond lengths



Bond angles

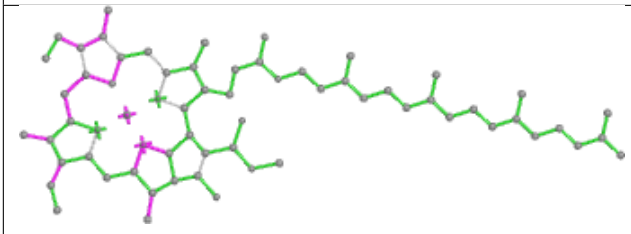


Torsions

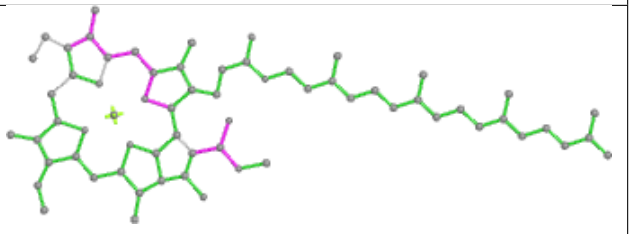


Rings

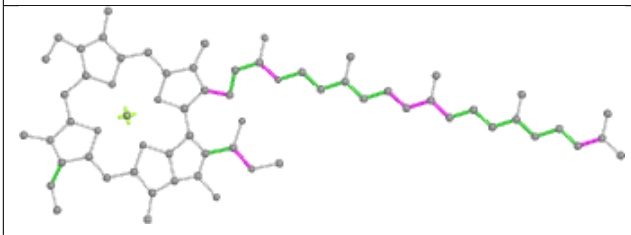
Ligand CLA cA 833



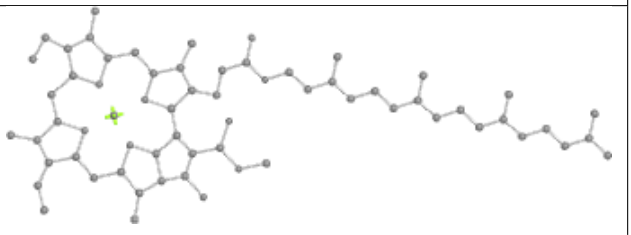
Bond lengths



Bond angles

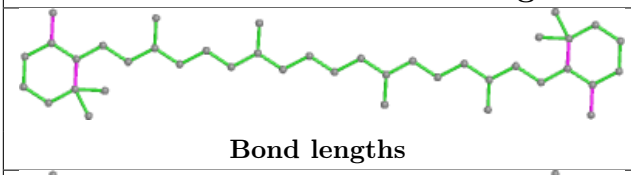


Torsions

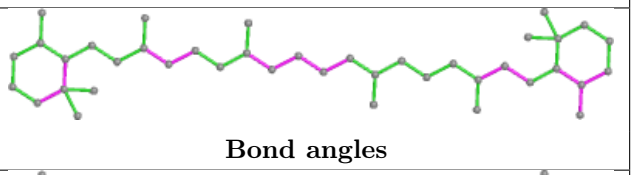


Rings

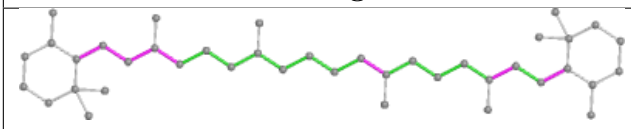
Ligand BCR aJ 205



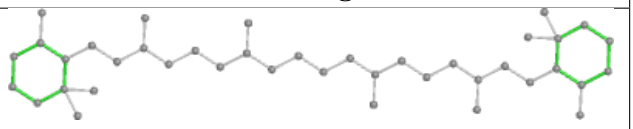
Bond lengths



Bond angles

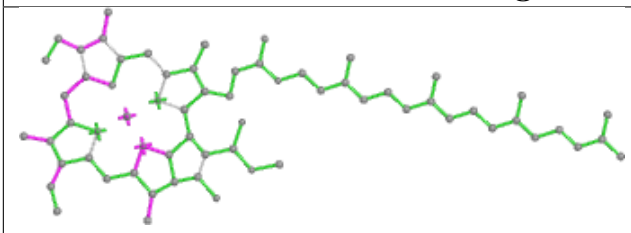


Torsions

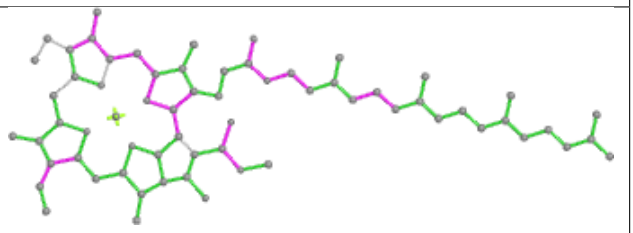


Rings

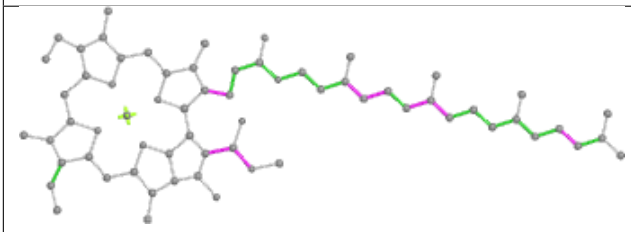
Ligand CLA bB 811



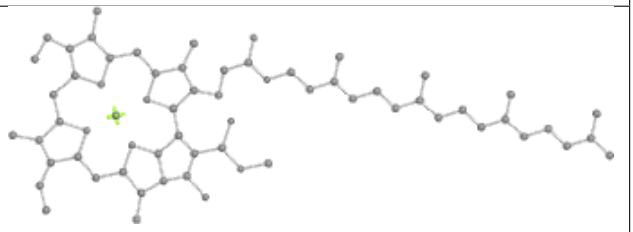
Bond lengths



Bond angles

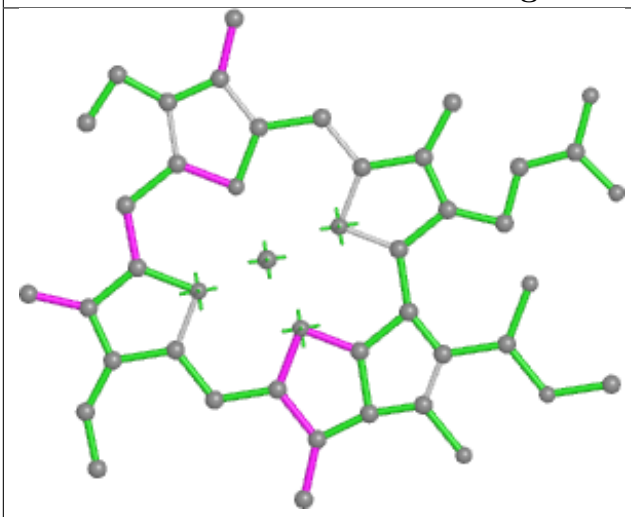


Torsions

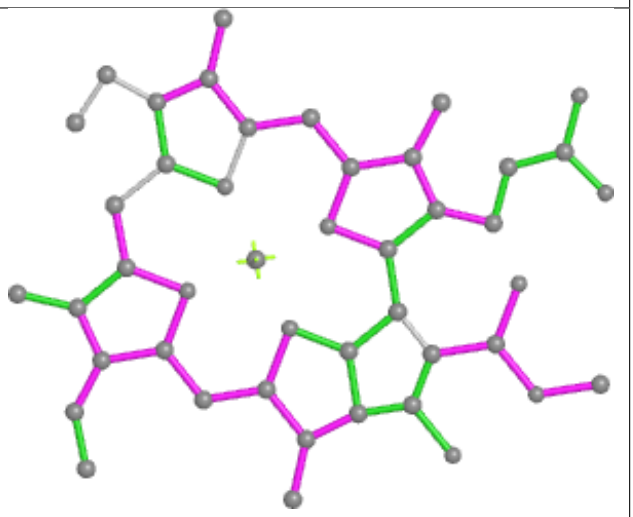


Rings

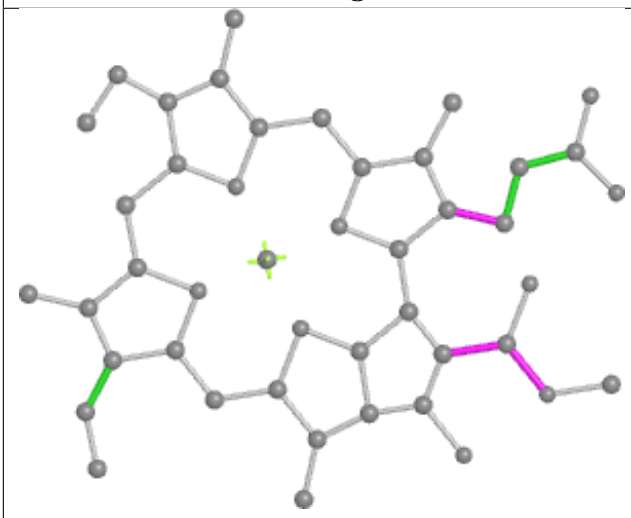
Ligand CLA c5 405



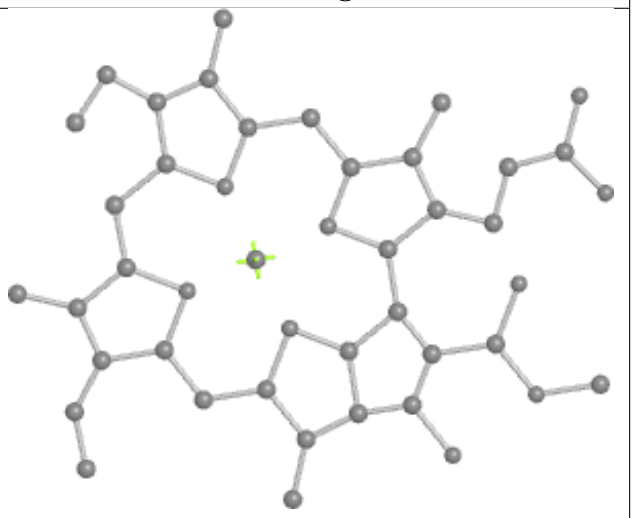
Bond lengths



Bond angles

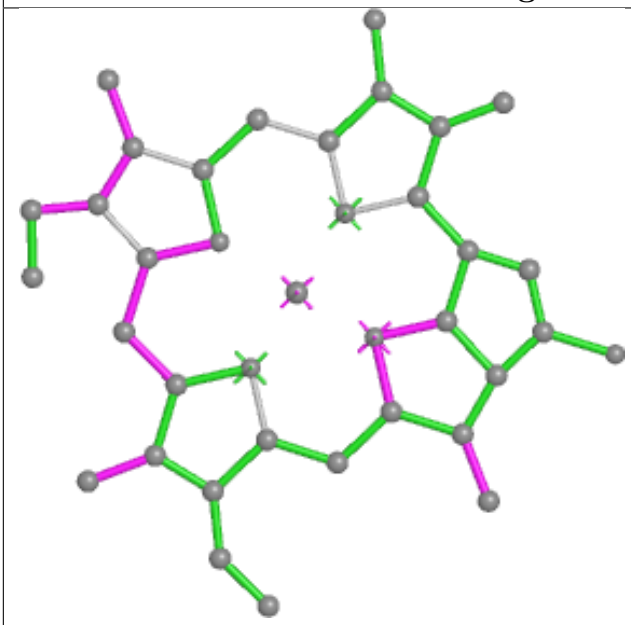


Torsions

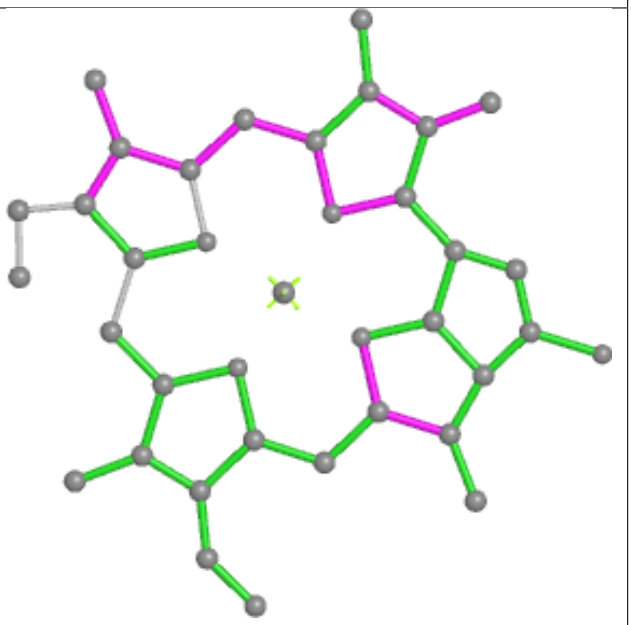


Rings

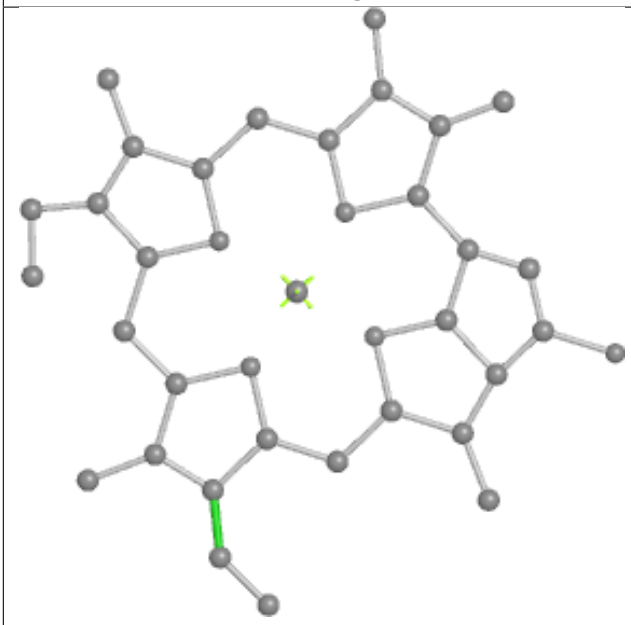
Ligand CLA bJ 102



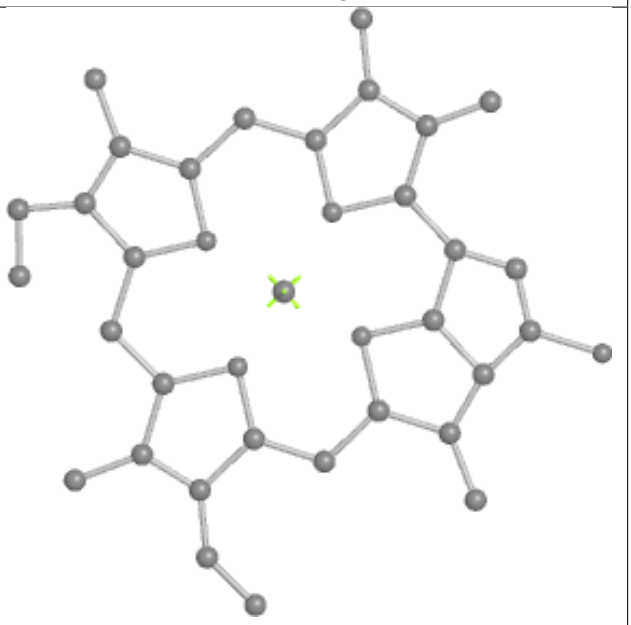
Bond lengths



Bond angles

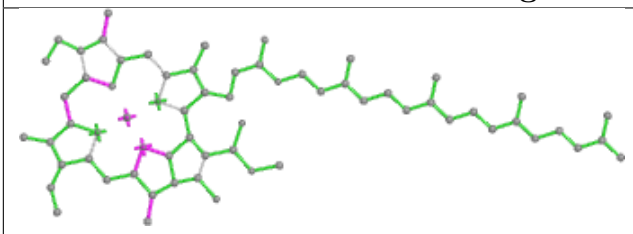


Torsions

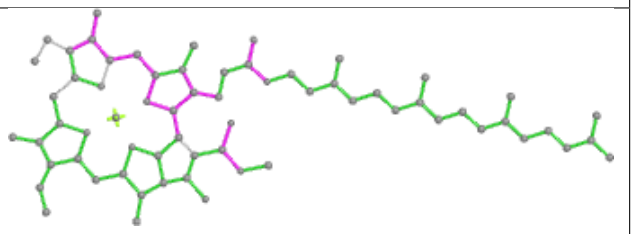


Rings

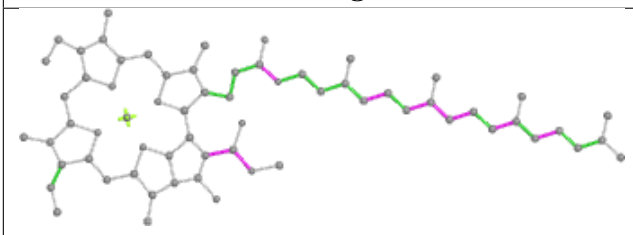
Ligand CLA a5 403



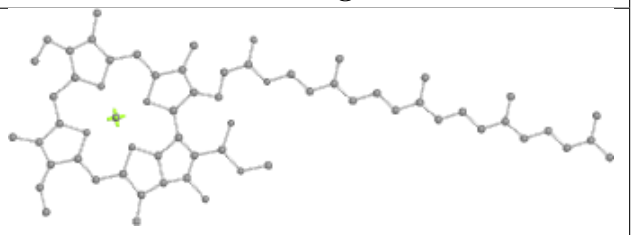
Bond lengths



Bond angles

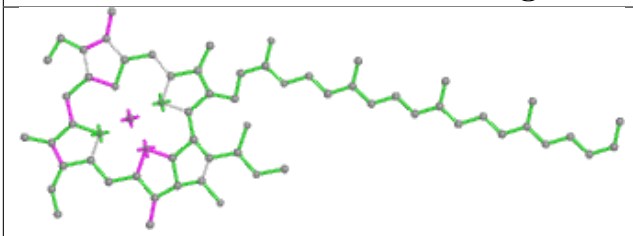


Torsions

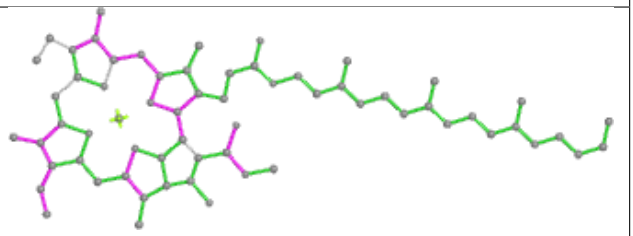


Rings

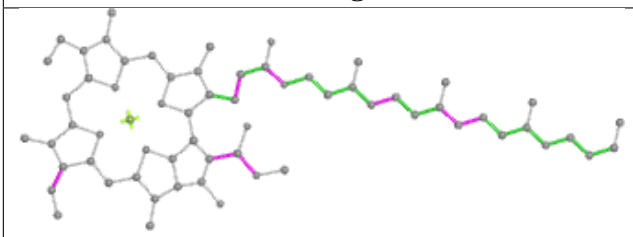
Ligand CLA a1 409



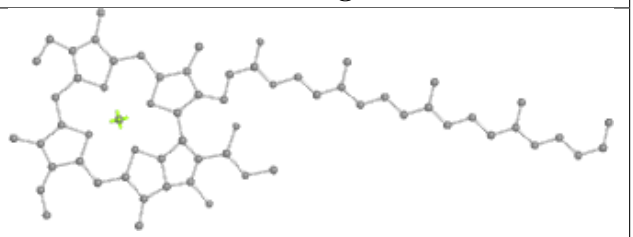
Bond lengths



Bond angles

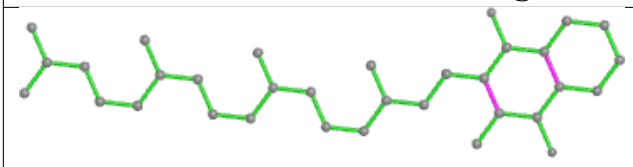


Torsions

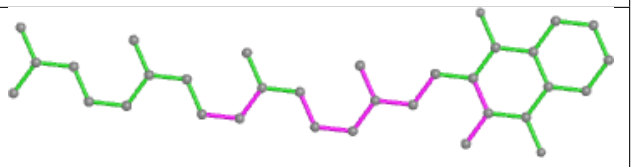


Rings

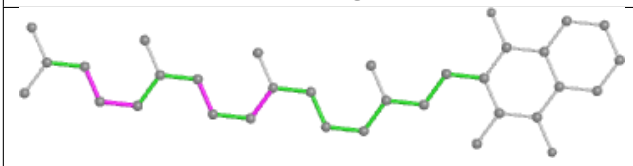
Ligand PQN cA 845



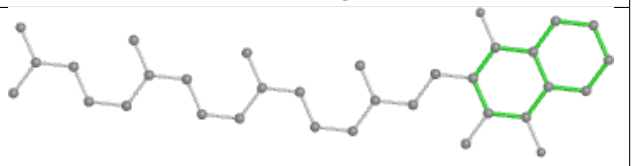
Bond lengths



Bond angles

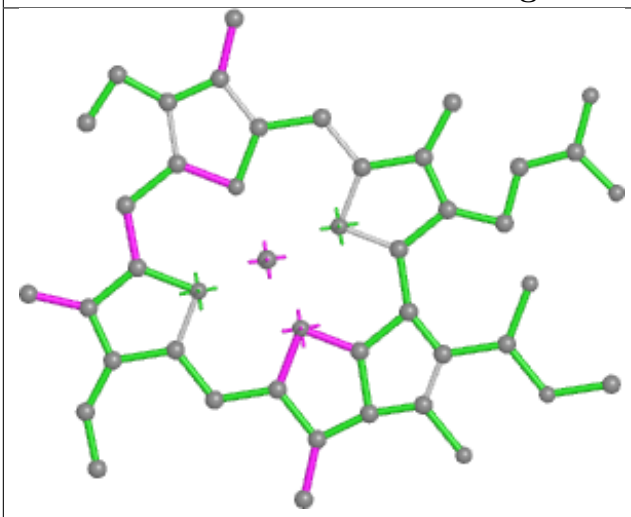


Torsions

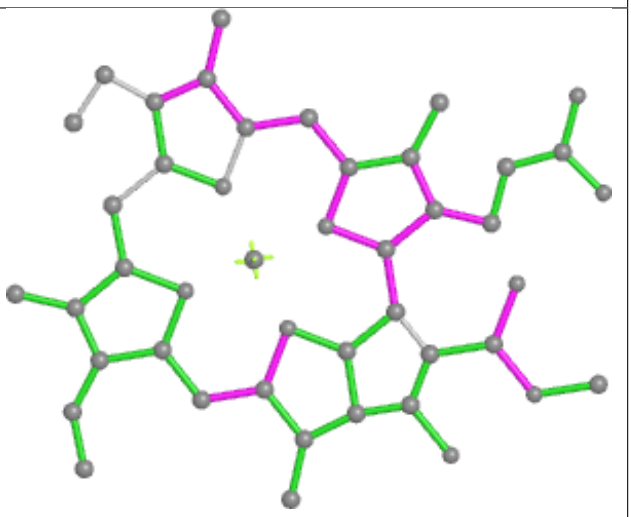


Rings

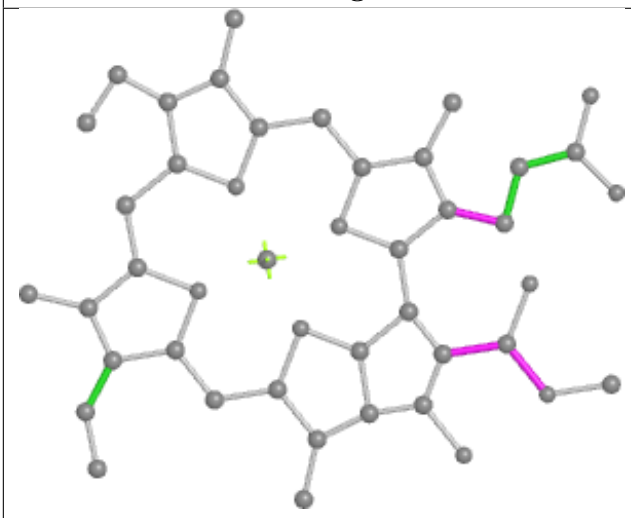
Ligand CLA a3 411



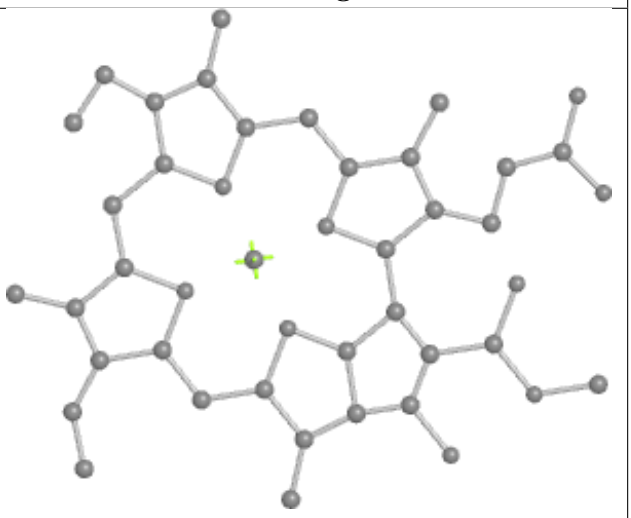
Bond lengths



Bond angles

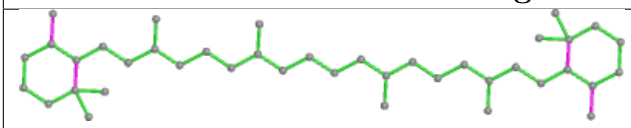


Torsions

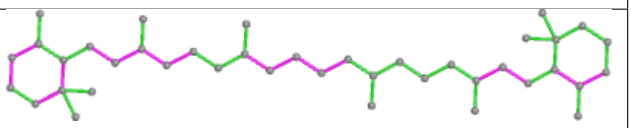


Rings

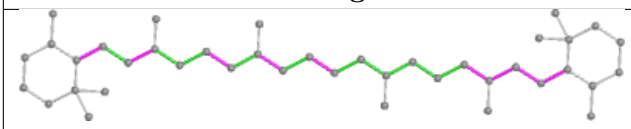
Ligand BCR aB 848



Bond lengths



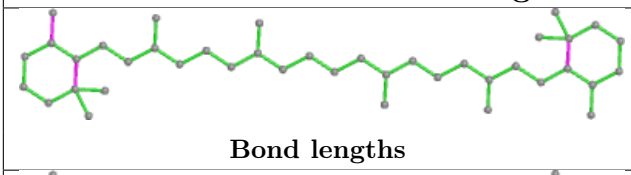
Bond angles



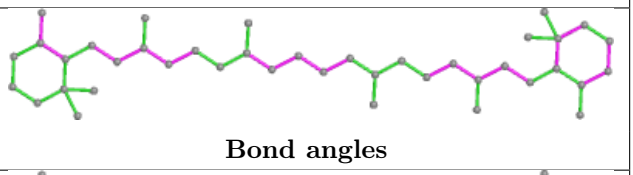
Torsions

Rings

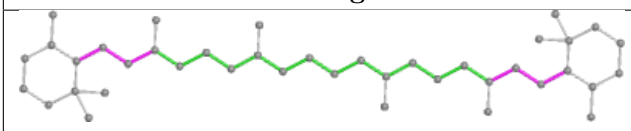
Ligand BCR aK 101



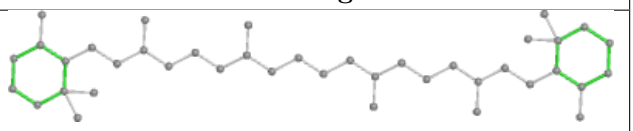
Bond lengths



Bond angles

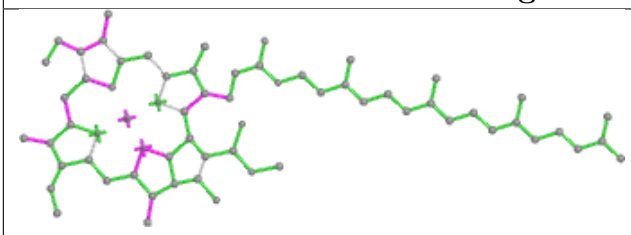


Torsions

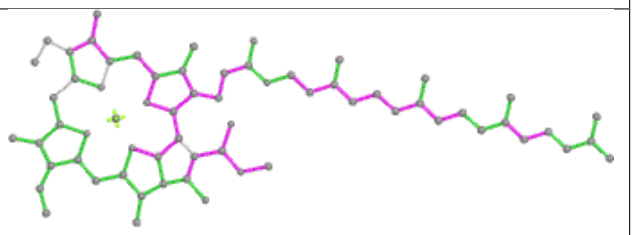


Rings

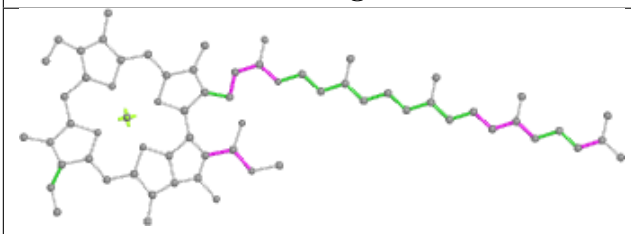
Ligand CLA b6 422



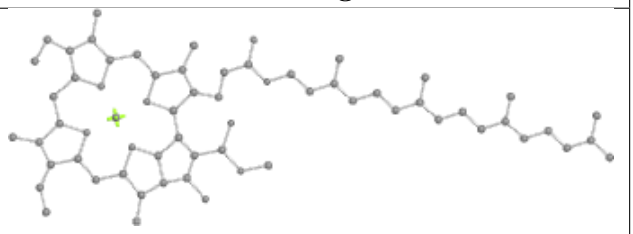
Bond lengths



Bond angles

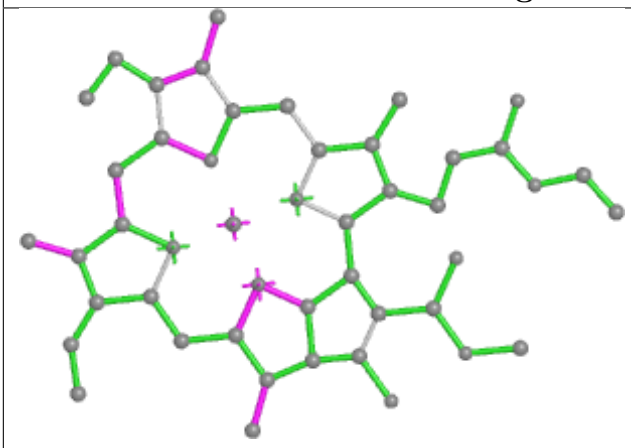


Torsions

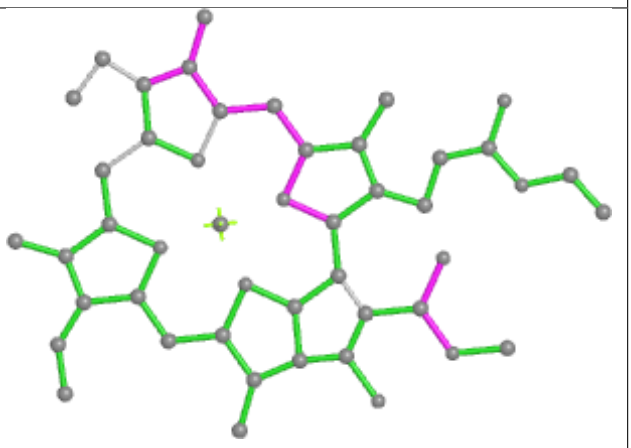


Rings

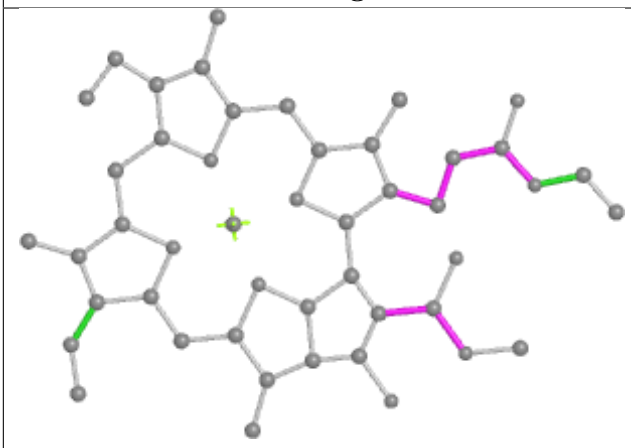
Ligand CLA aB 821



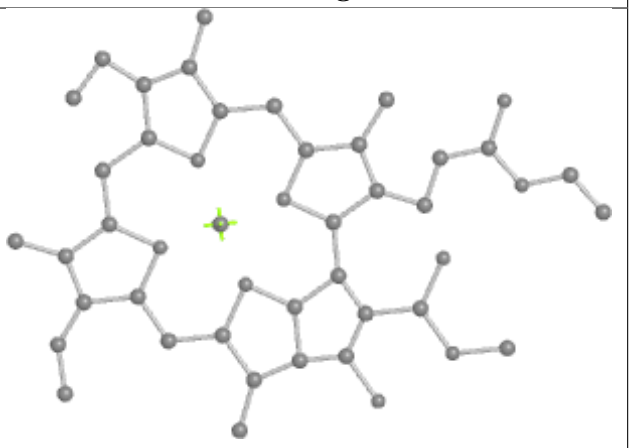
Bond lengths



Bond angles

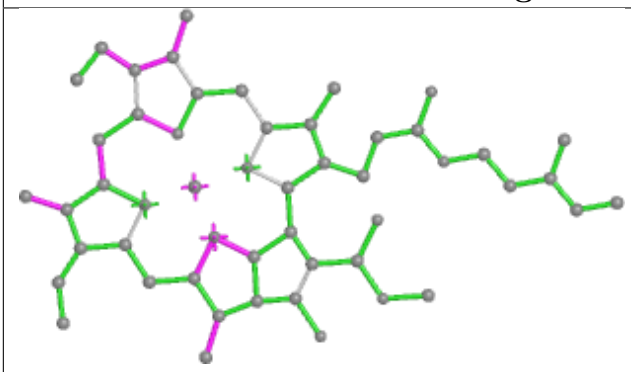


Torsions

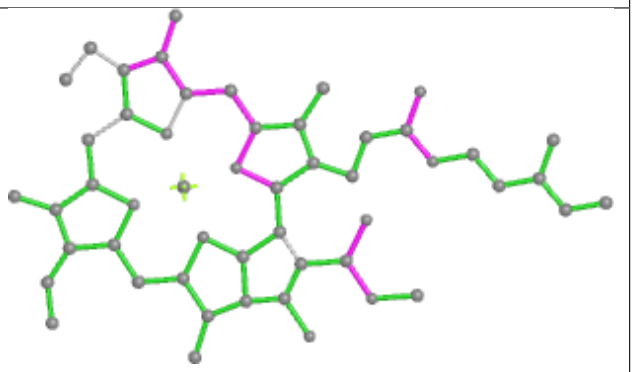


Rings

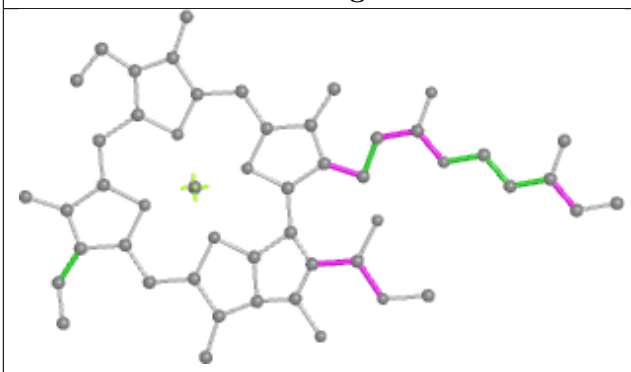
Ligand CLA aA 824



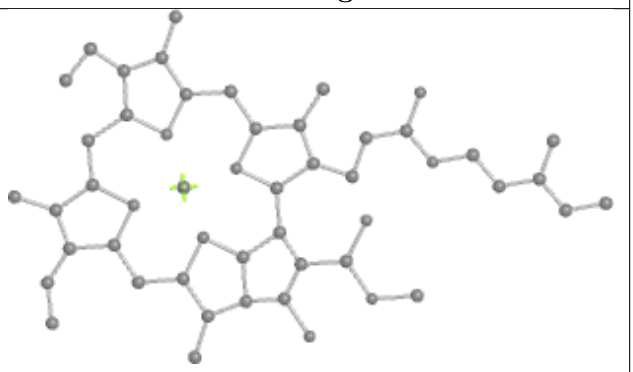
Bond lengths



Bond angles

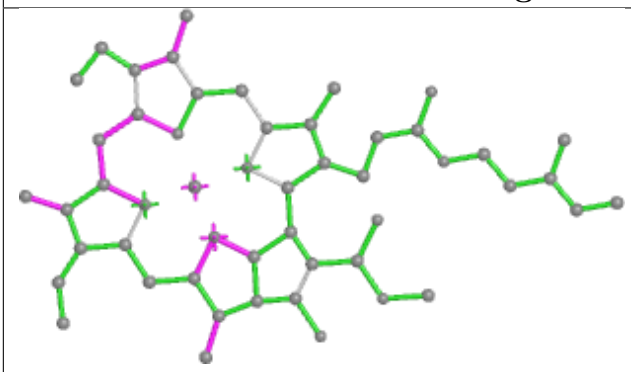


Torsions

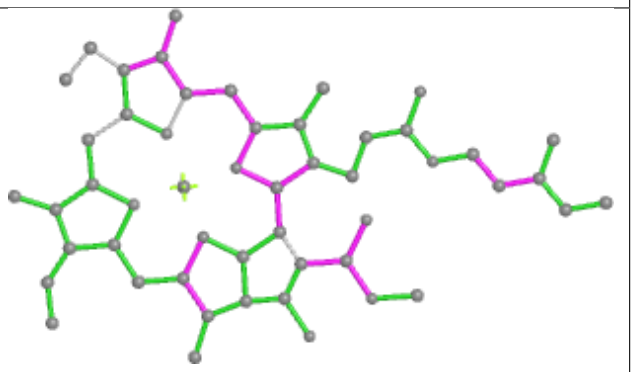


Rings

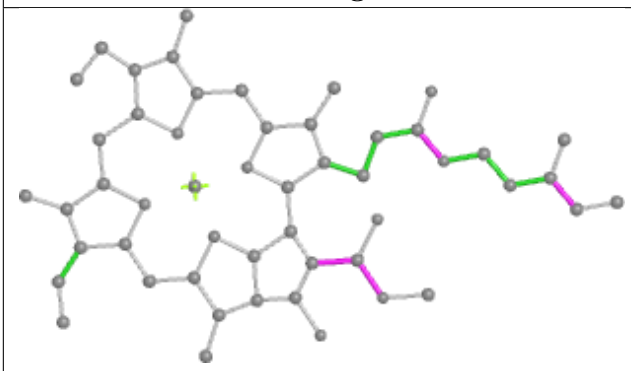
Ligand CLA aA 838



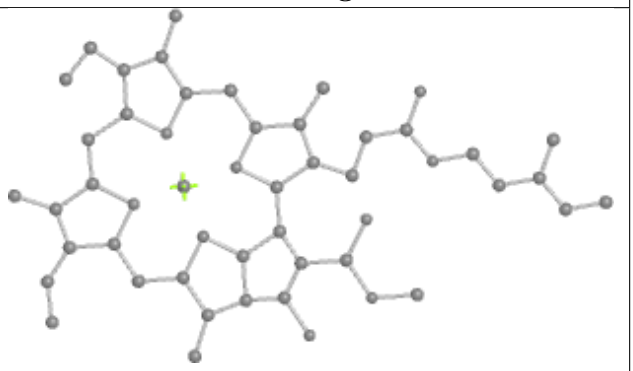
Bond lengths



Bond angles

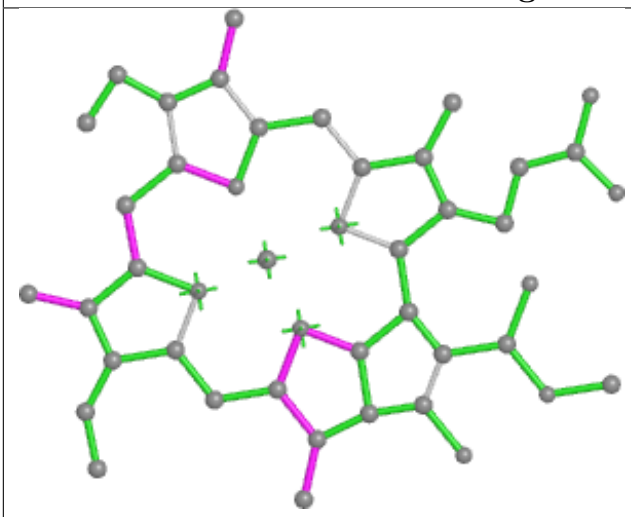


Torsions

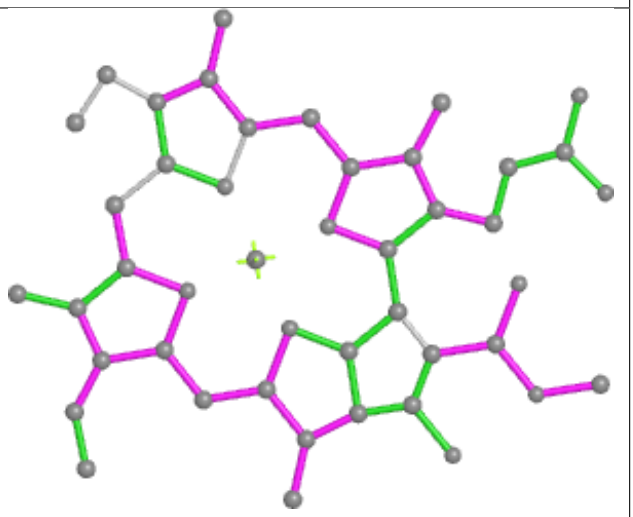


Rings

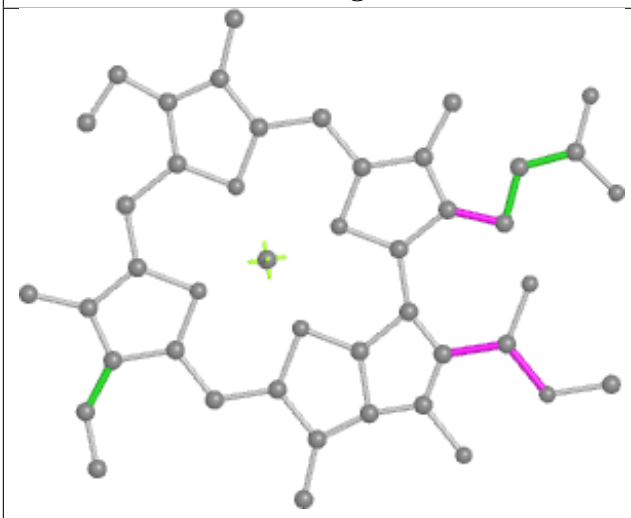
Ligand CLA b5 405



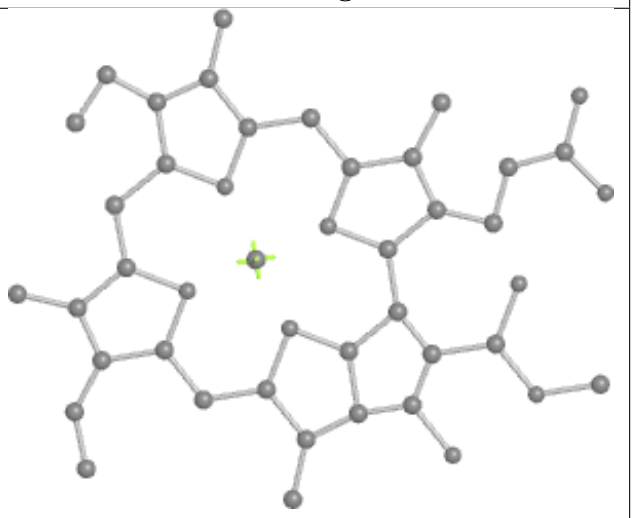
Bond lengths



Bond angles

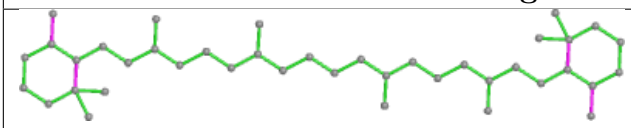


Torsions

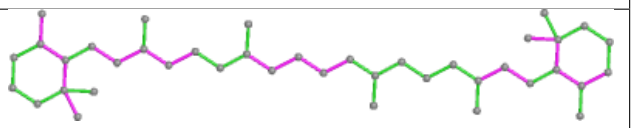


Rings

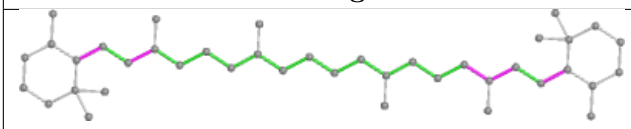
Ligand BCR aI 103



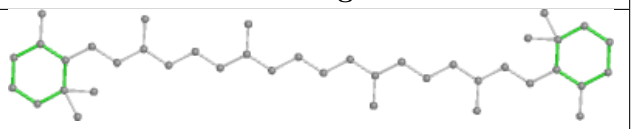
Bond lengths



Bond angles

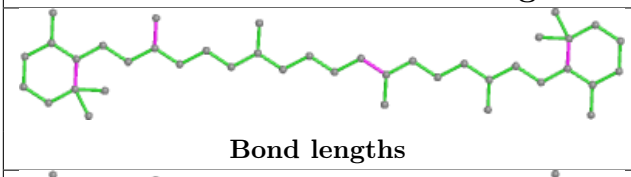


Torsions

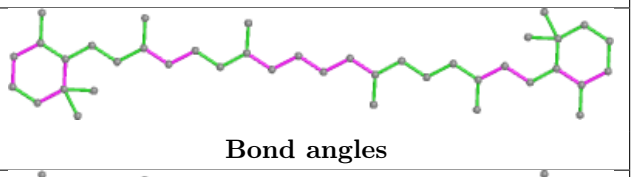


Rings

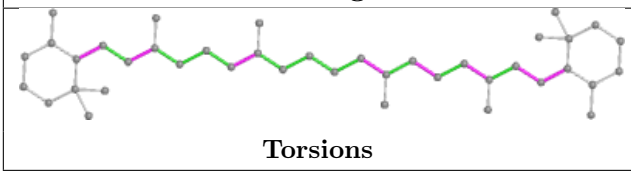
Ligand BCR bI 102



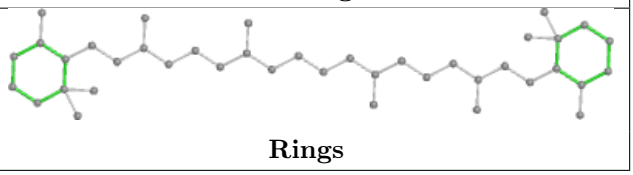
Bond lengths



Bond angles

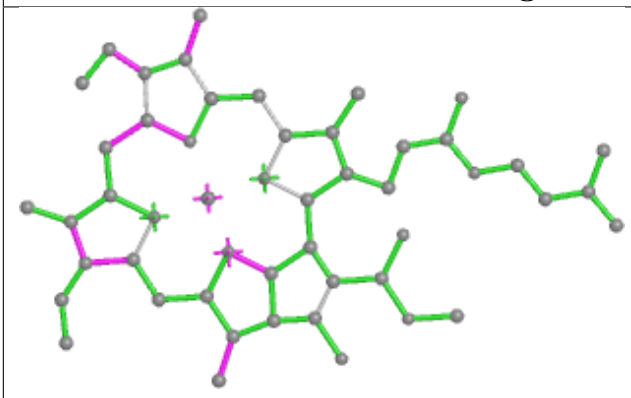


Torsions

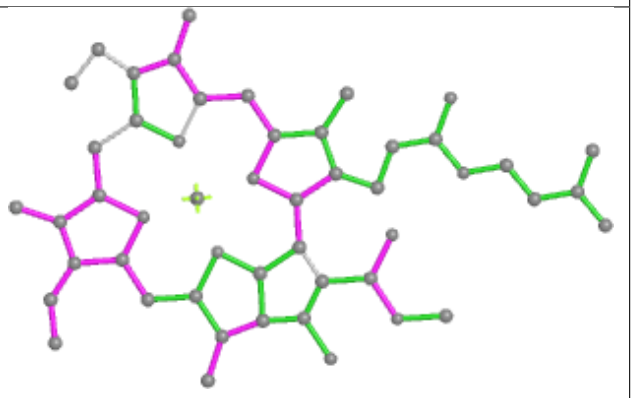


Rings

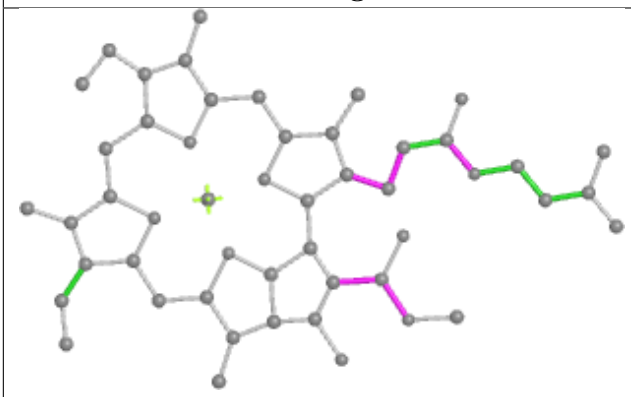
Ligand CLA b5 416



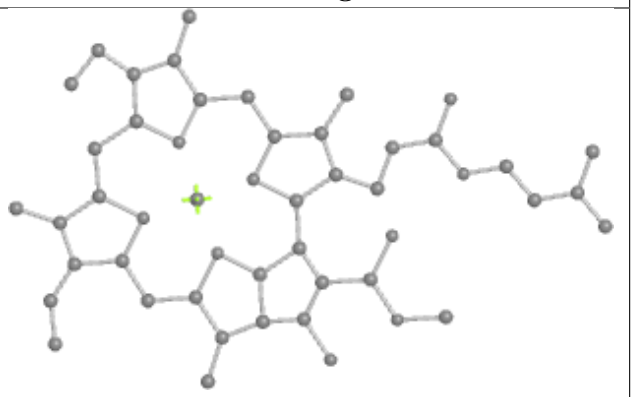
Bond lengths



Bond angles

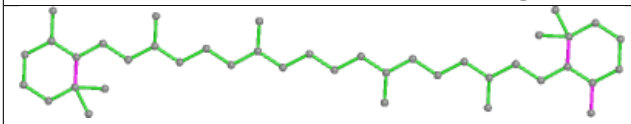


Torsions

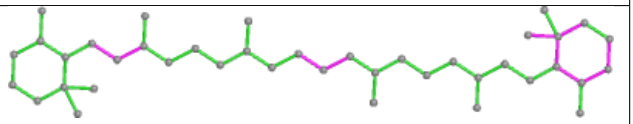


Rings

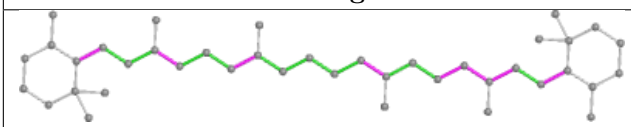
Ligand BCR cB 845



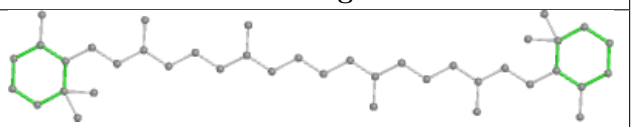
Bond lengths



Bond angles

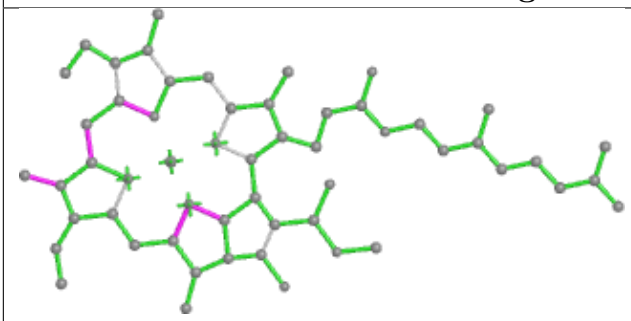


Torsions

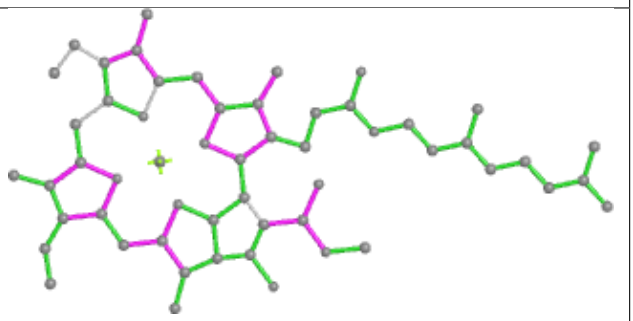


Rings

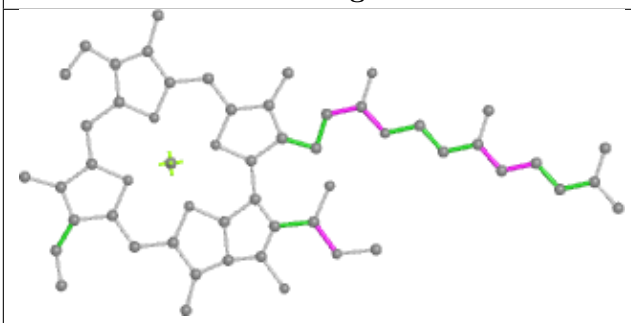
Ligand CLA b5 417



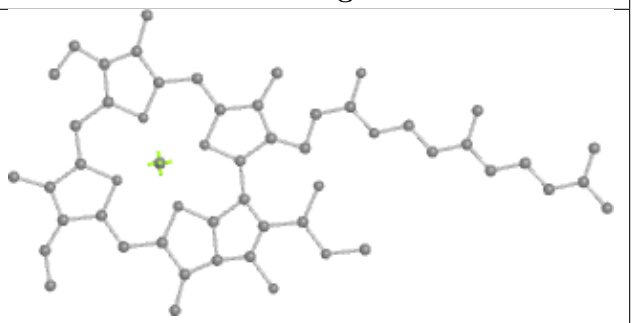
Bond lengths



Bond angles

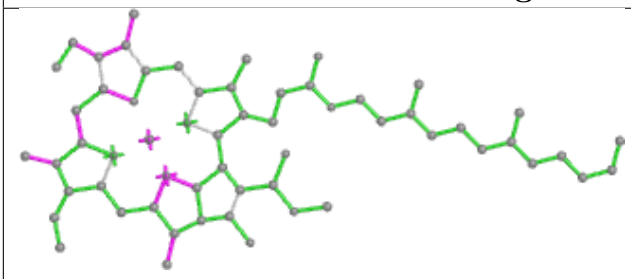


Torsions

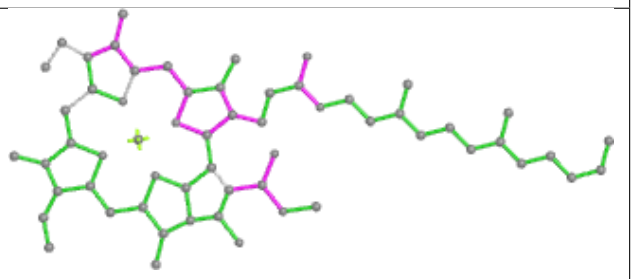


Rings

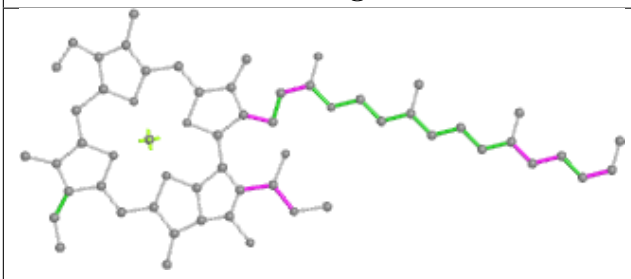
Ligand CLA aA 805



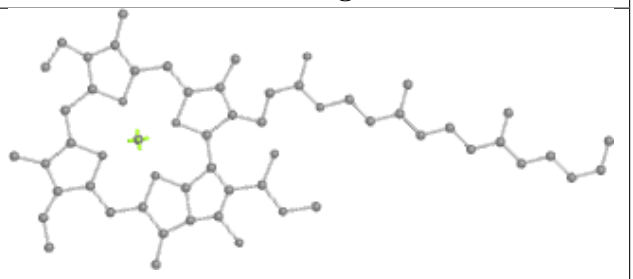
Bond lengths



Bond angles

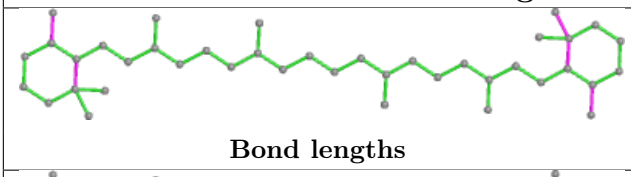


Torsions

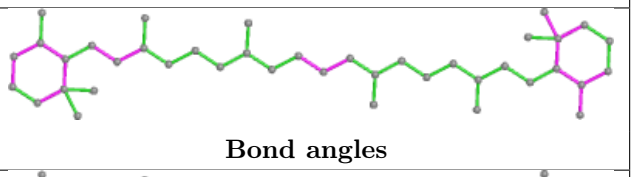


Rings

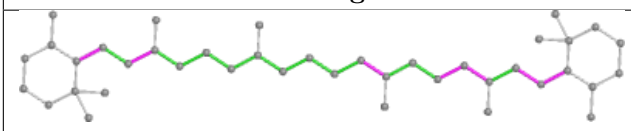
Ligand BCR b6 419



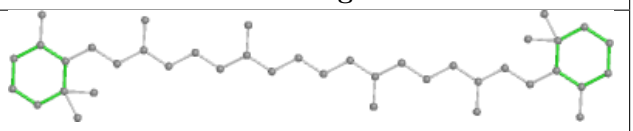
Bond lengths



Bond angles

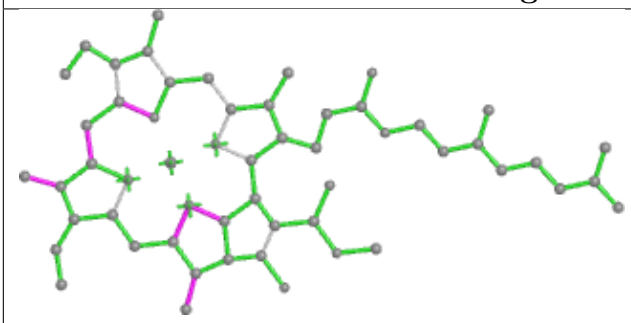


Torsions

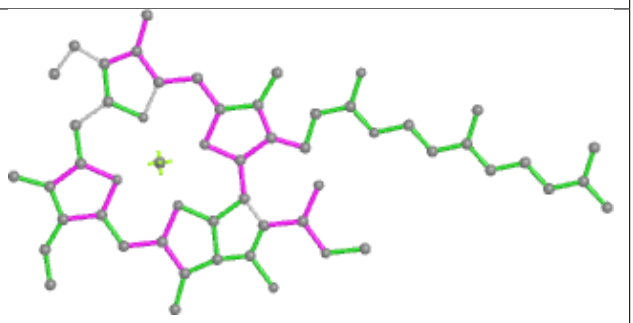


Rings

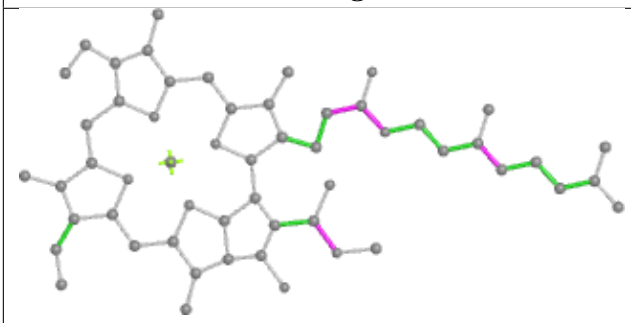
Ligand CLA c1 417



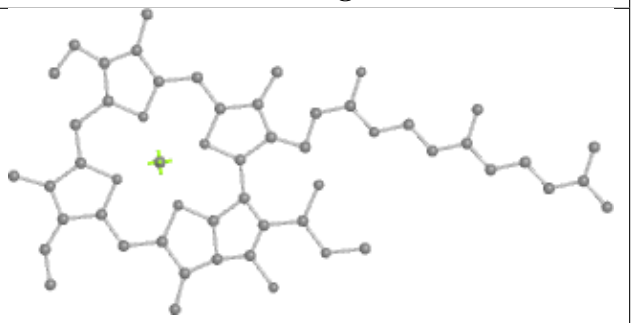
Bond lengths



Bond angles

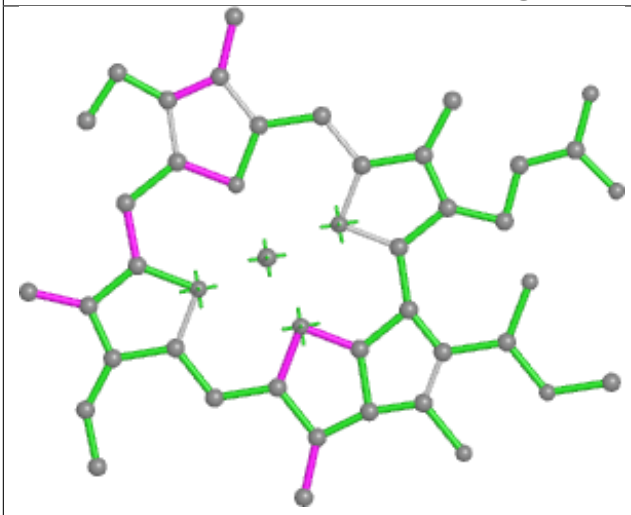


Torsions

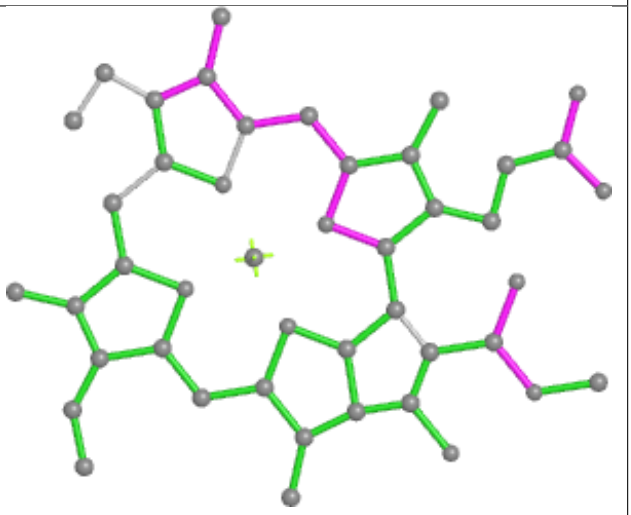


Rings

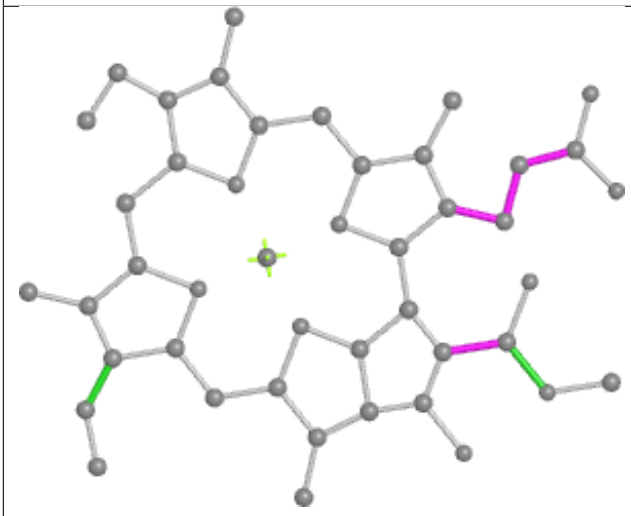
Ligand CLA aA 837



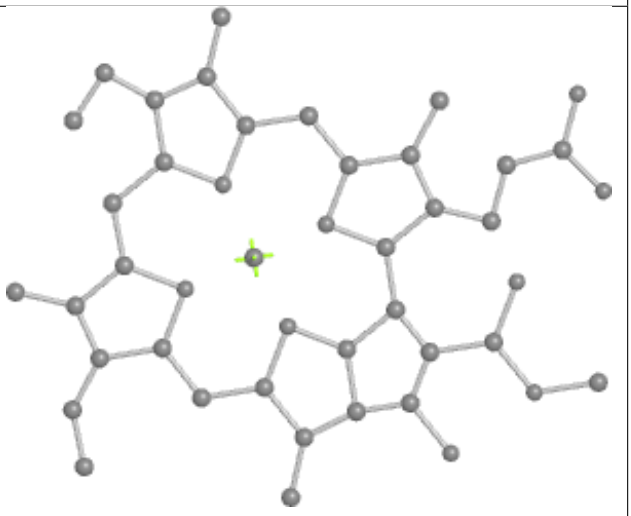
Bond lengths



Bond angles

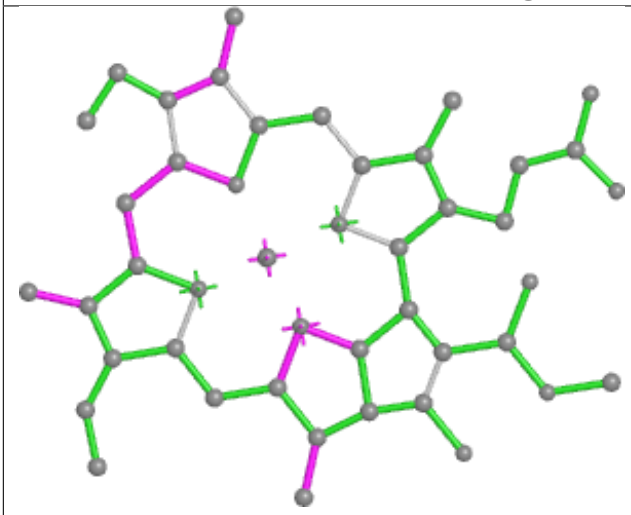


Torsions

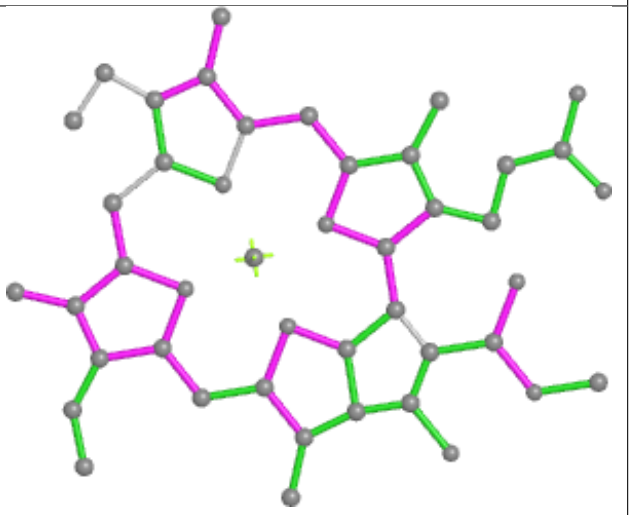


Rings

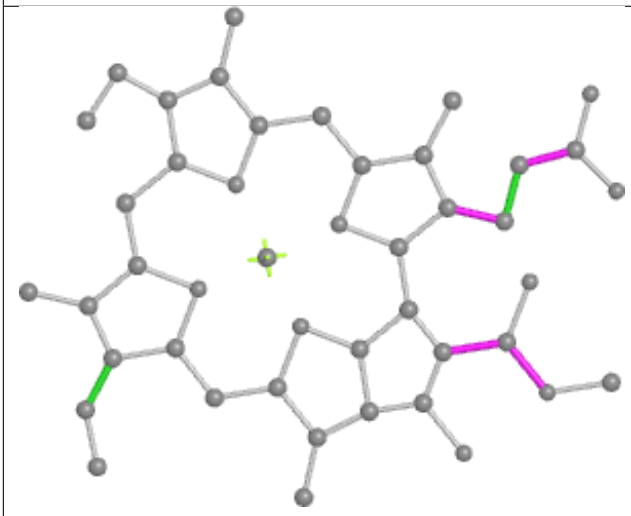
Ligand CLA a1 411



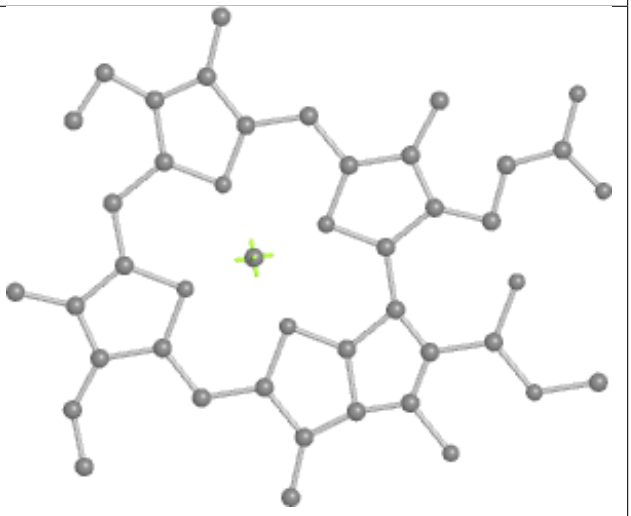
Bond lengths



Bond angles

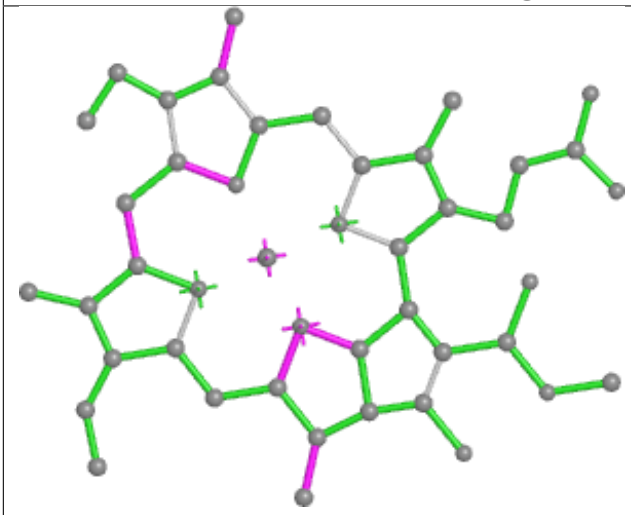


Torsions

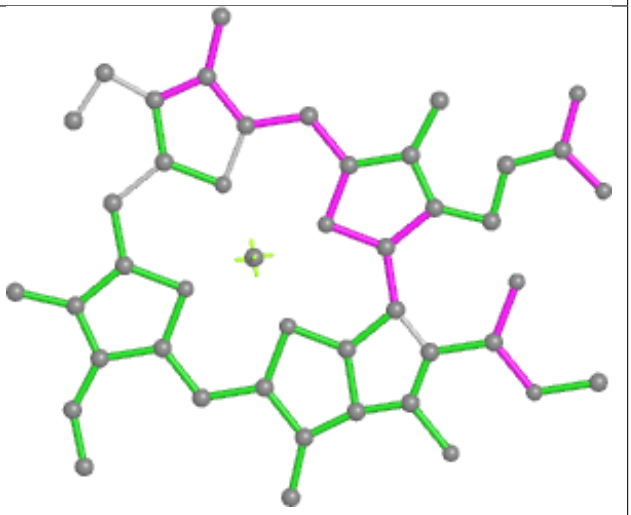


Rings

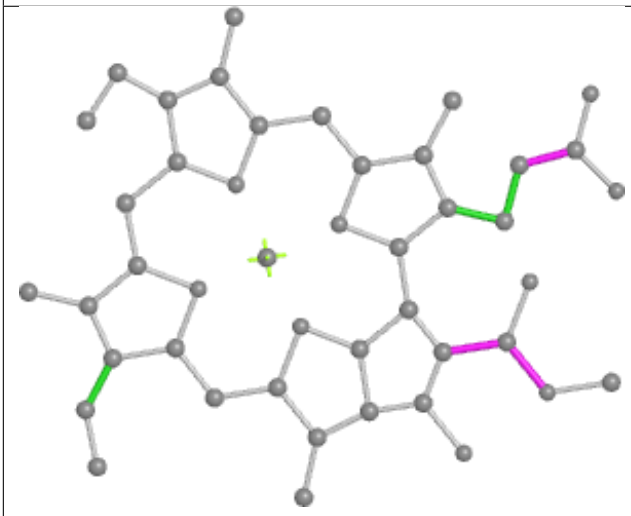
Ligand CLA b5 407



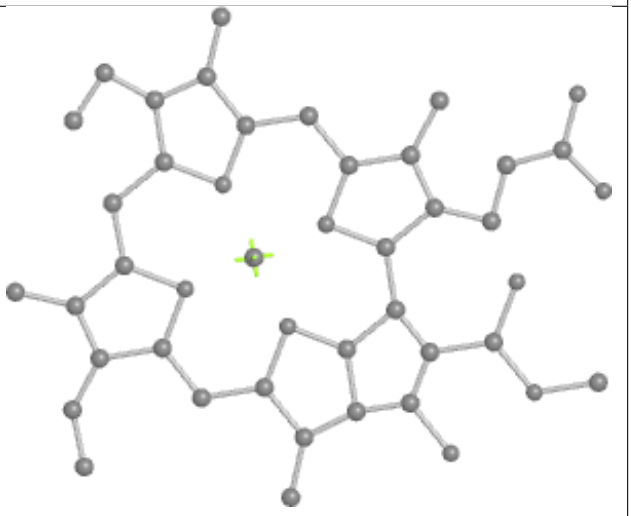
Bond lengths



Bond angles

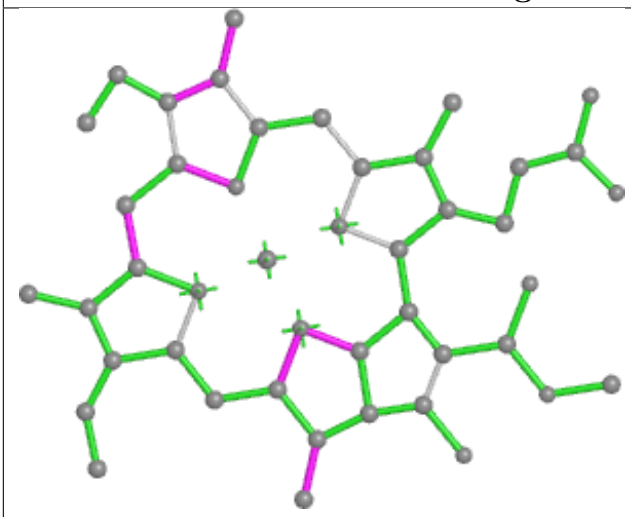


Torsions

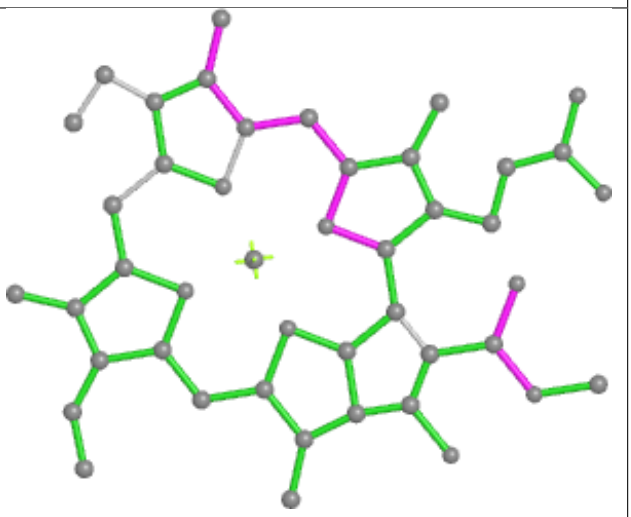


Rings

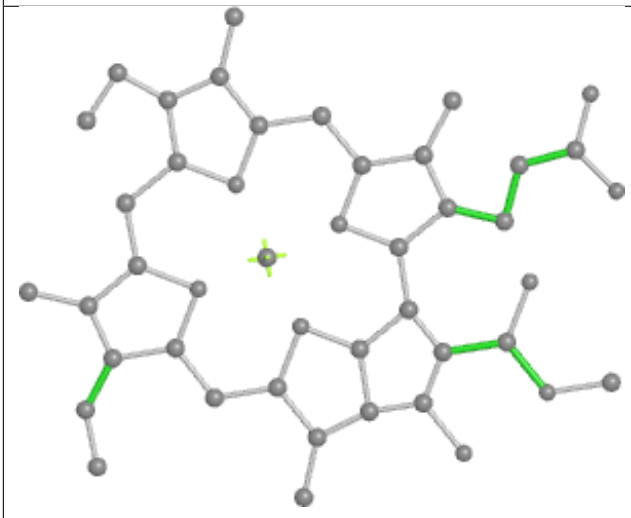
Ligand CLA bB 842



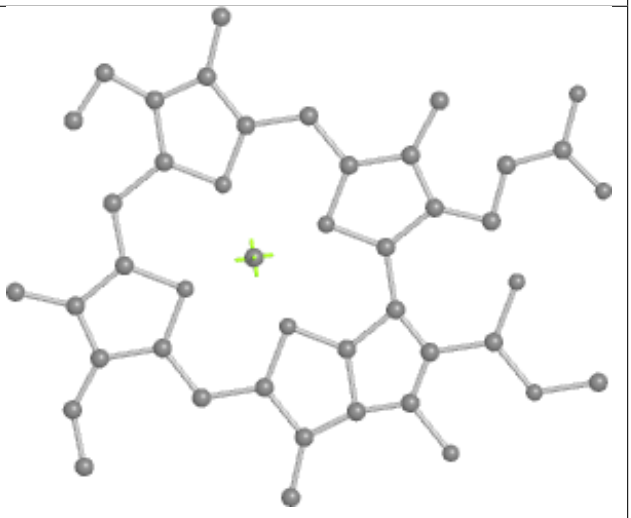
Bond lengths



Bond angles

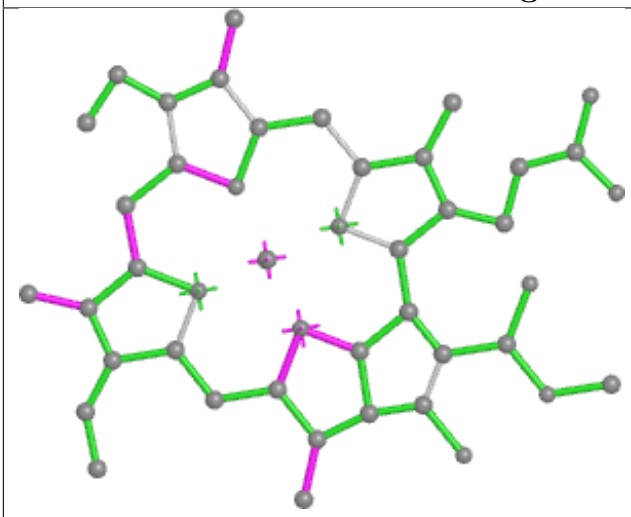


Torsions

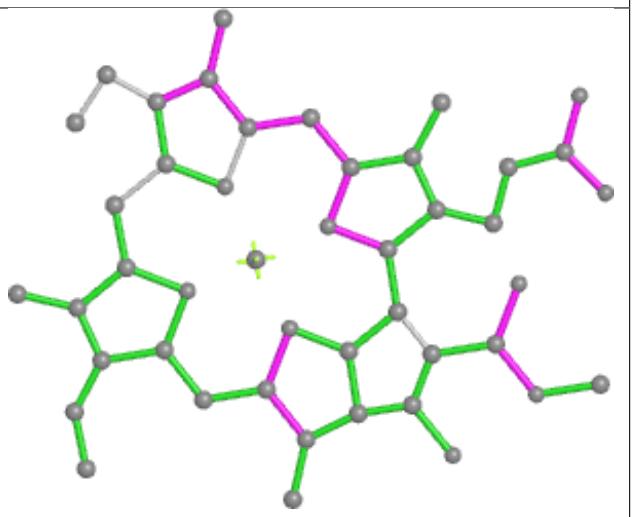


Rings

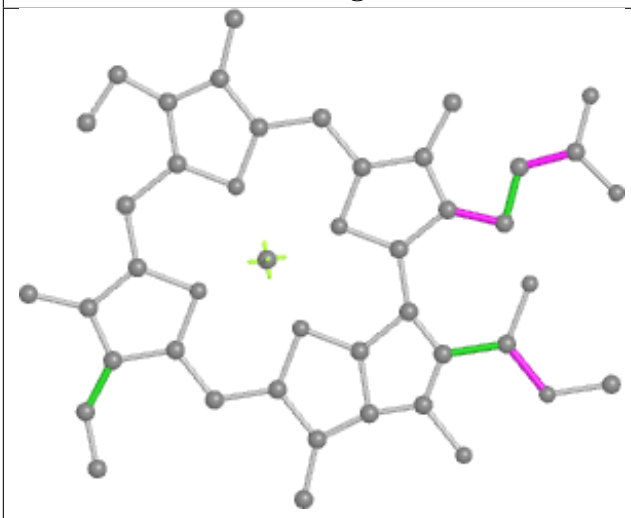
Ligand CLA c6 409



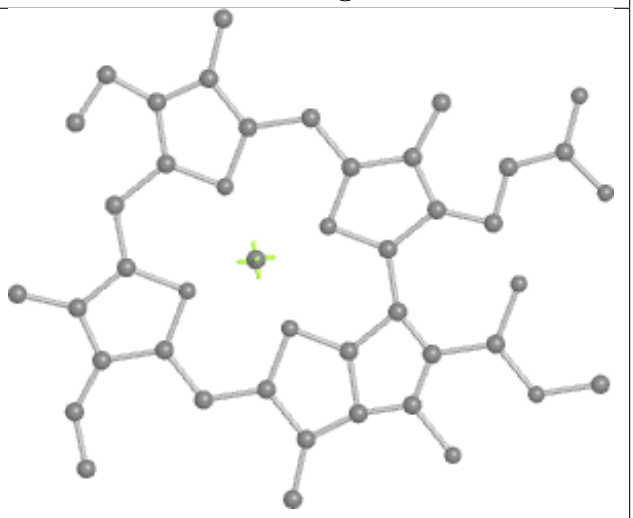
Bond lengths



Bond angles

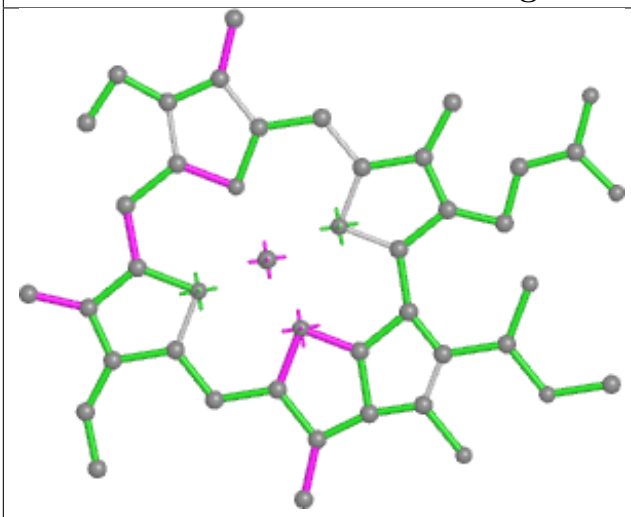


Torsions

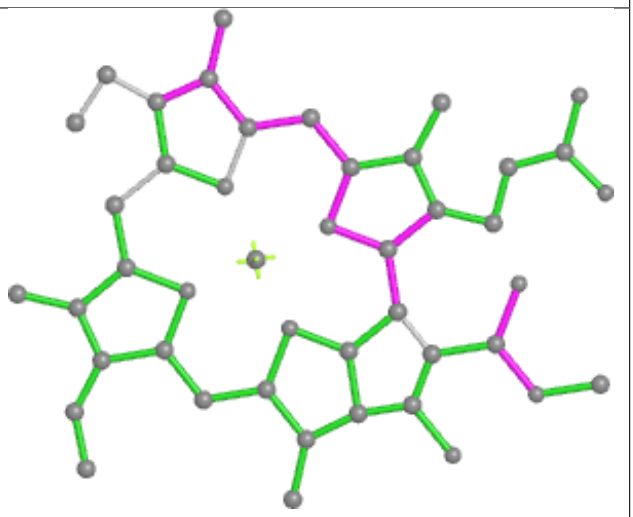


Rings

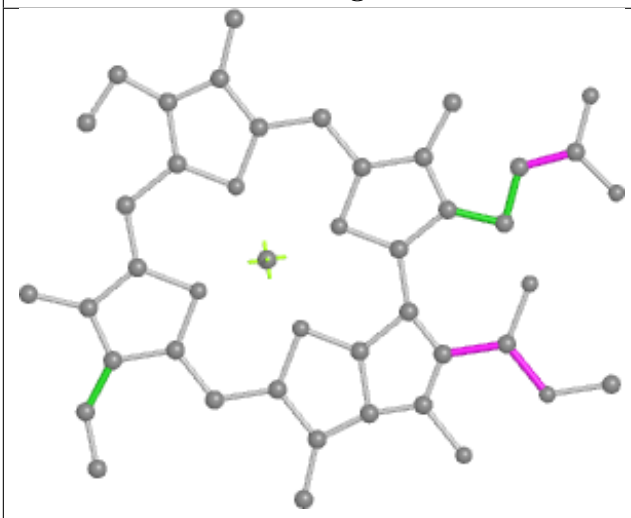
Ligand CLA a3 407



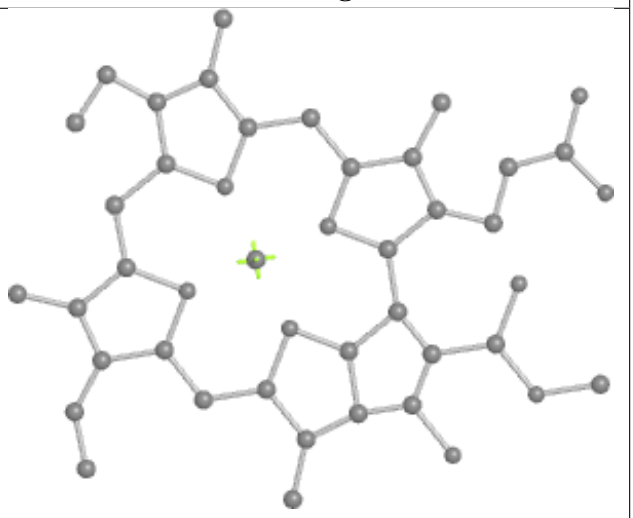
Bond lengths



Bond angles

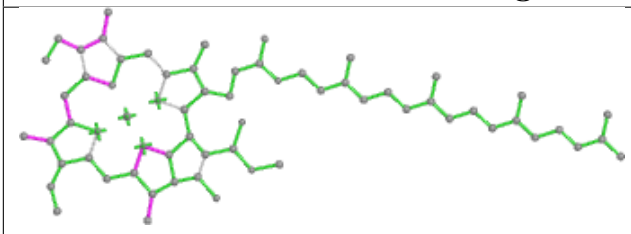


Torsions

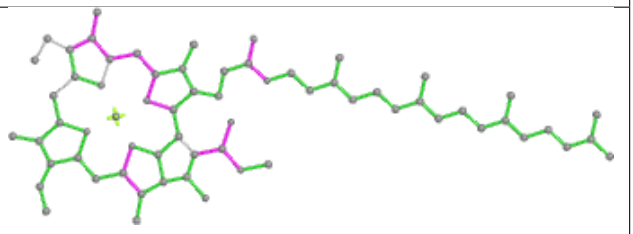


Rings

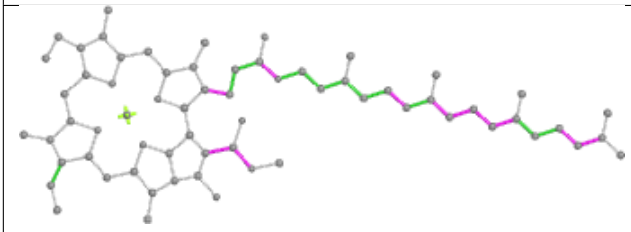
Ligand CLA bB 815



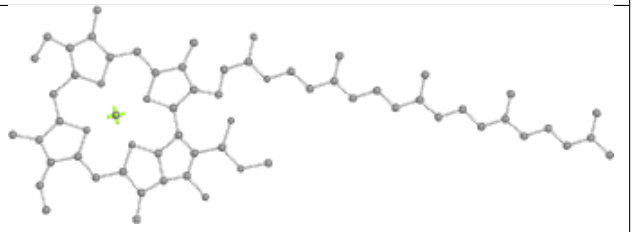
Bond lengths



Bond angles

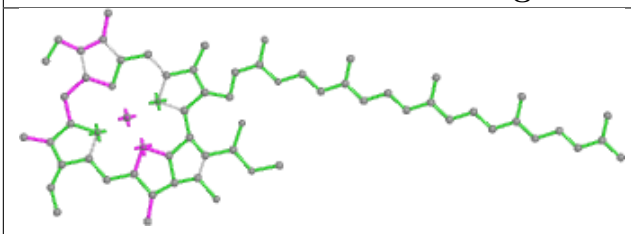


Torsions

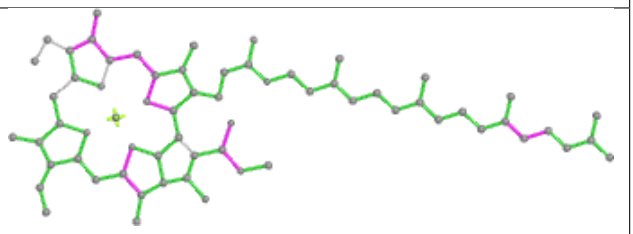


Rings

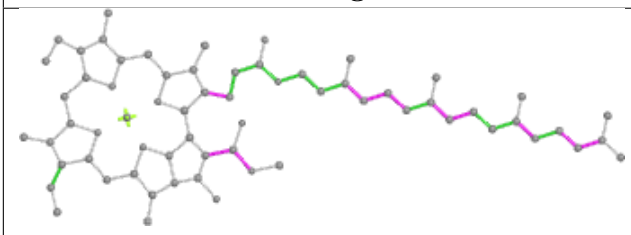
Ligand CLA bA 822



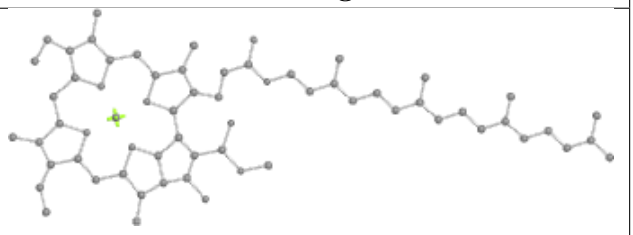
Bond lengths



Bond angles

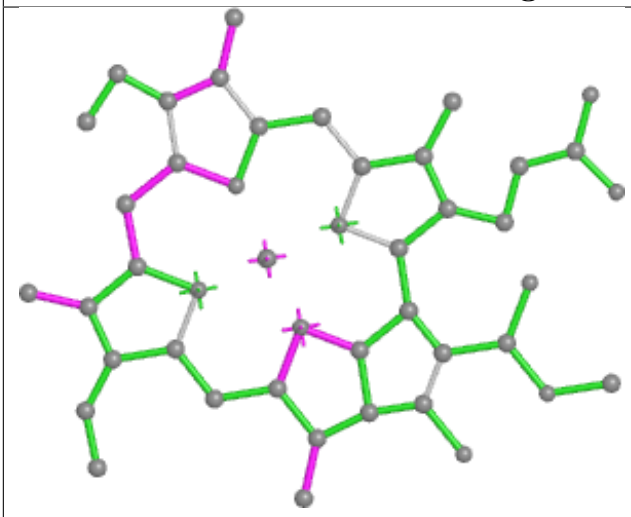


Torsions

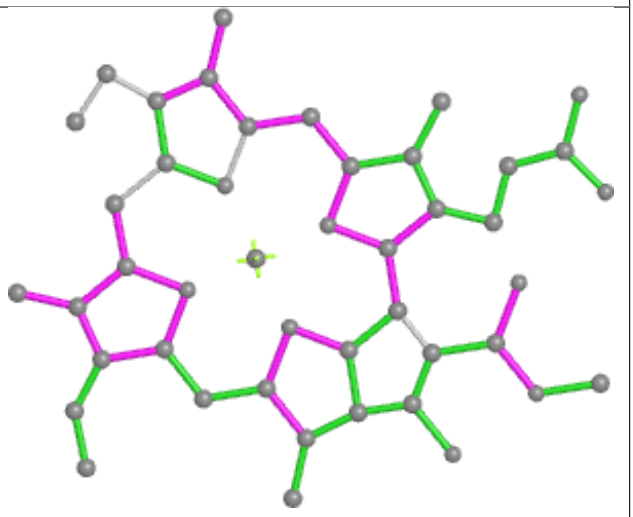


Rings

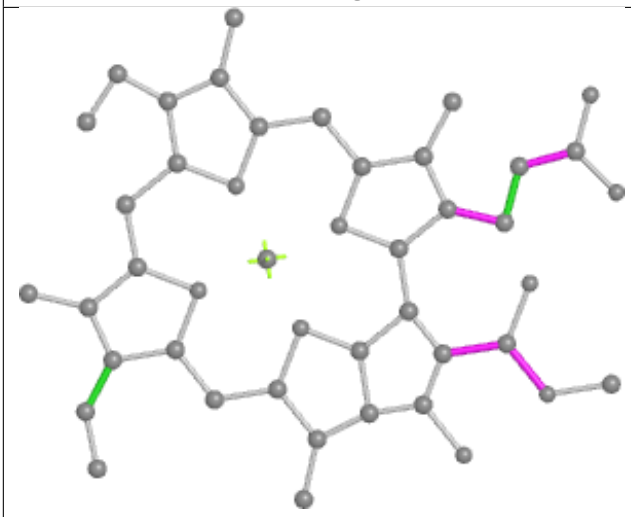
Ligand CLA a3 412



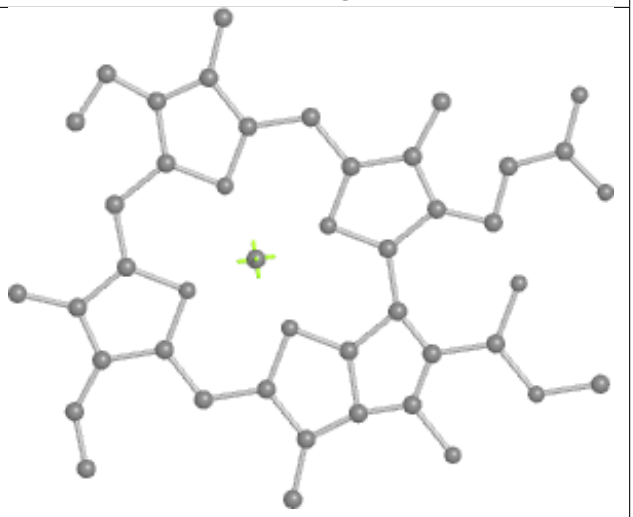
Bond lengths



Bond angles

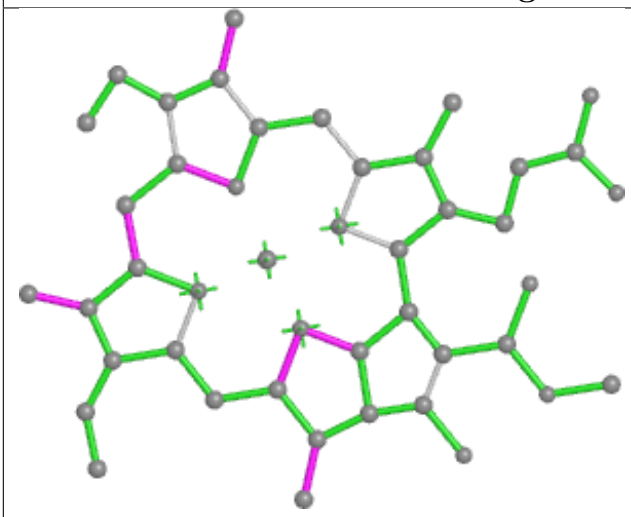


Torsions

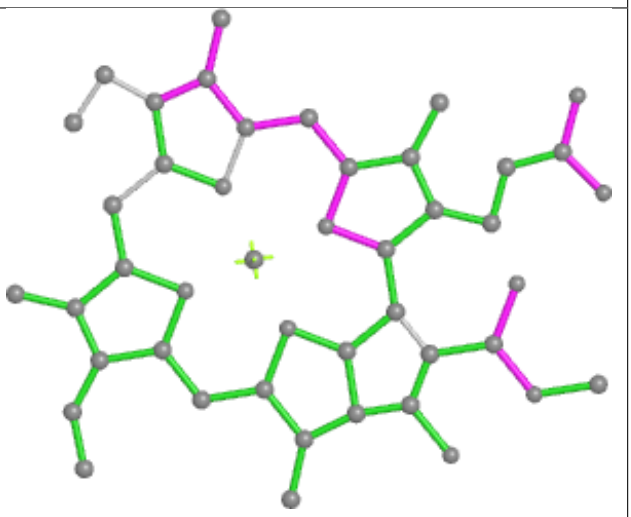


Rings

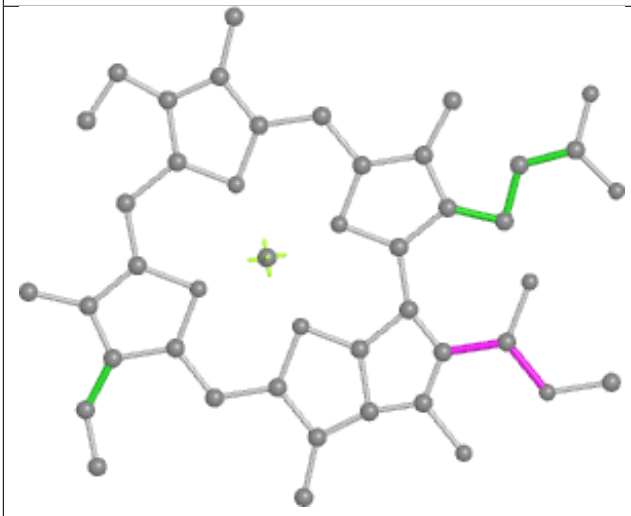
Ligand CLA b4 406



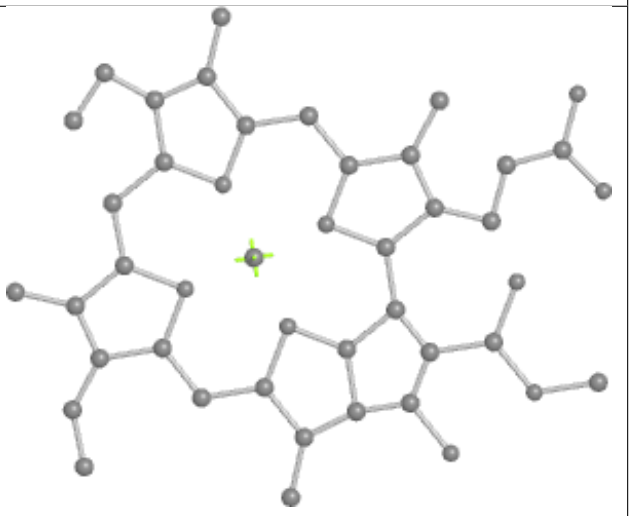
Bond lengths



Bond angles

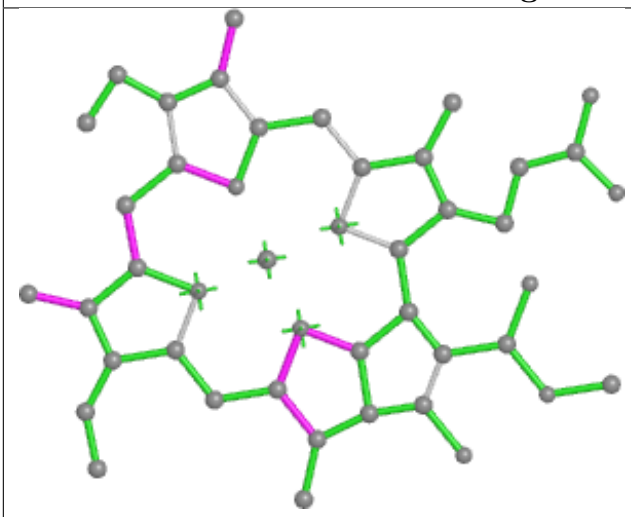


Torsions

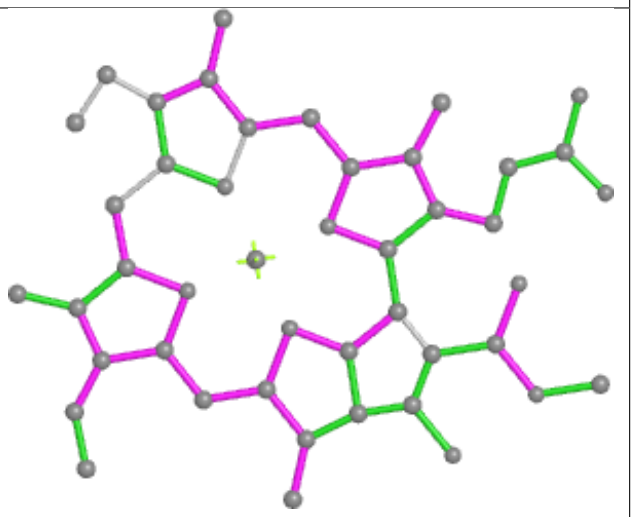


Rings

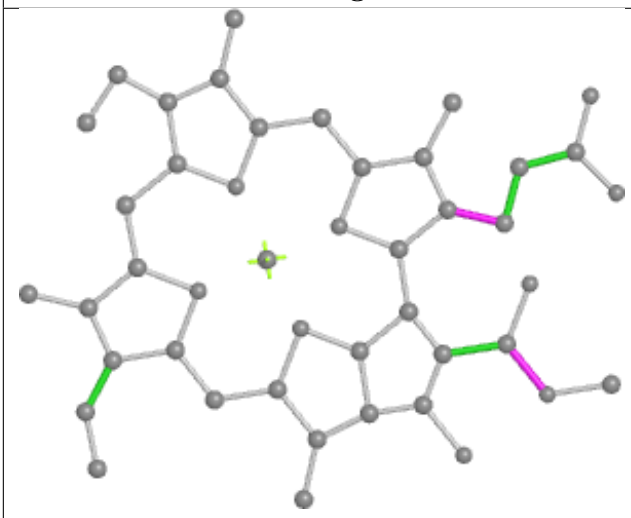
Ligand CLA c2 405



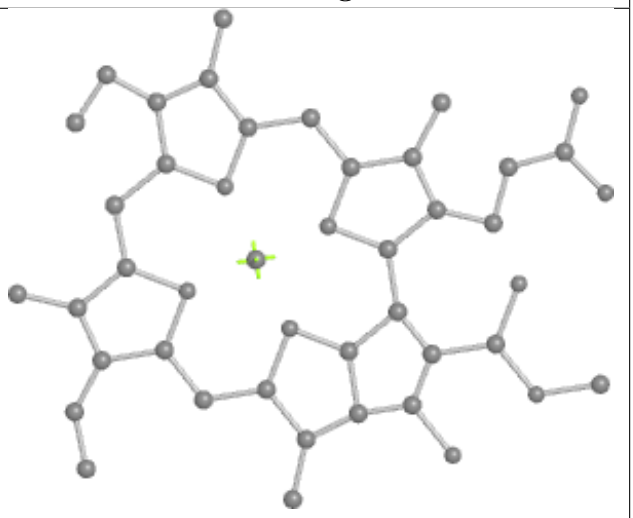
Bond lengths



Bond angles

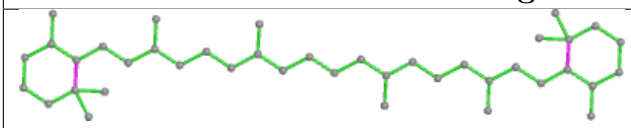


Torsions

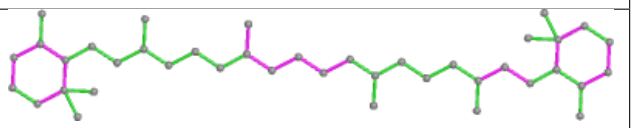


Rings

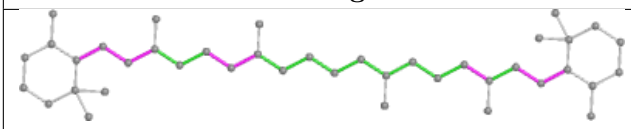
Ligand BCR a2 421



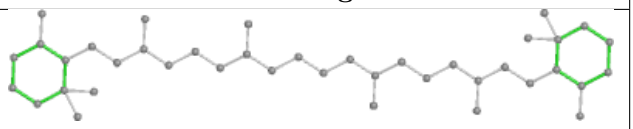
Bond lengths



Bond angles

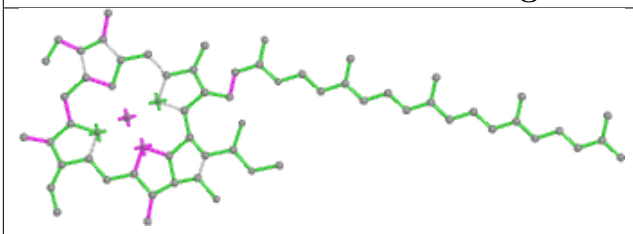


Torsions

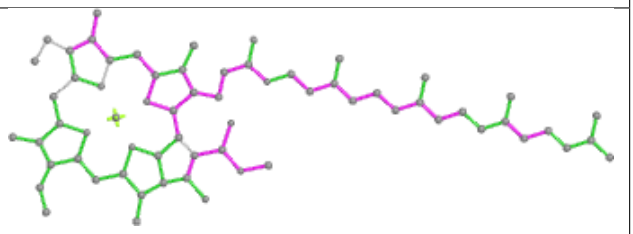


Rings

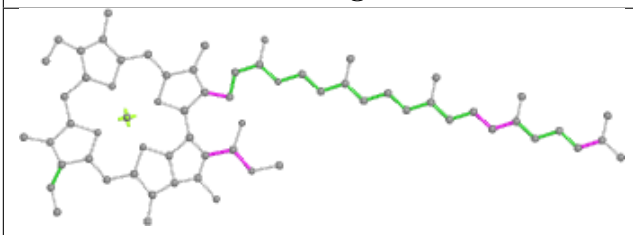
Ligand CLA c2 406



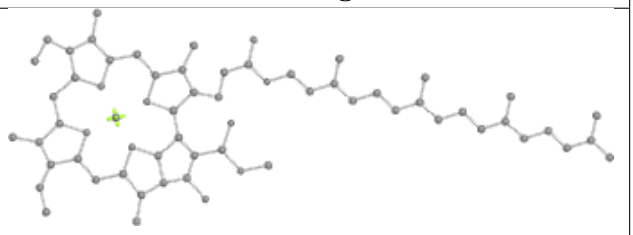
Bond lengths



Bond angles

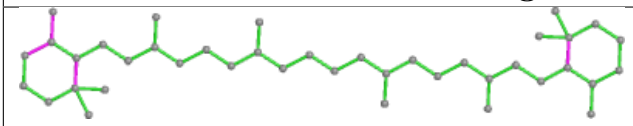


Torsions

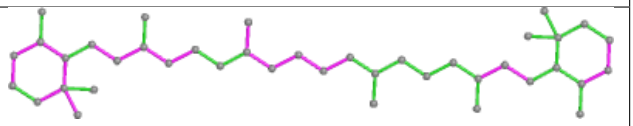


Rings

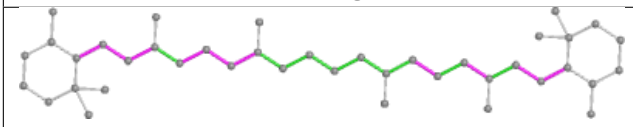
Ligand BCR c2 401



Bond lengths



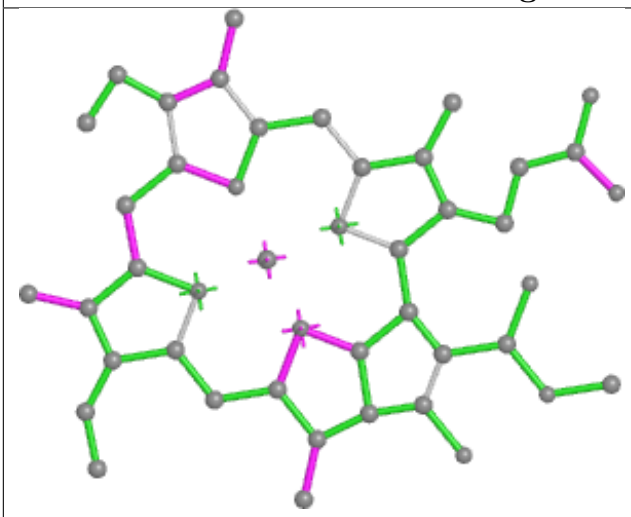
Bond angles



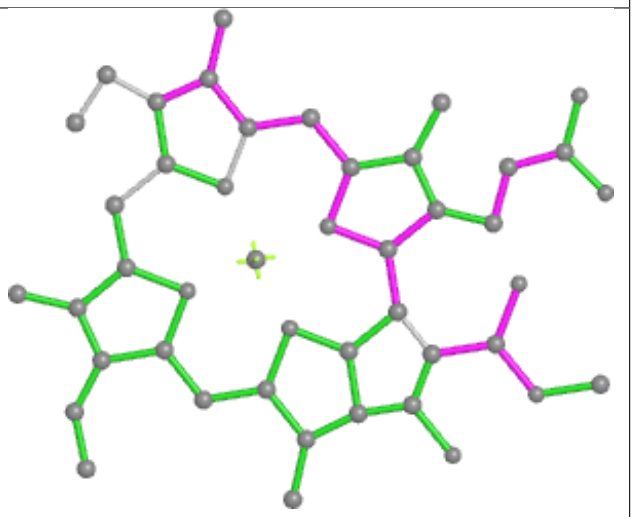
Torsions

Rings

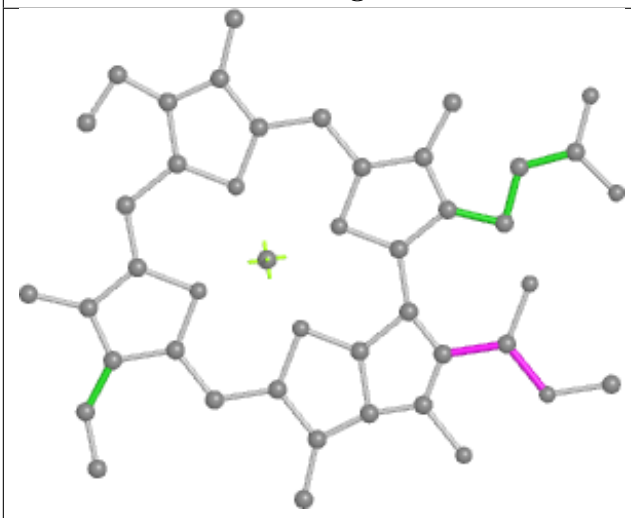
Ligand CLA aJ 202



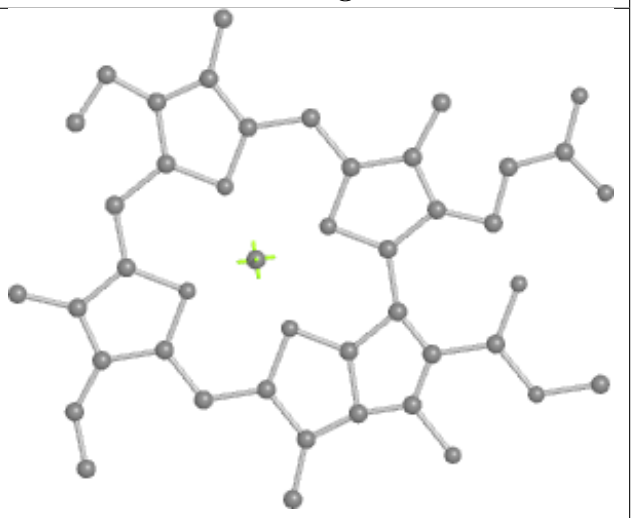
Bond lengths



Bond angles

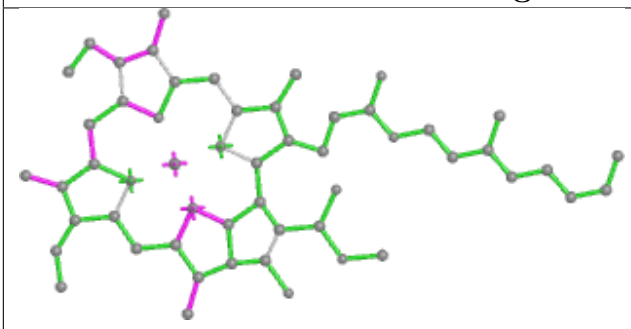


Torsions

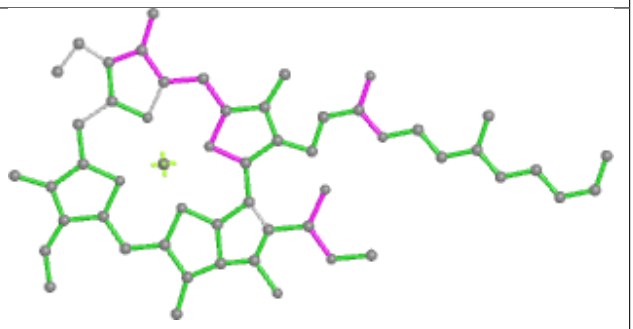


Rings

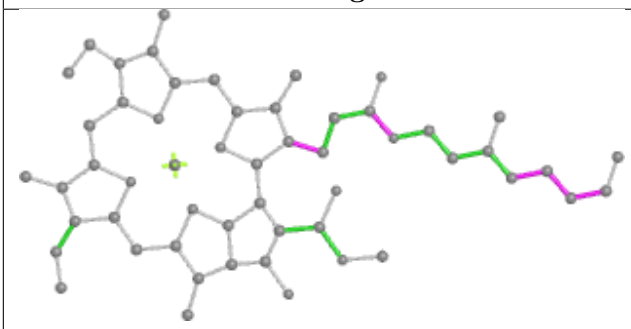
Ligand CLA bA 836



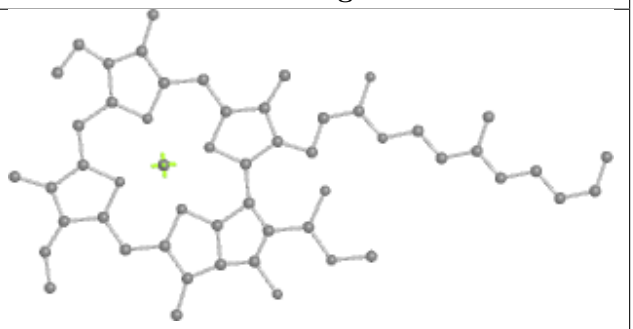
Bond lengths



Bond angles

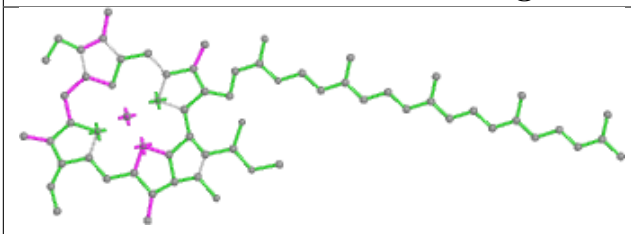


Torsions

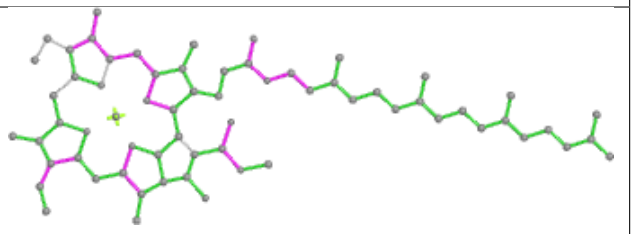


Rings

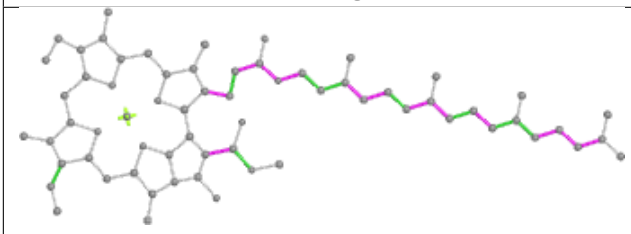
Ligand CLA aB 806



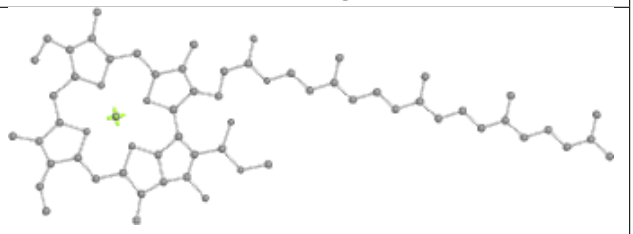
Bond lengths



Bond angles

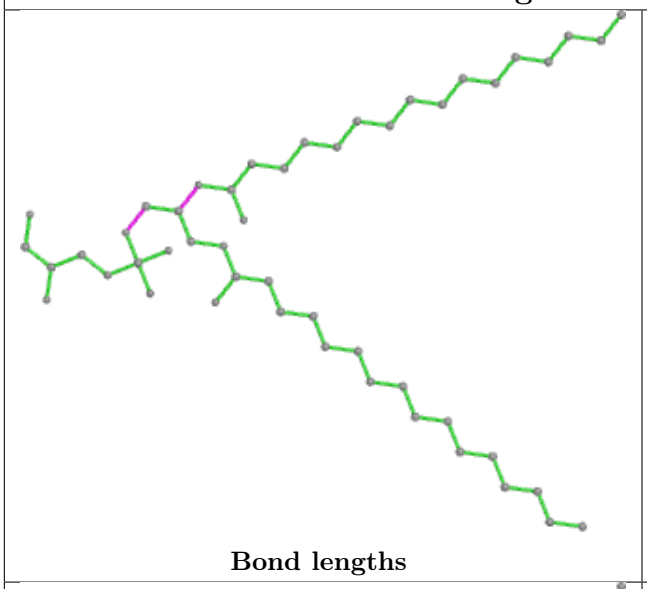


Torsions

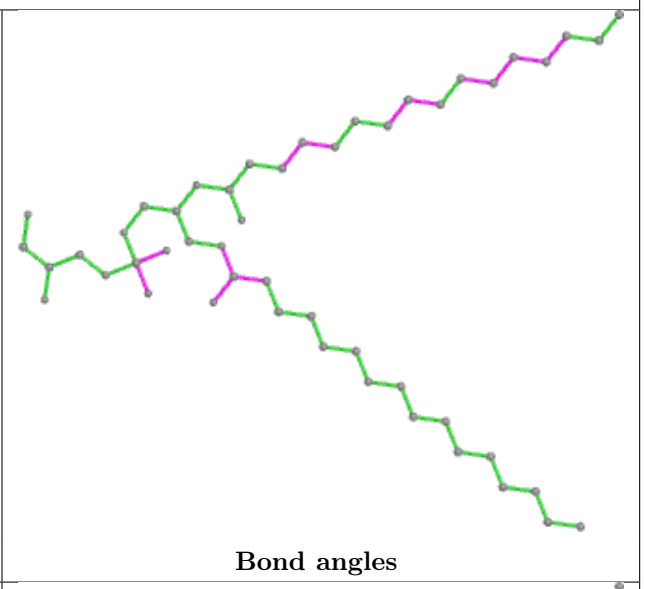


Rings

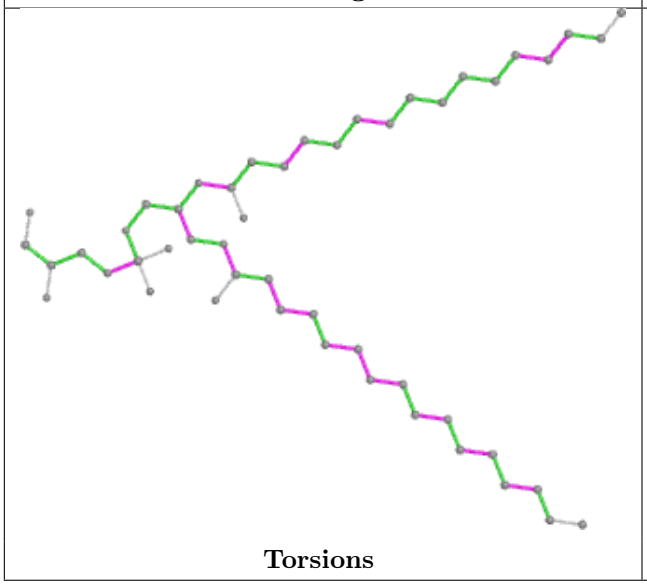
Ligand LHG cA 852



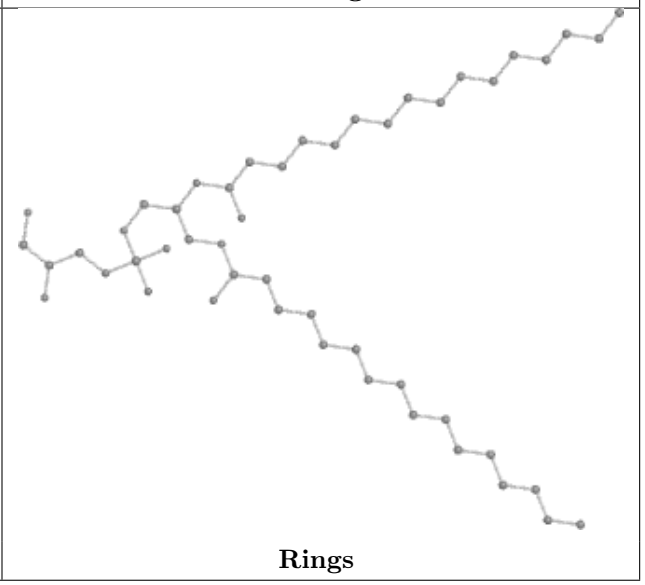
Bond lengths



Bond angles

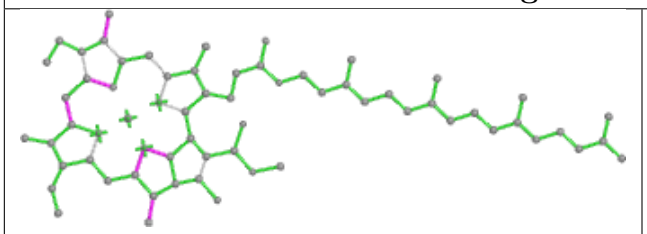


Torsions

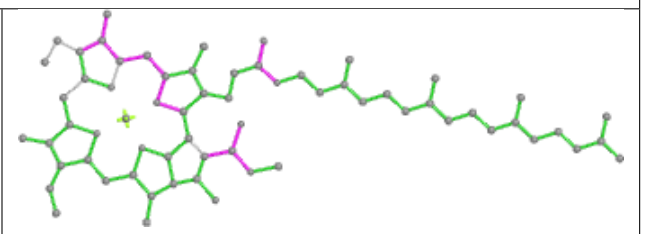


Rings

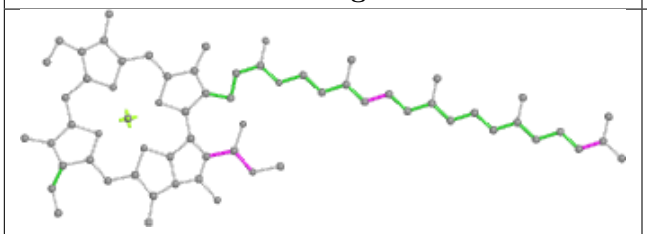
Ligand CLA a6 410



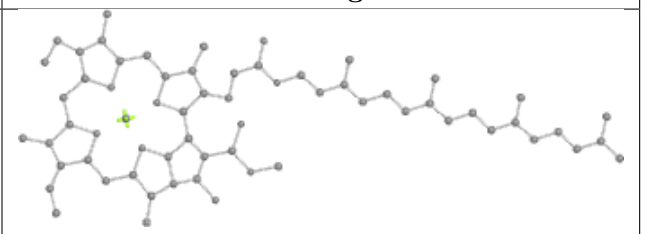
Bond lengths



Bond angles

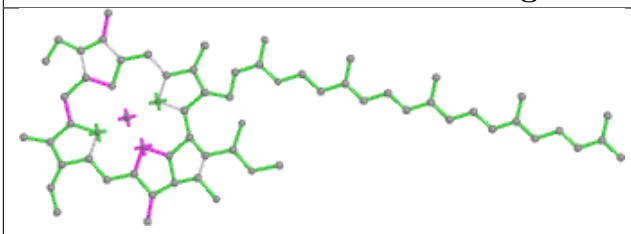


Torsions

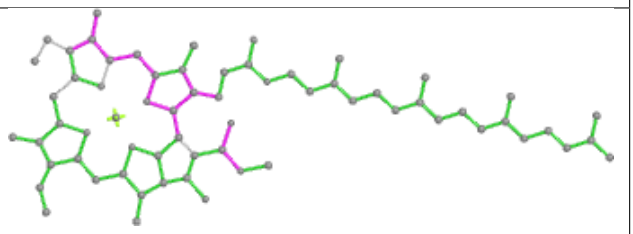


Rings

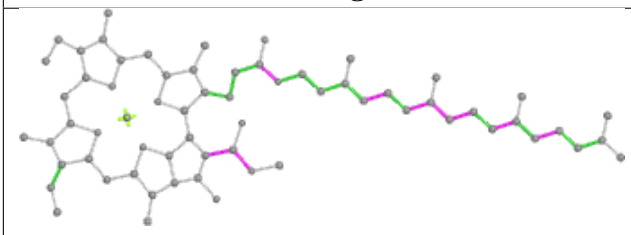
Ligand CLA c1 403



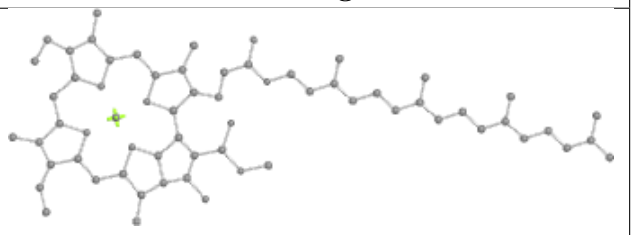
Bond lengths



Bond angles

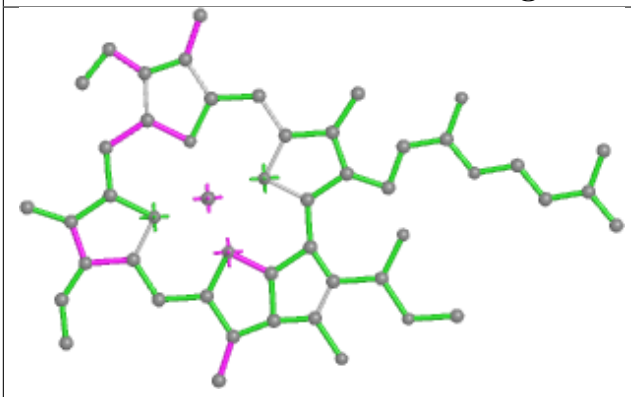


Torsions

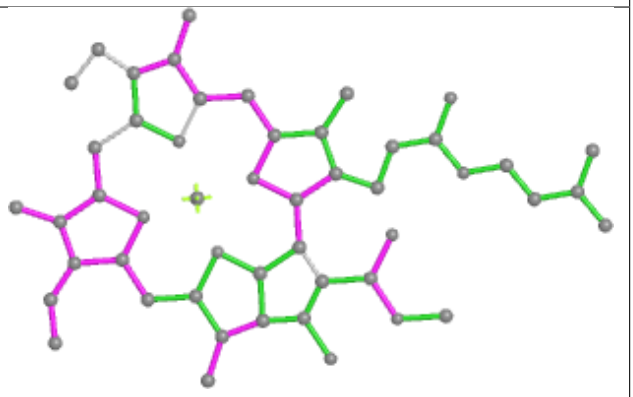


Rings

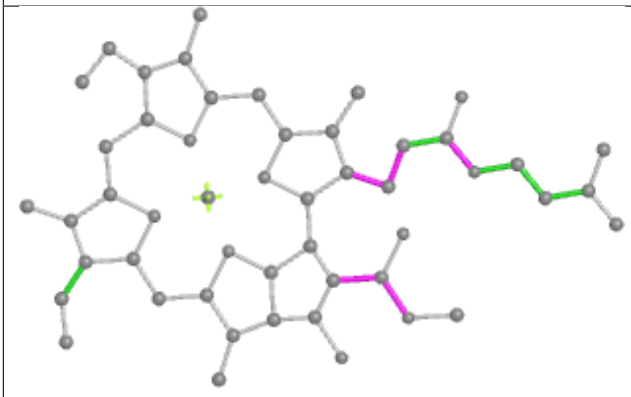
Ligand CLA a4 416



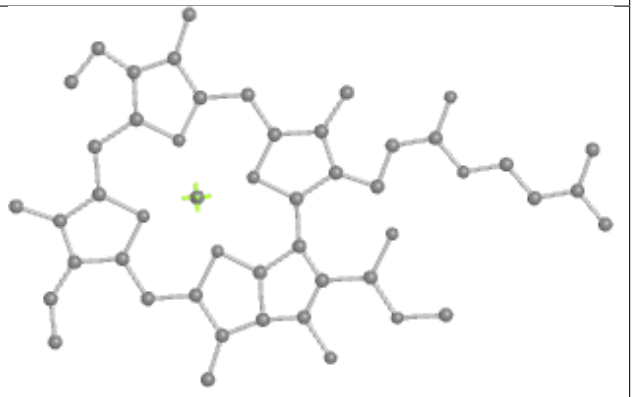
Bond lengths



Bond angles

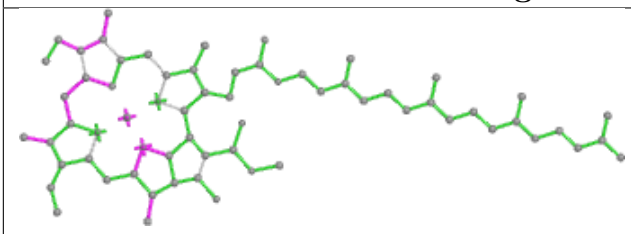


Torsions

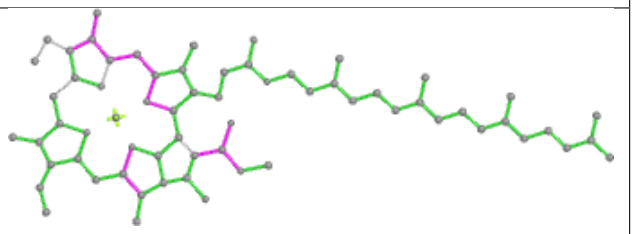


Rings

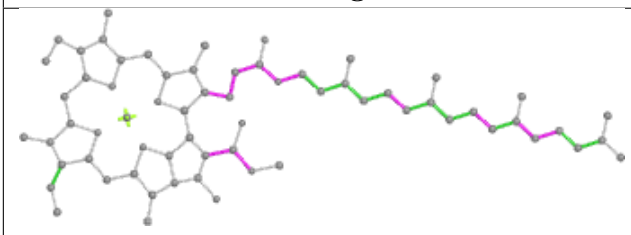
Ligand CLA bB 829



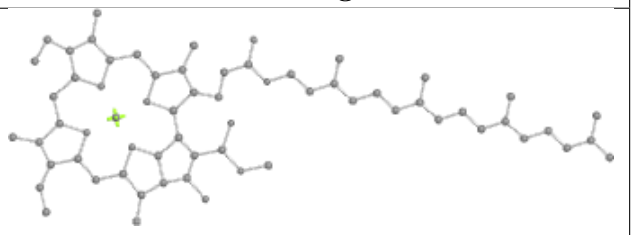
Bond lengths



Bond angles

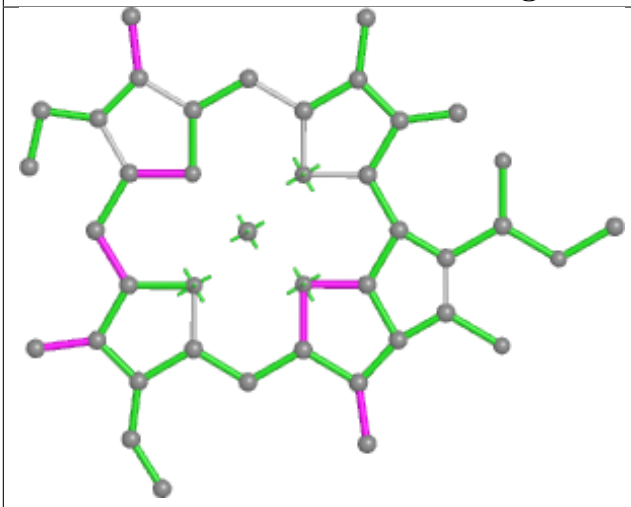


Torsions

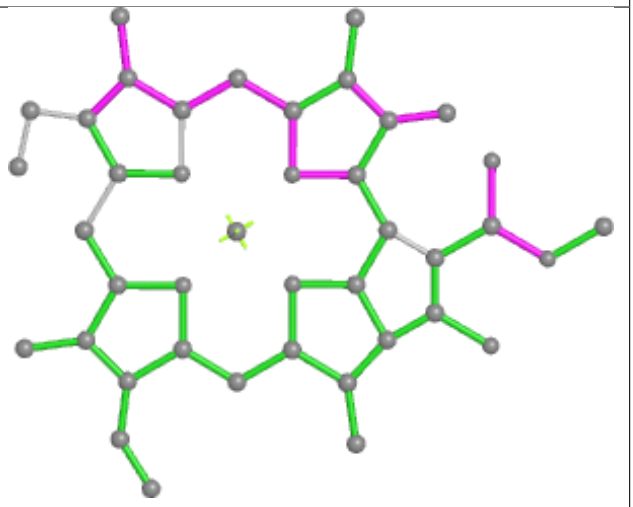


Rings

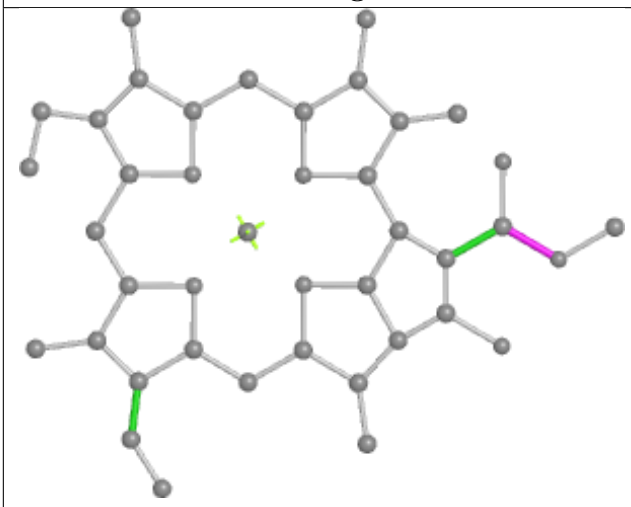
Ligand CLA c2 415



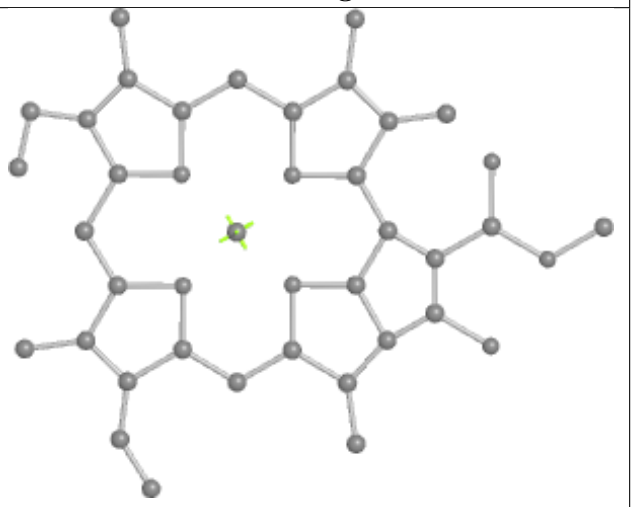
Bond lengths



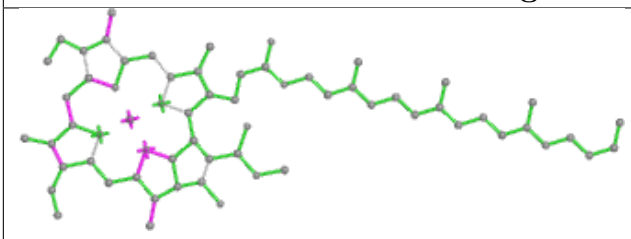
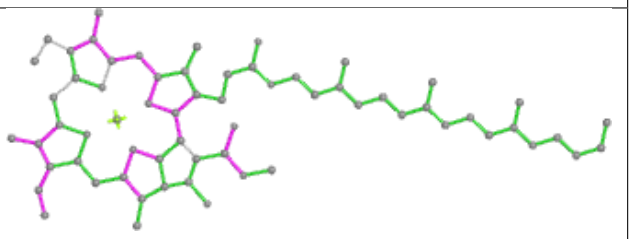
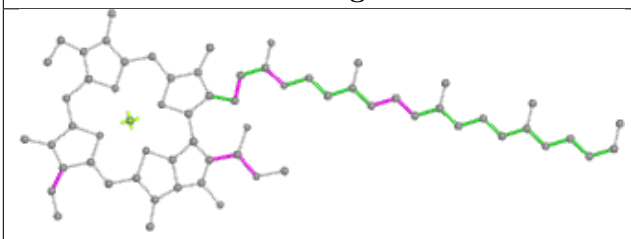
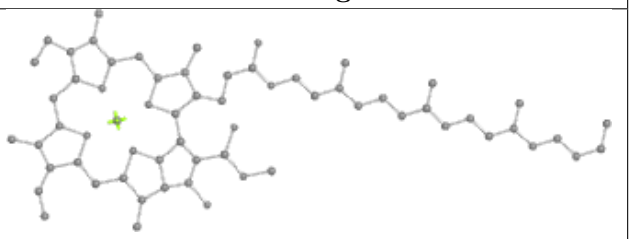
Bond angles

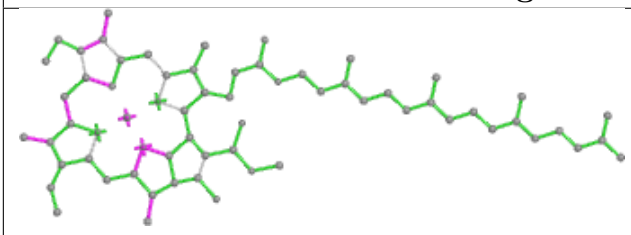
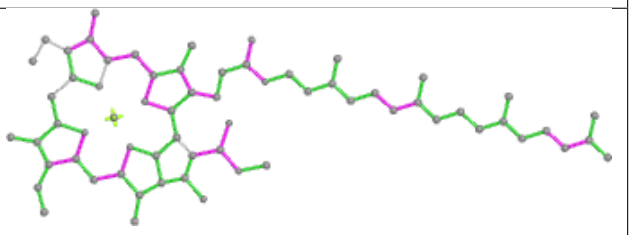
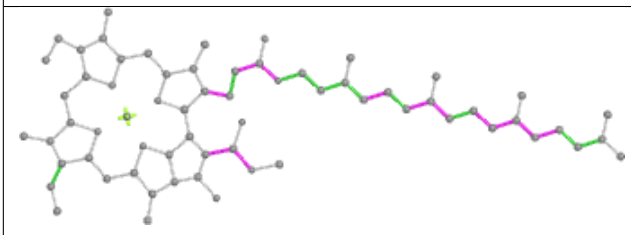
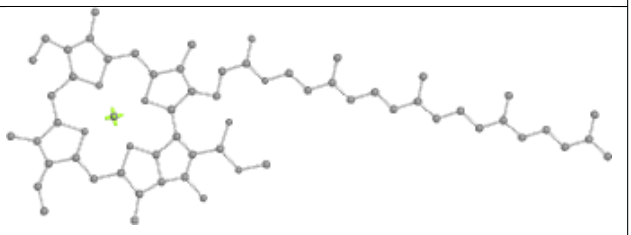


Torsions

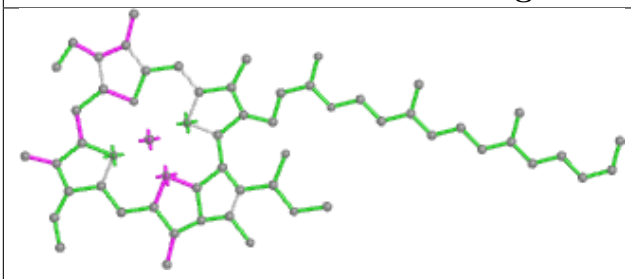


Rings

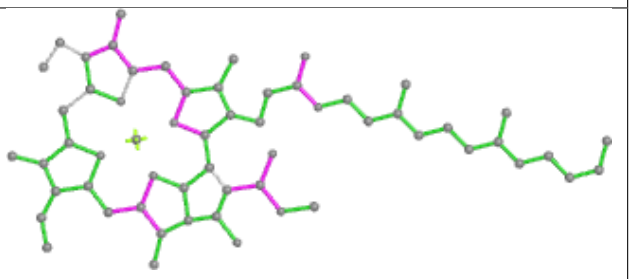
Ligand CLA c6 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cB 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

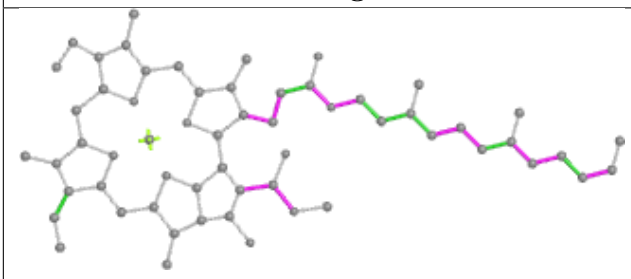
Ligand CLA aA 825



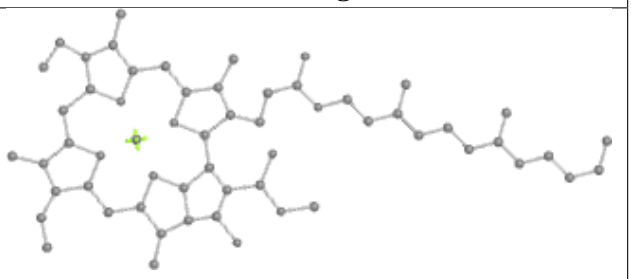
Bond lengths



Bond angles

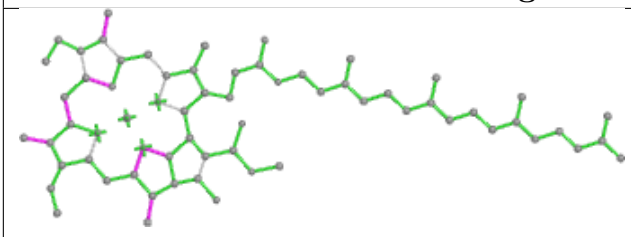


Torsions

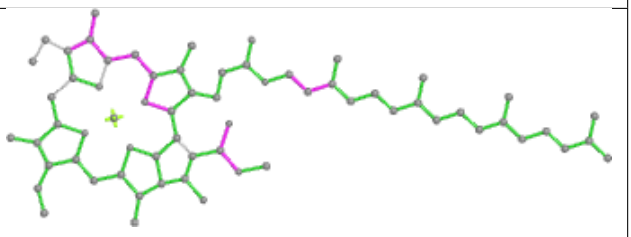


Rings

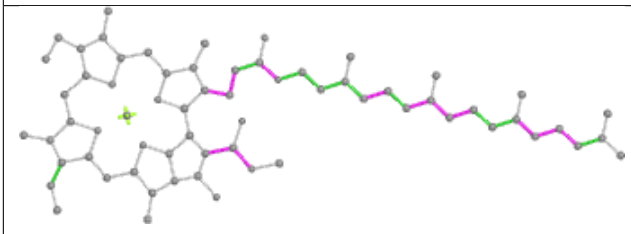
Ligand CLA b1 402



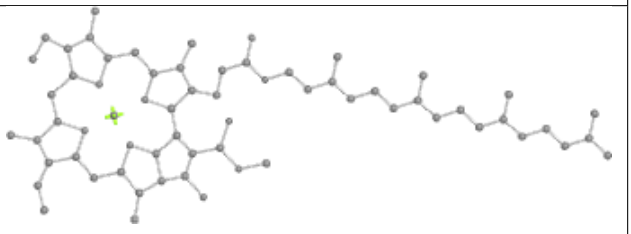
Bond lengths



Bond angles

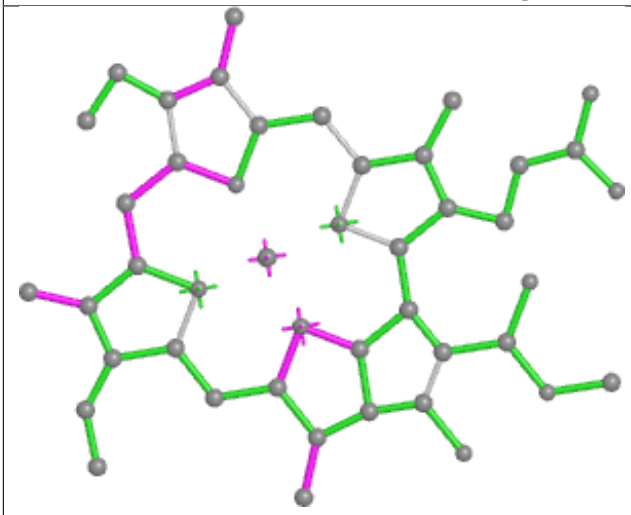


Torsions

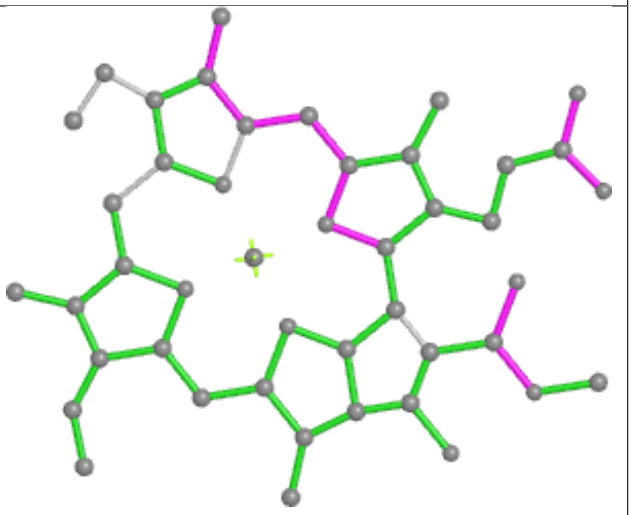


Rings

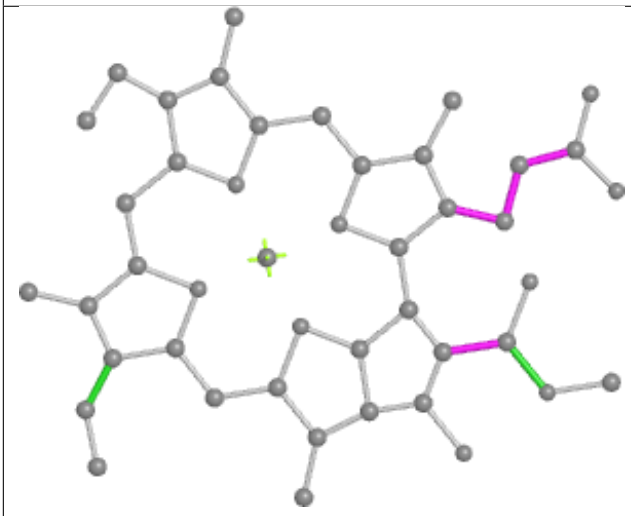
Ligand CLA cB 831



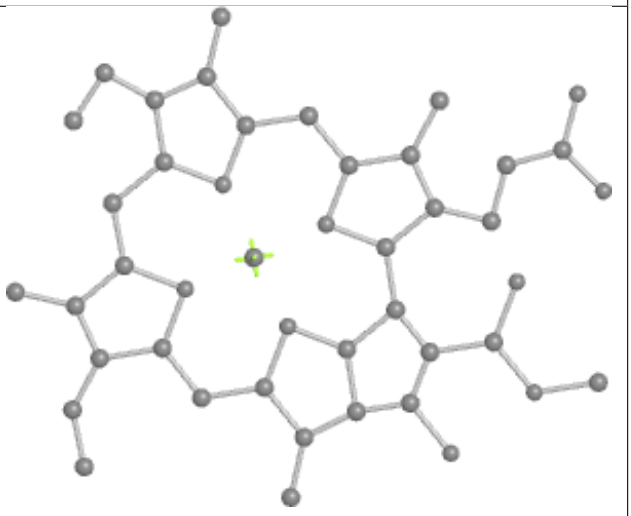
Bond lengths



Bond angles

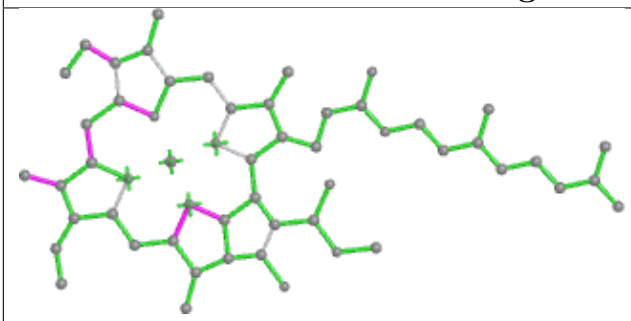


Torsions

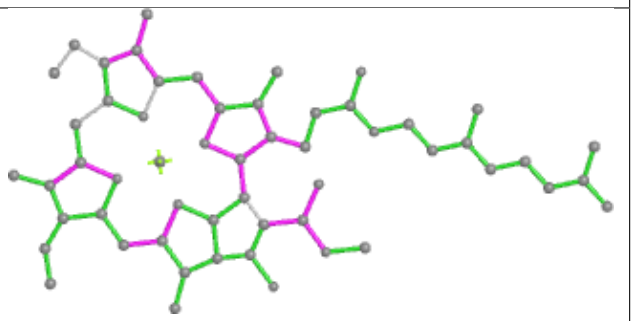


Rings

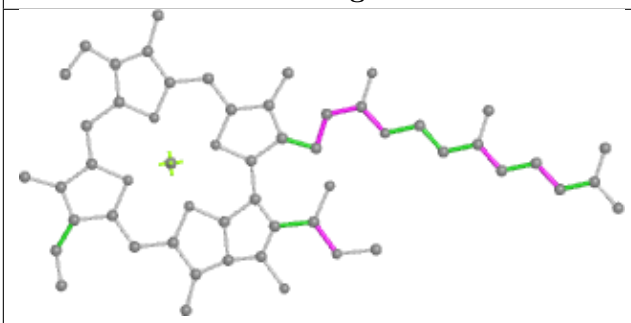
Ligand CLA b2 418



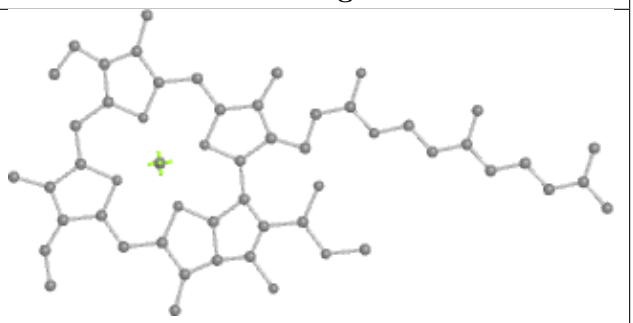
Bond lengths



Bond angles

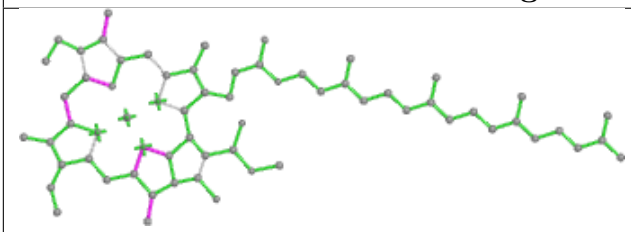


Torsions

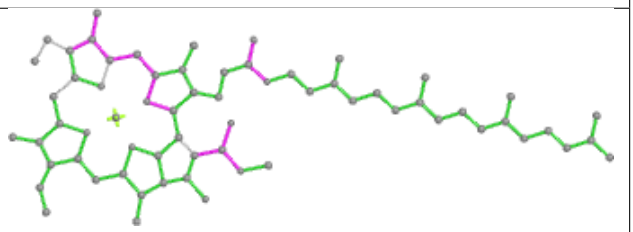


Rings

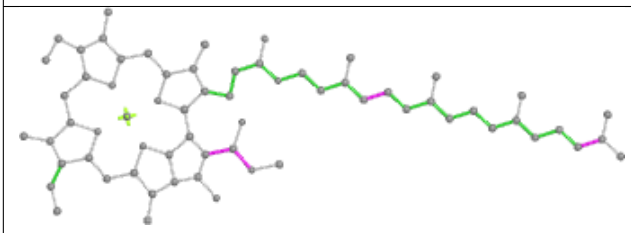
Ligand CLA c2 410



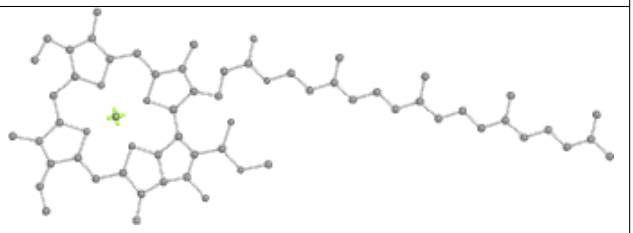
Bond lengths



Bond angles

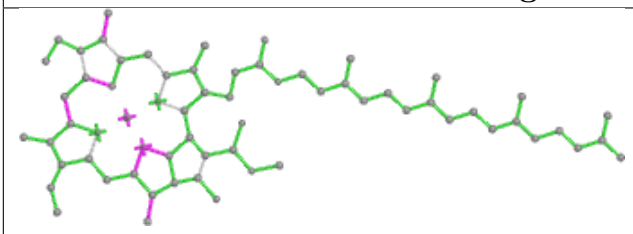


Torsions

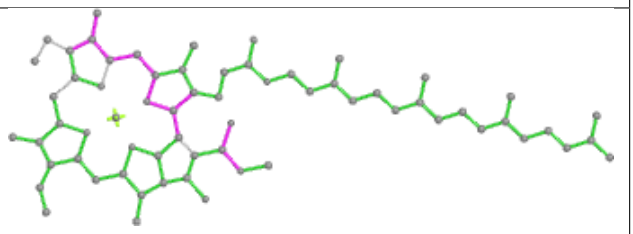


Rings

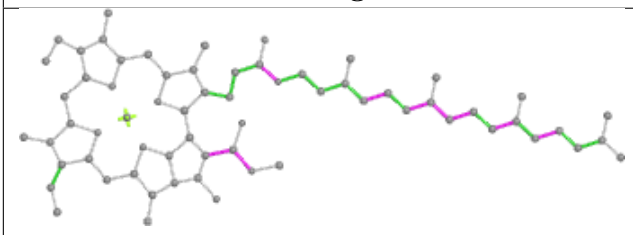
Ligand CLA a2 403



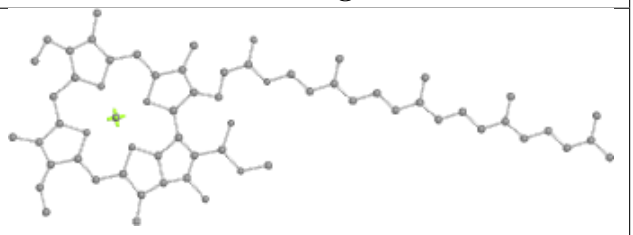
Bond lengths



Bond angles

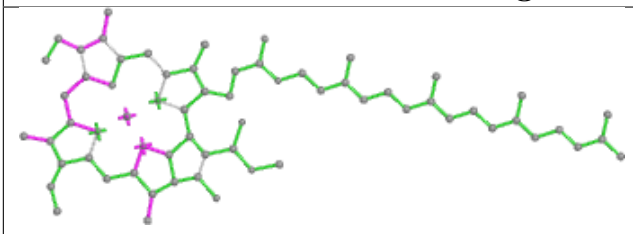


Torsions

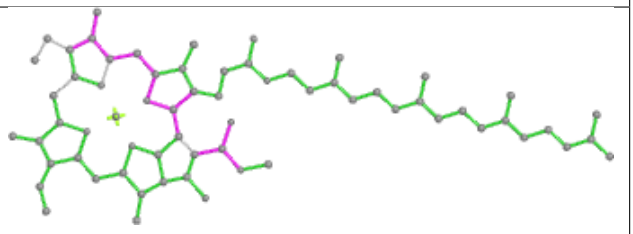


Rings

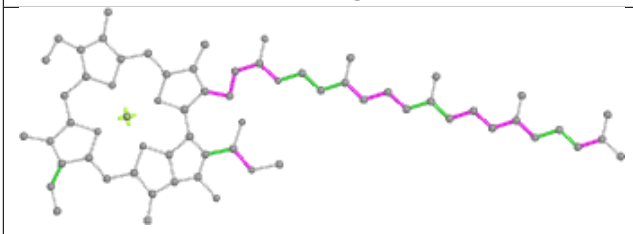
Ligand CLA aB 828



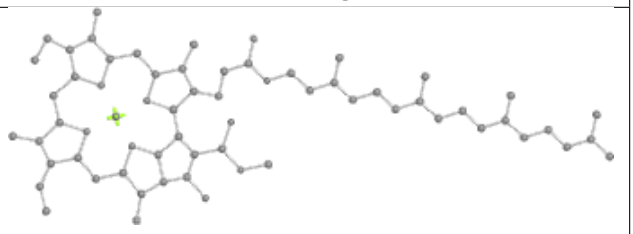
Bond lengths



Bond angles

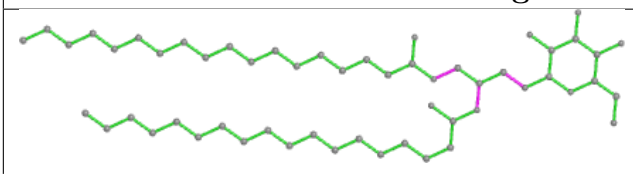


Torsions

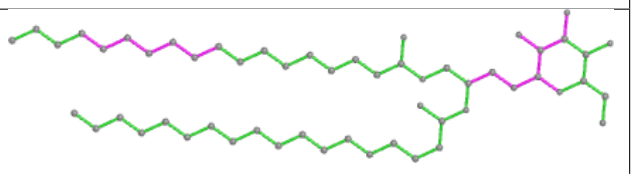


Rings

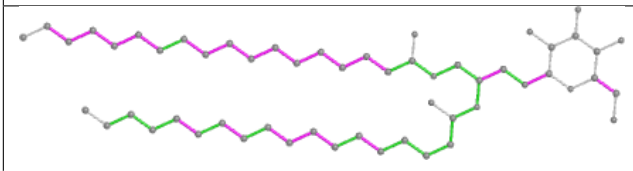
Ligand LMG cB 850



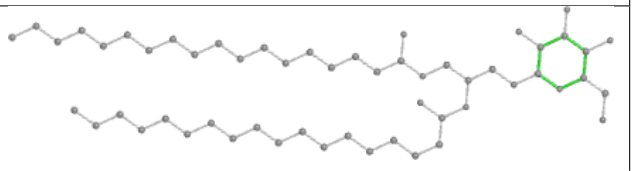
Bond lengths



Bond angles

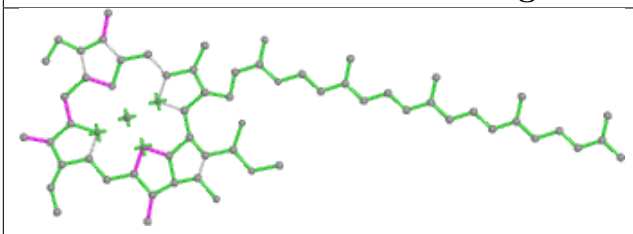


Torsions

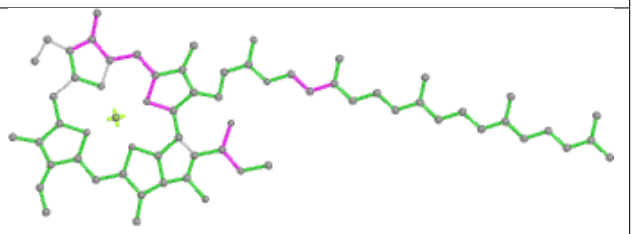


Rings

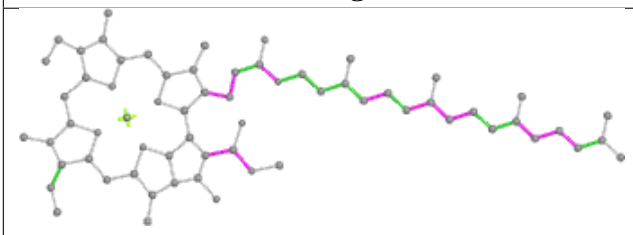
Ligand CLA b5 402



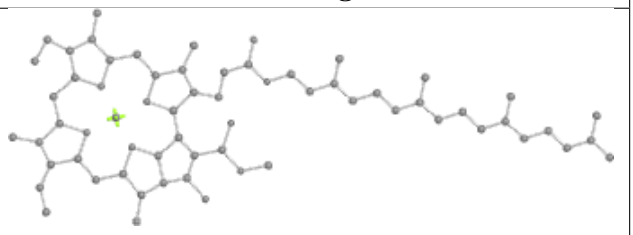
Bond lengths



Bond angles

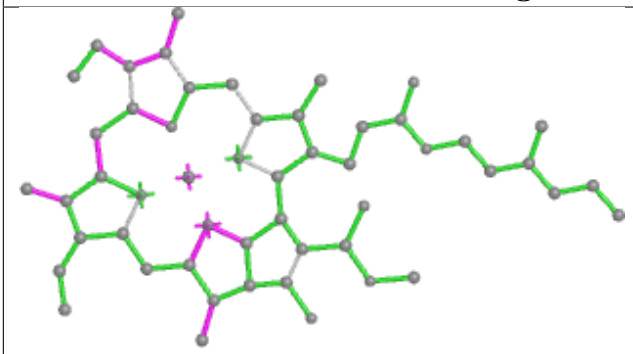


Torsions

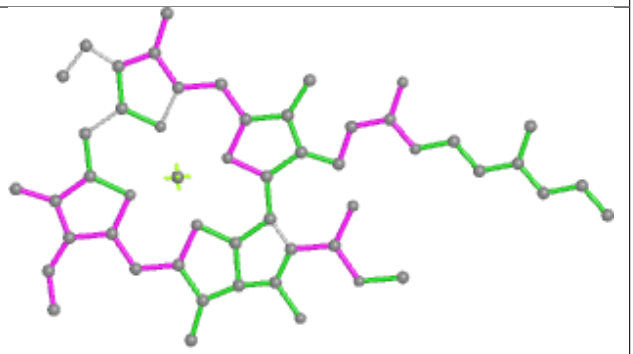


Rings

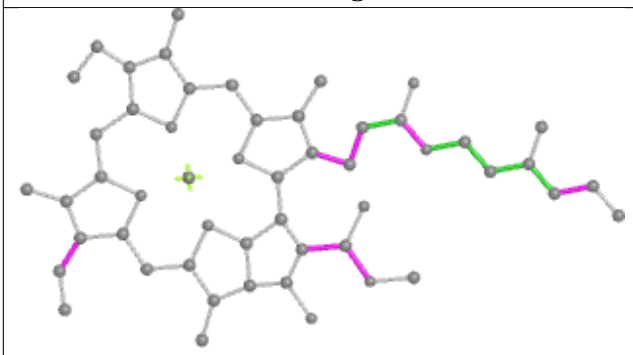
Ligand CLA aA 845



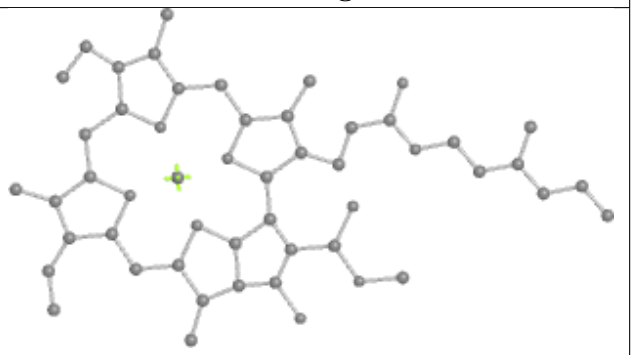
Bond lengths



Bond angles

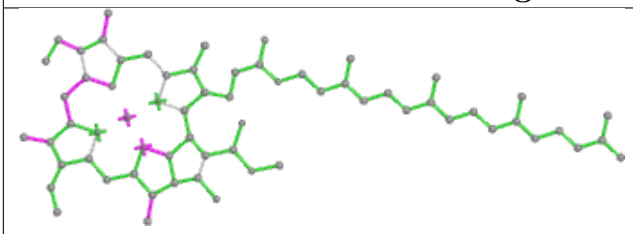


Torsions

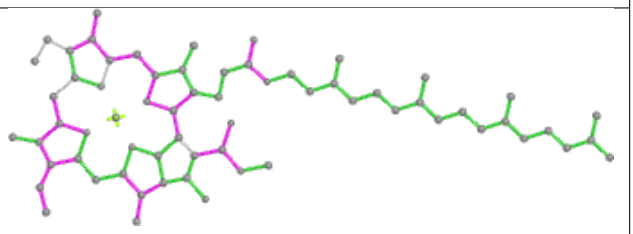


Rings

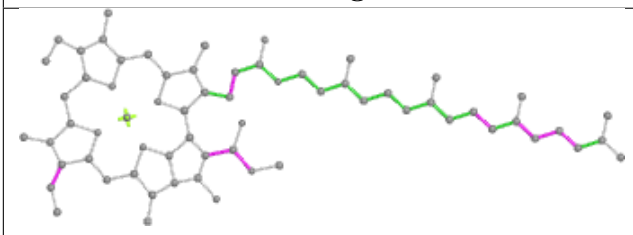
Ligand CLA bB 804



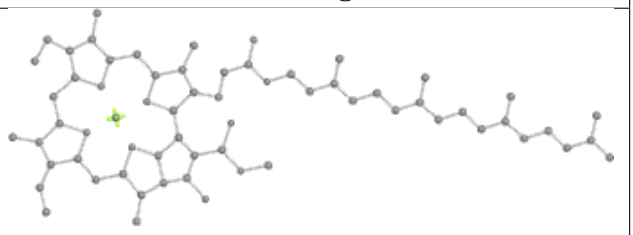
Bond lengths



Bond angles

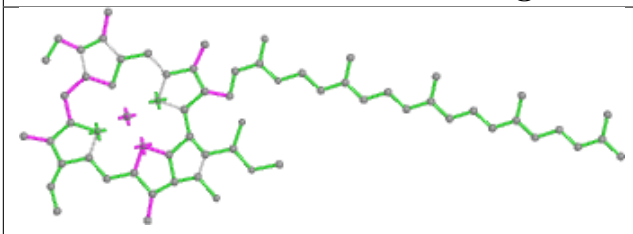


Torsions

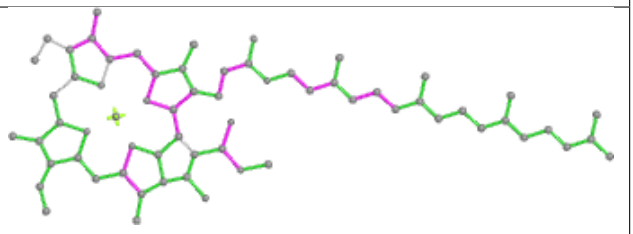


Rings

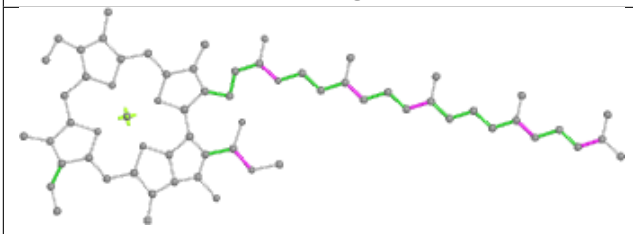
Ligand CLA cA 834



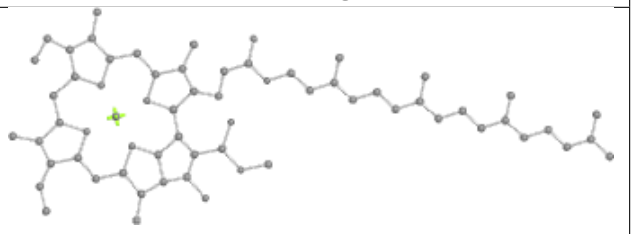
Bond lengths



Bond angles

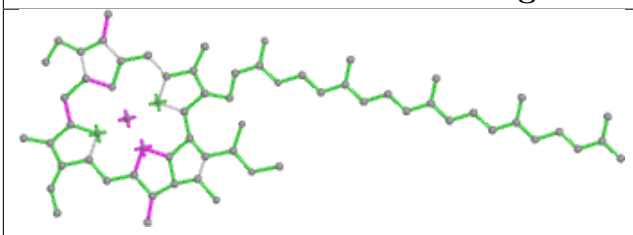


Torsions

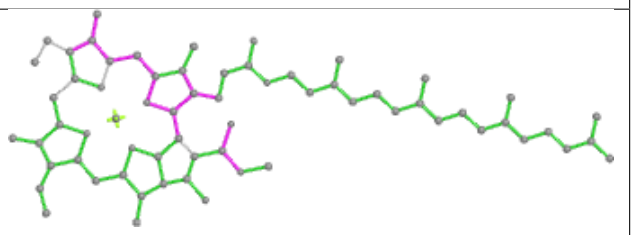


Rings

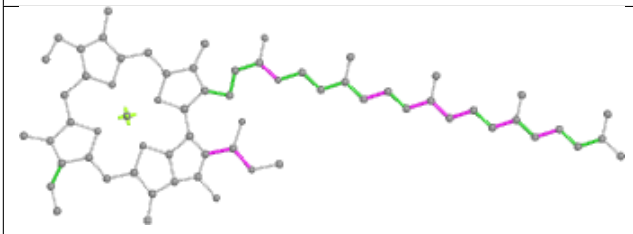
Ligand CLA b6 404



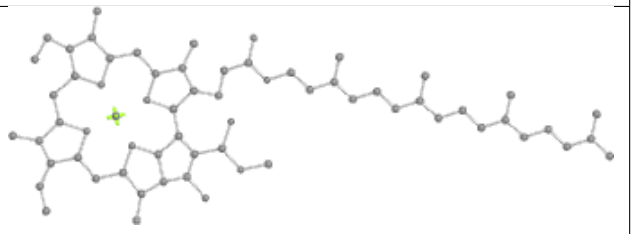
Bond lengths



Bond angles

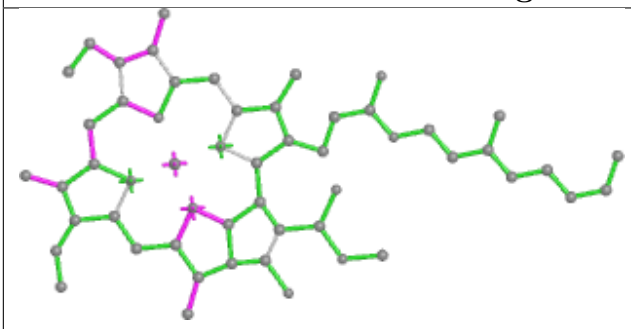


Torsions

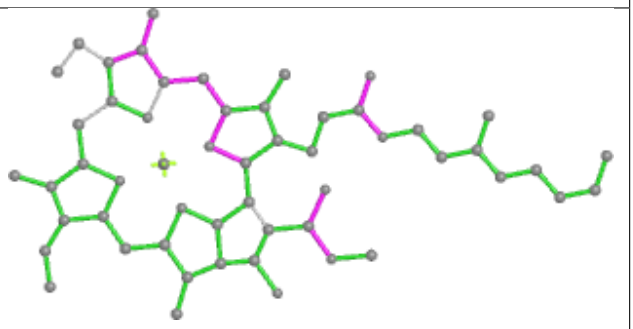


Rings

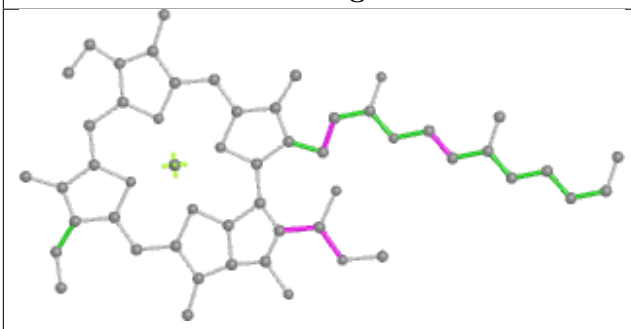
Ligand CLA aB 805



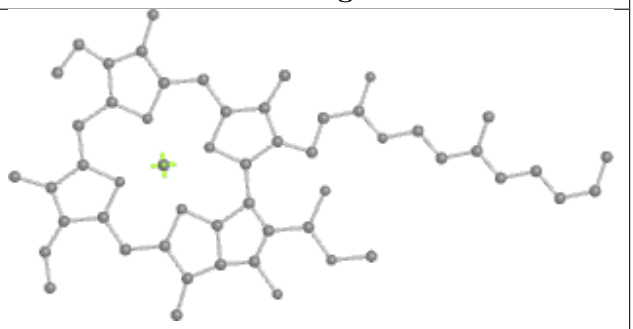
Bond lengths



Bond angles

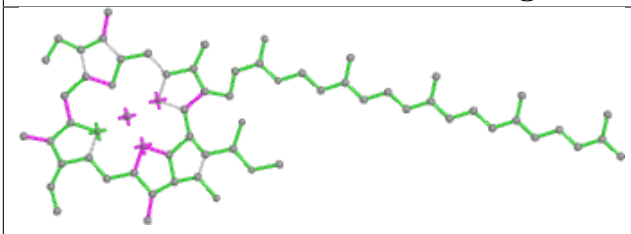


Torsions

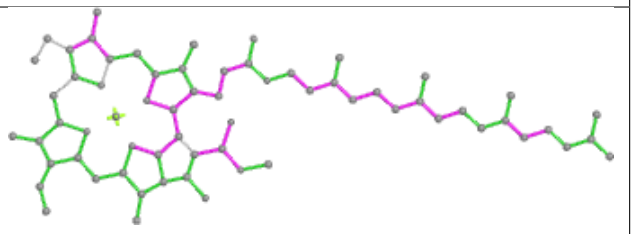


Rings

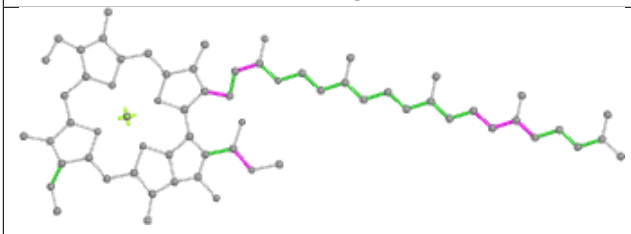
Ligand CLA b3 421



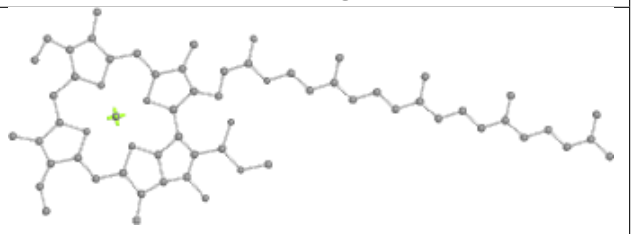
Bond lengths



Bond angles

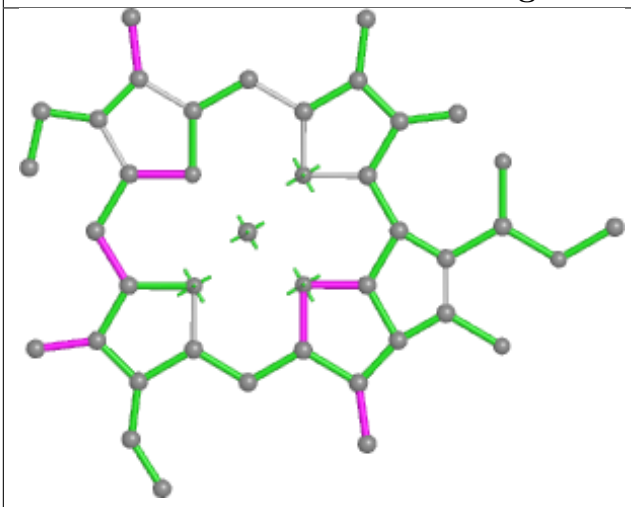


Torsions

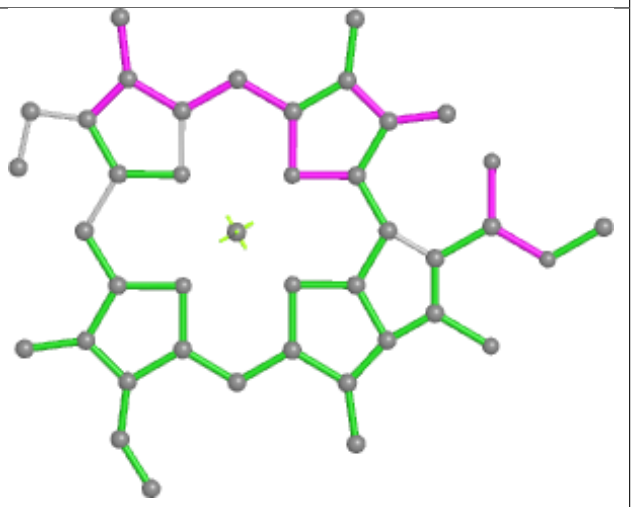


Rings

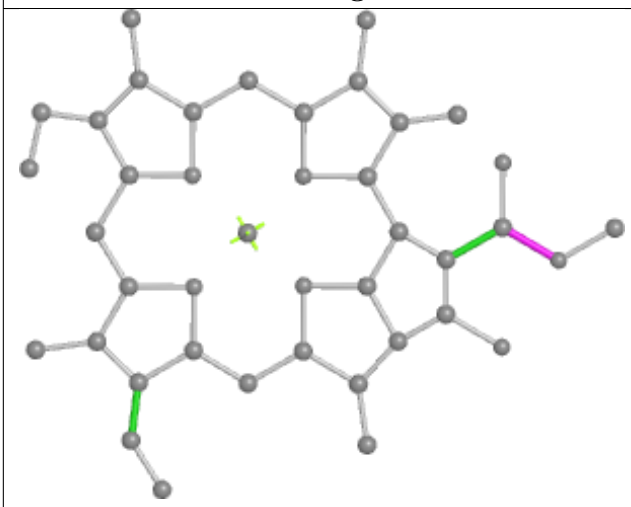
Ligand CLA b6 415



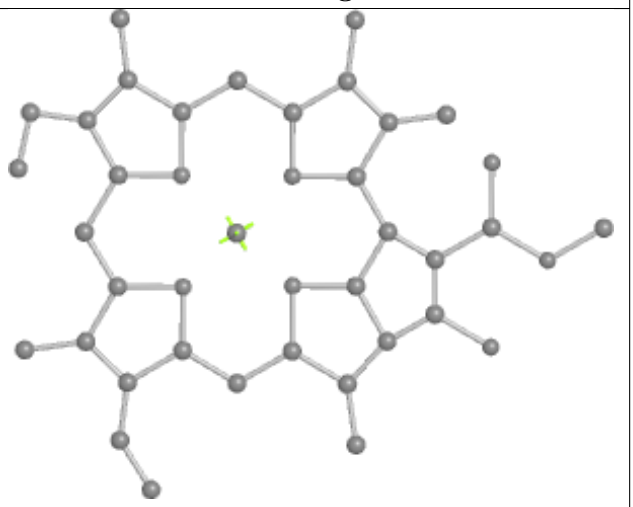
Bond lengths



Bond angles

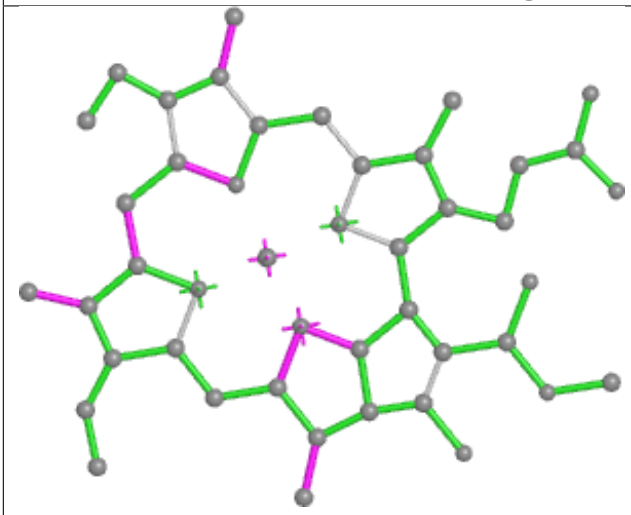


Torsions

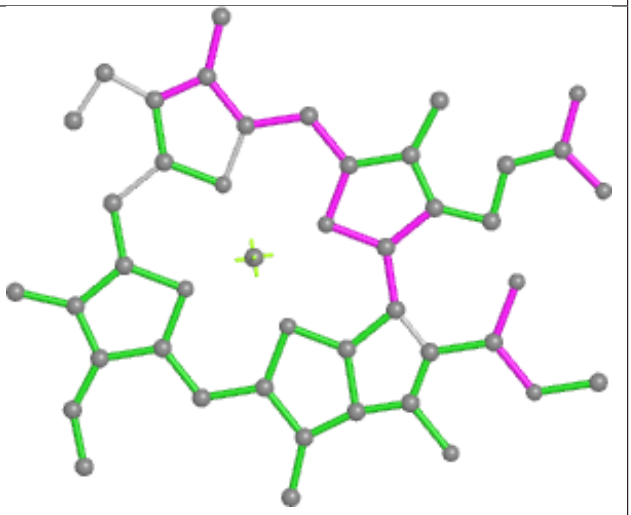


Rings

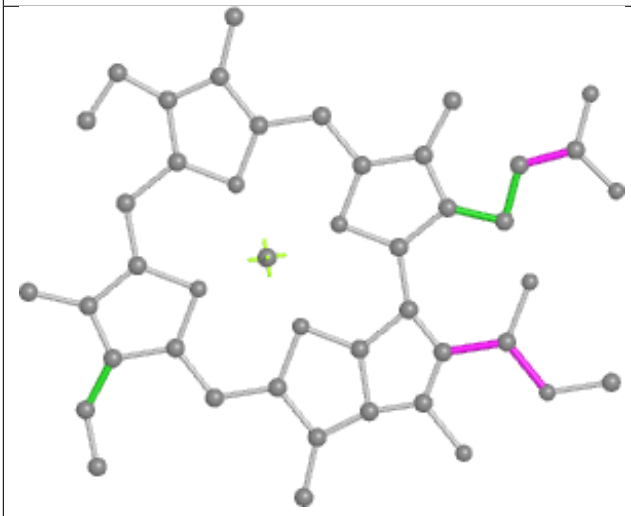
Ligand CLA c2 408



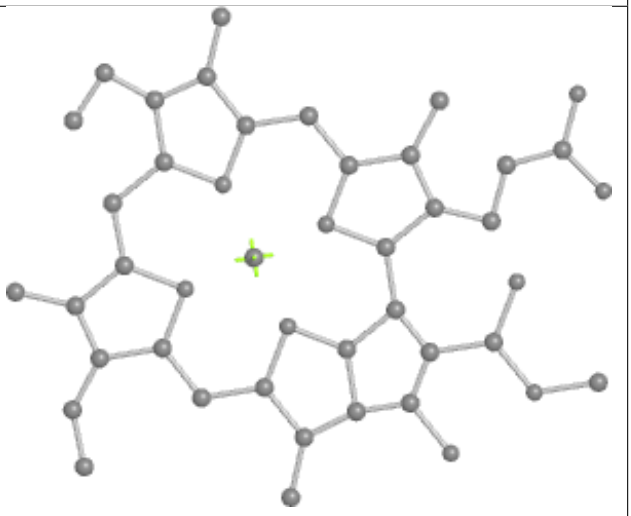
Bond lengths



Bond angles

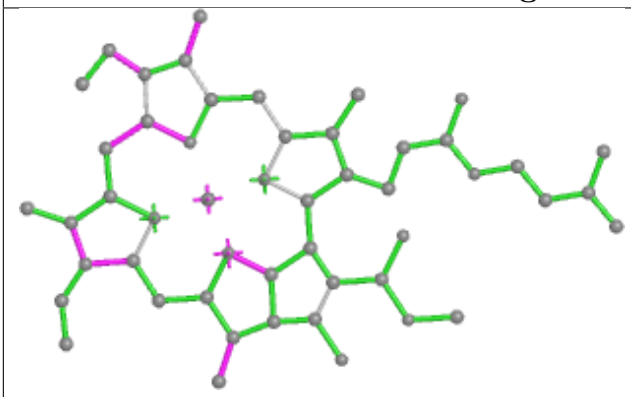


Torsions

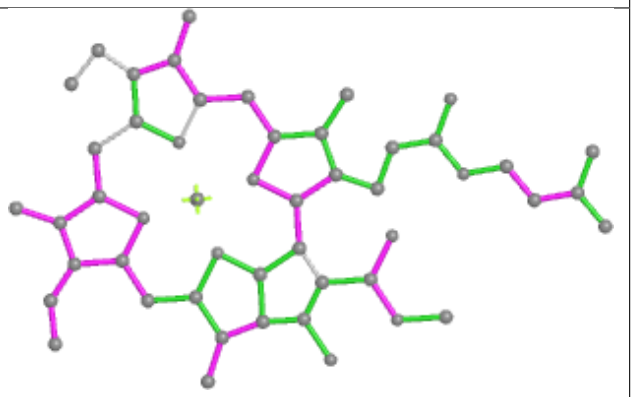


Rings

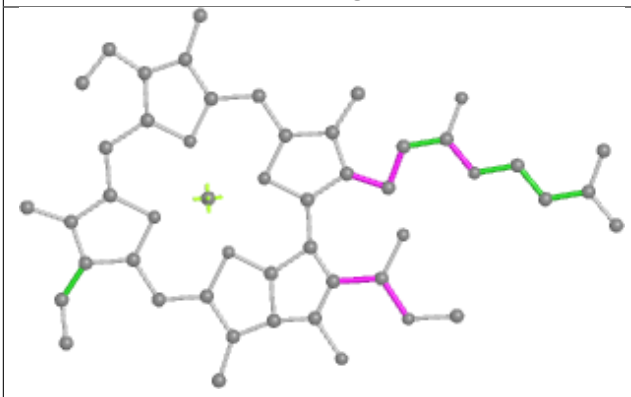
Ligand CLA a6 417



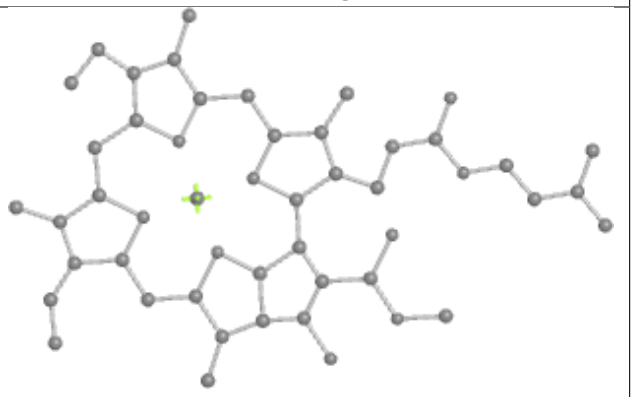
Bond lengths



Bond angles

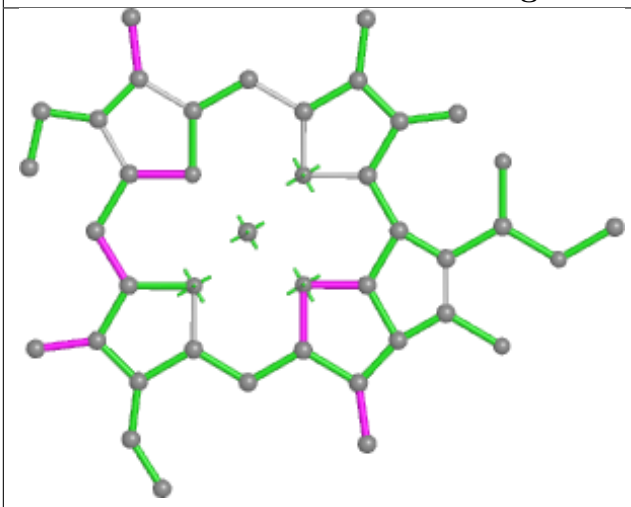


Torsions

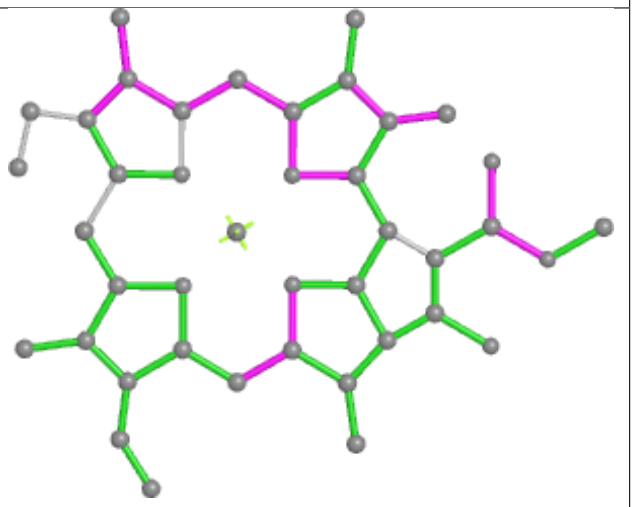


Rings

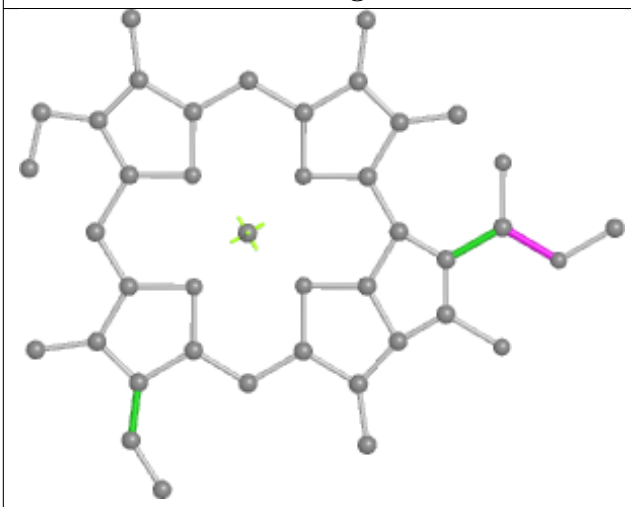
Ligand CLA c5 414



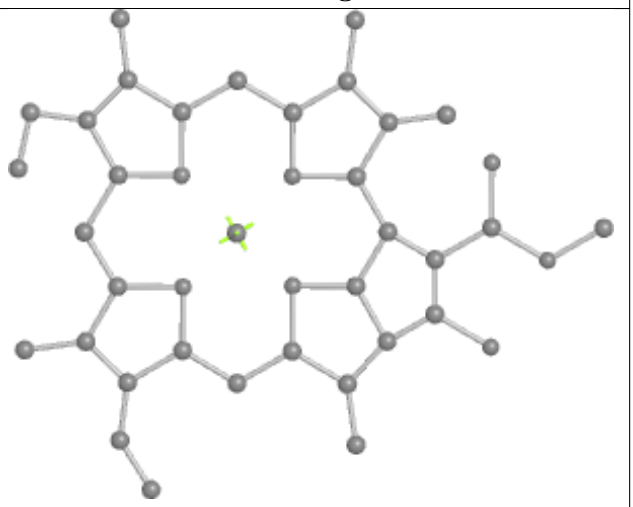
Bond lengths



Bond angles

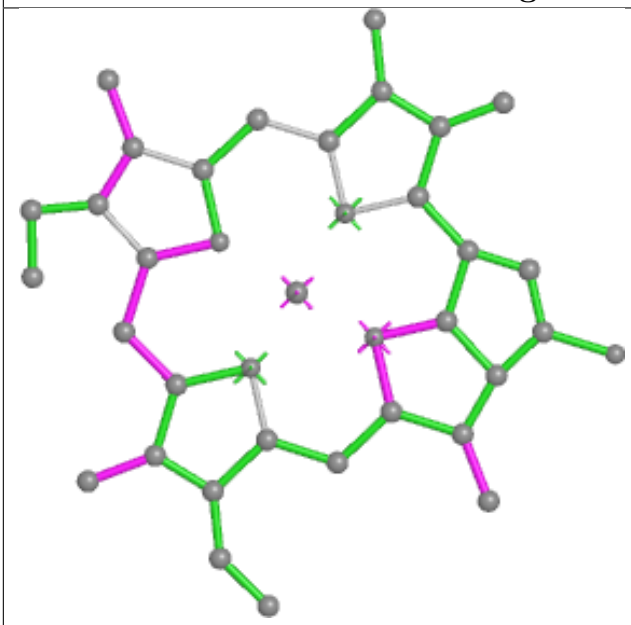


Torsions

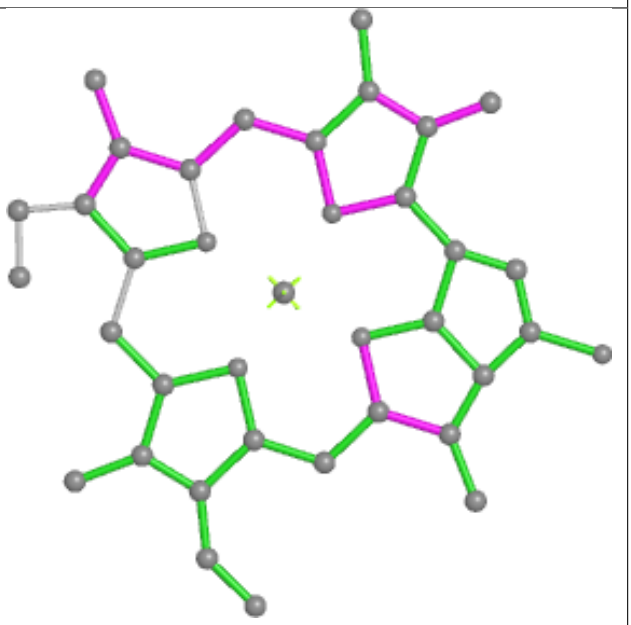


Rings

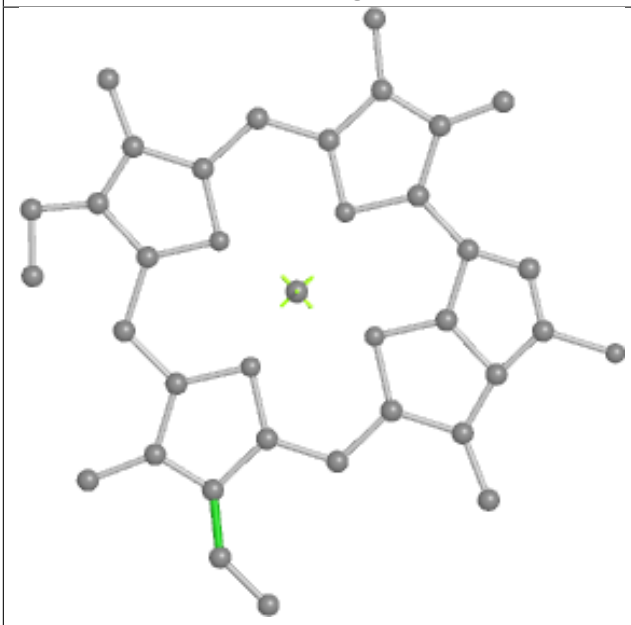
Ligand CLA aJ 203



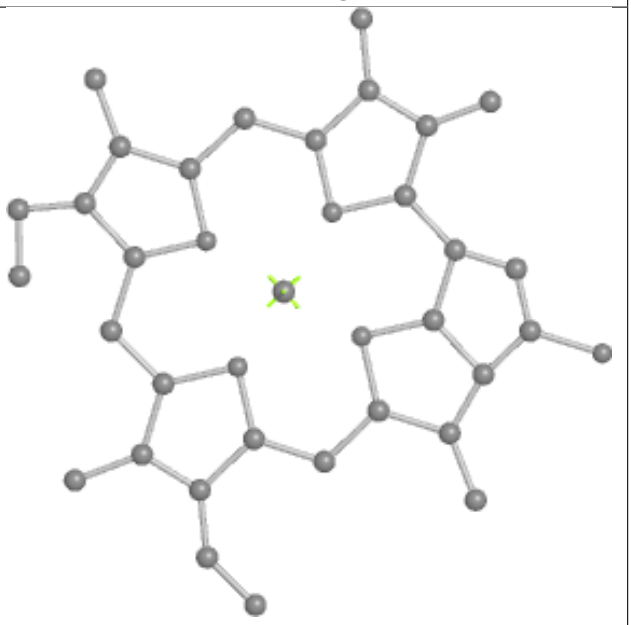
Bond lengths



Bond angles

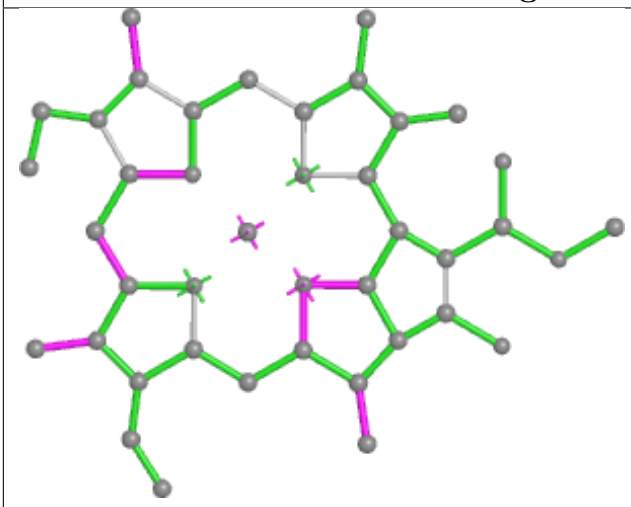


Torsions

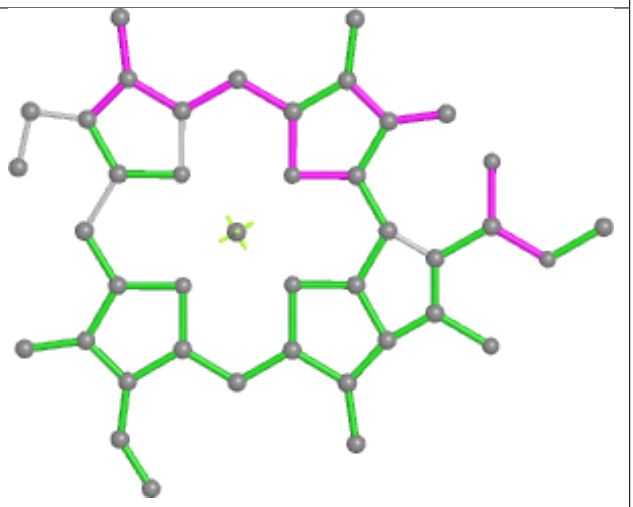


Rings

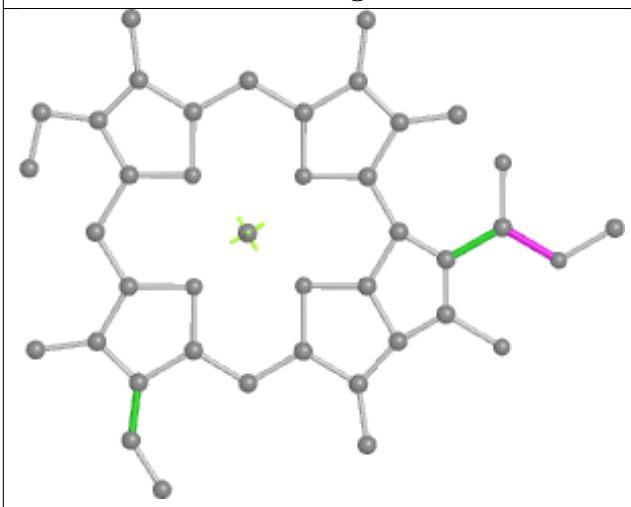
Ligand CLA a3 414



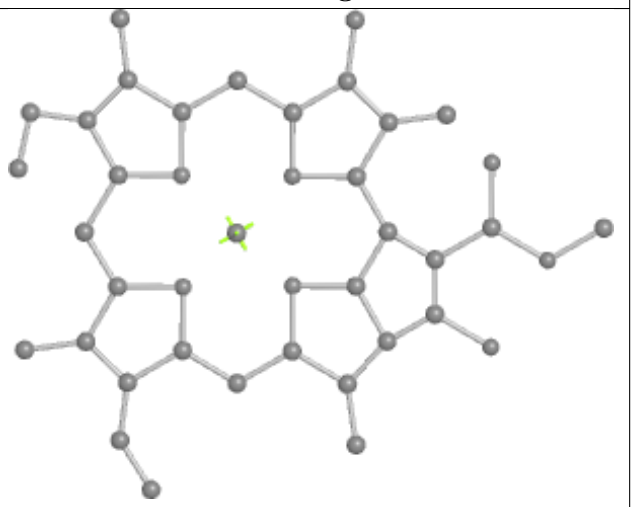
Bond lengths



Bond angles

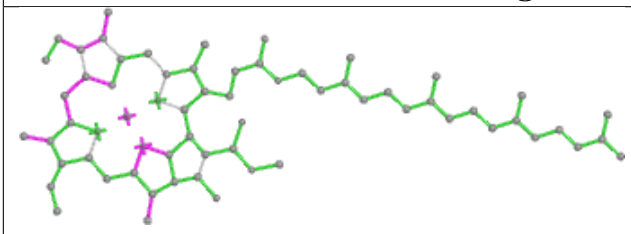


Torsions

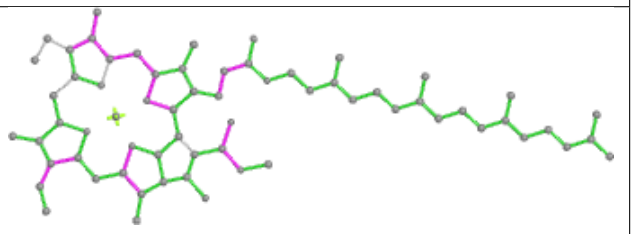


Rings

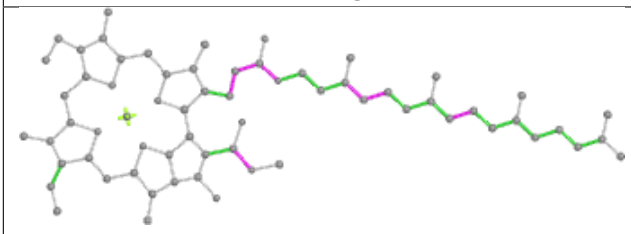
Ligand CLA cB 801



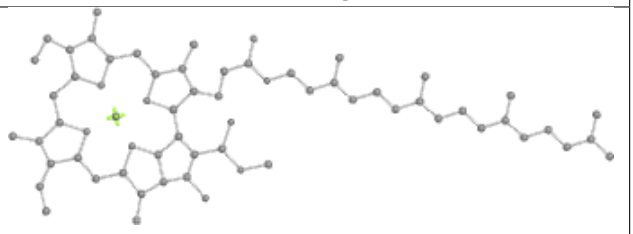
Bond lengths



Bond angles

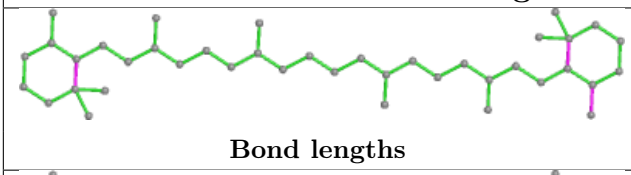


Torsions

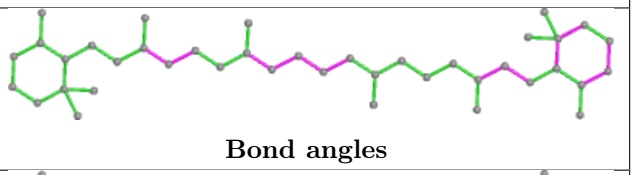


Rings

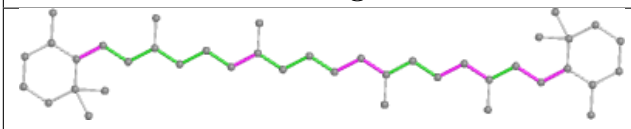
Ligand BCR aA 848



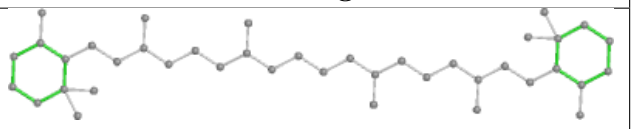
Bond lengths



Bond angles

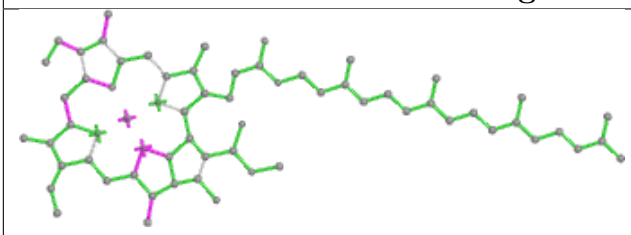


Torsions

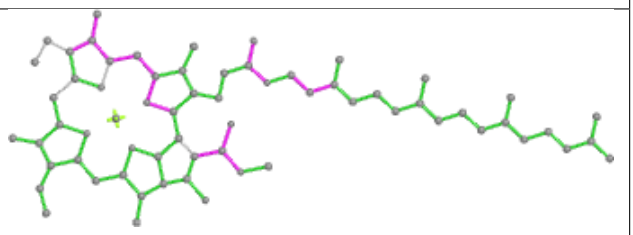


Rings

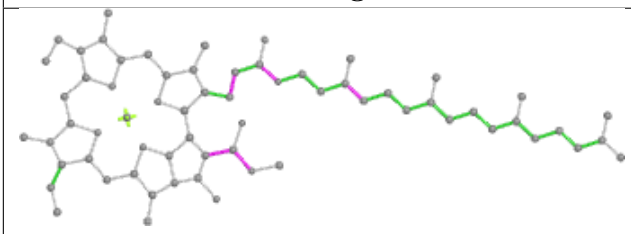
Ligand CLA b2 404



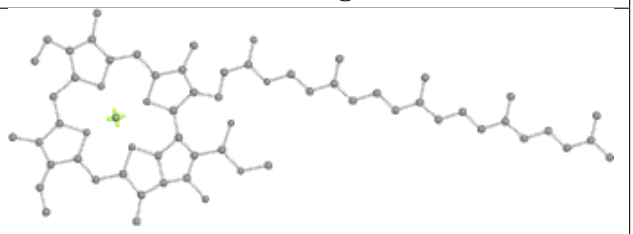
Bond lengths



Bond angles

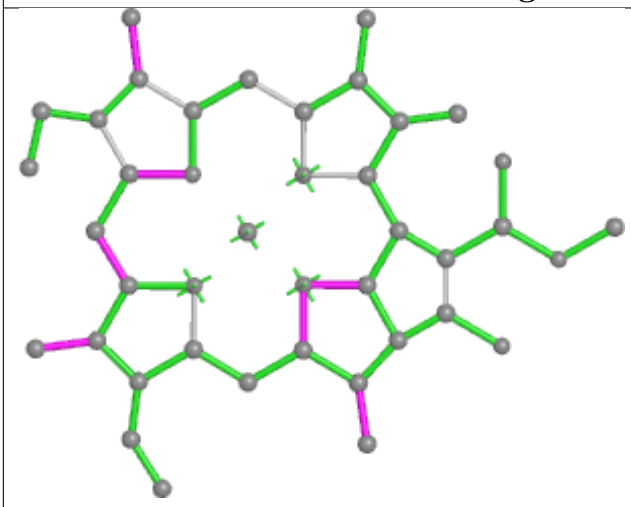


Torsions

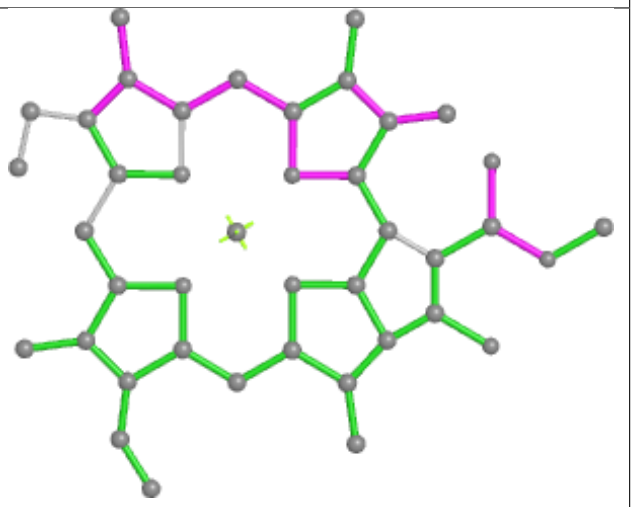


Rings

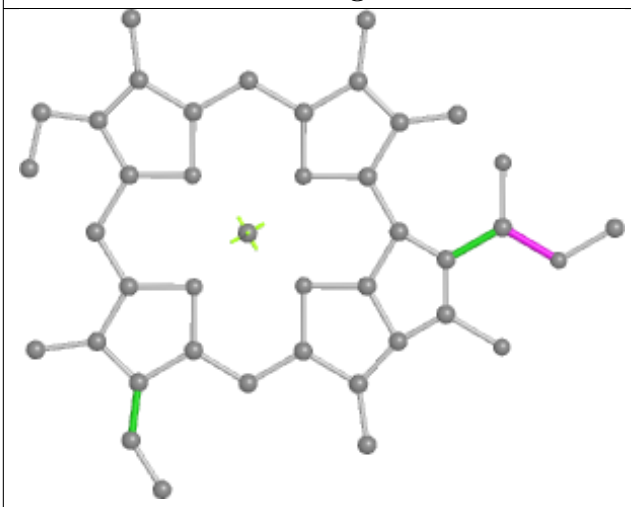
Ligand CLA b5 414



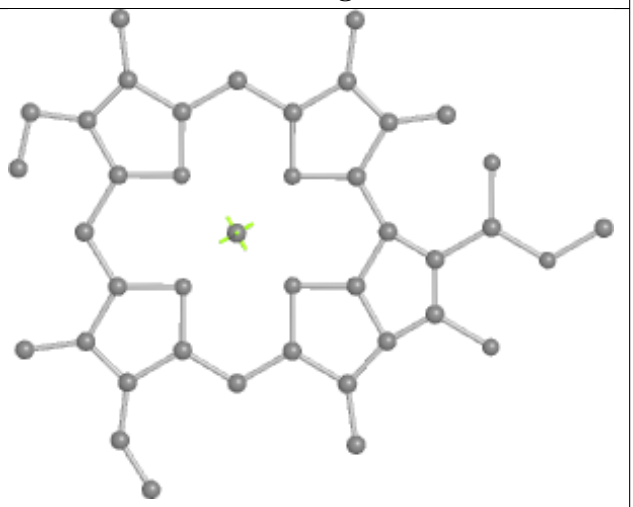
Bond lengths



Bond angles

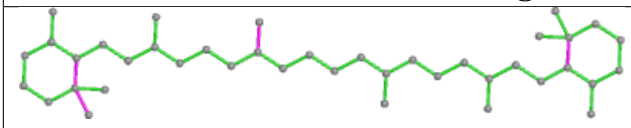


Torsions

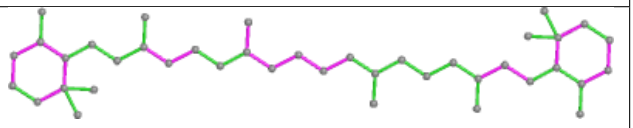


Rings

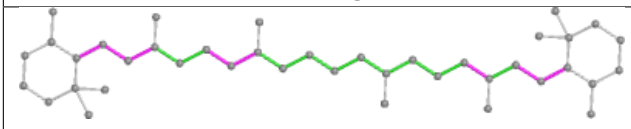
Ligand BCR b1 420



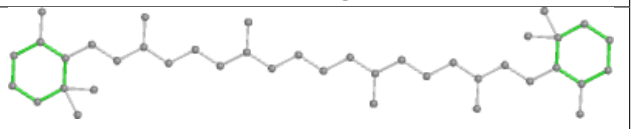
Bond lengths



Bond angles

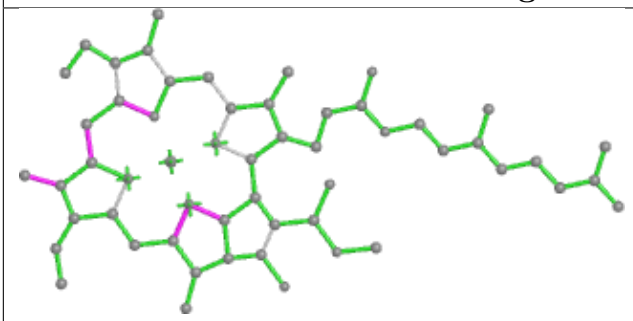


Torsions

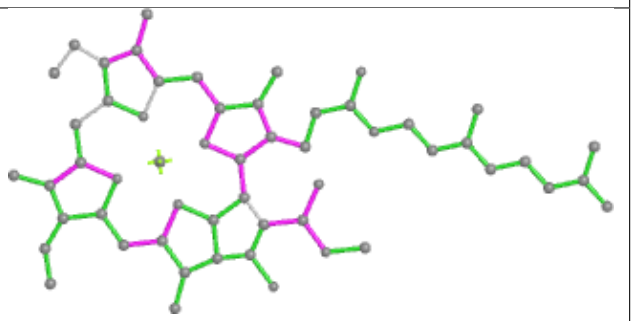


Rings

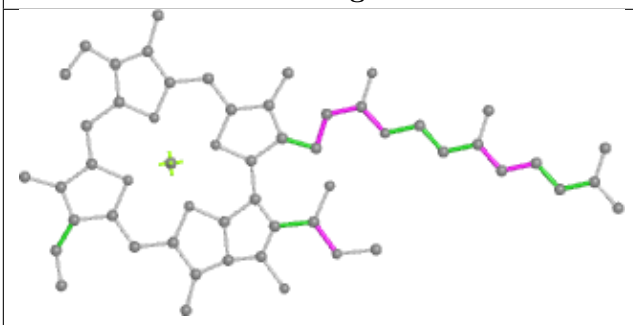
Ligand CLA b6 418



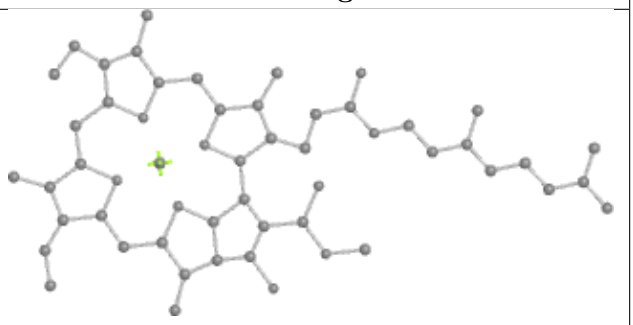
Bond lengths



Bond angles

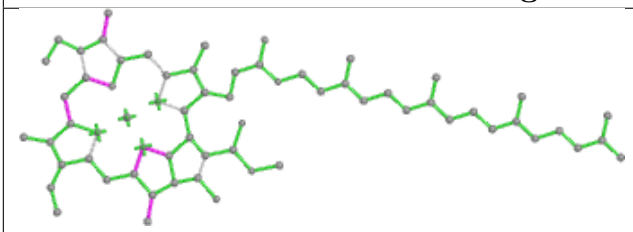


Torsions

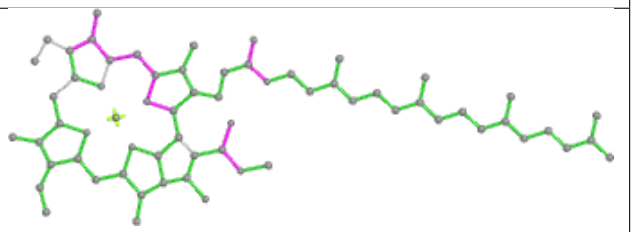


Rings

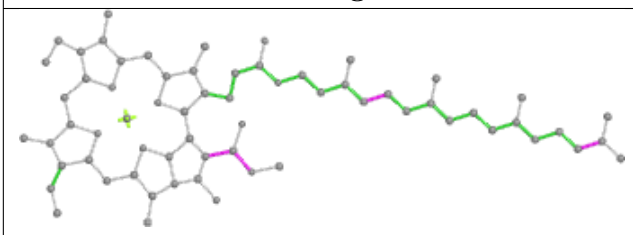
Ligand CLA c1 409



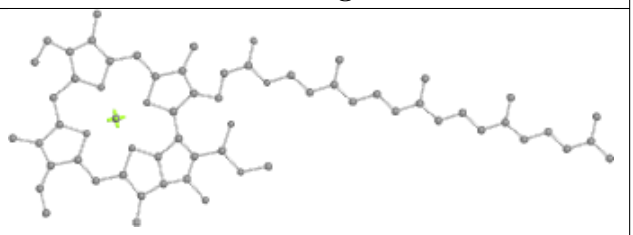
Bond lengths



Bond angles

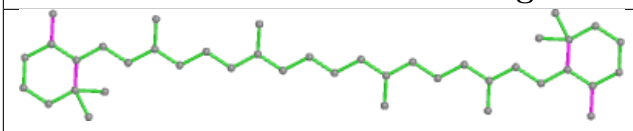


Torsions

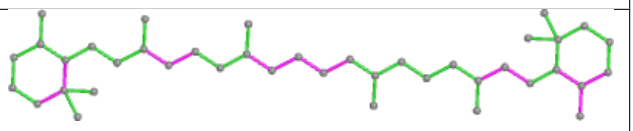


Rings

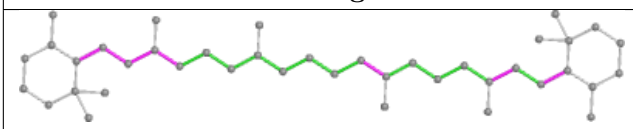
Ligand BCR bJ 104



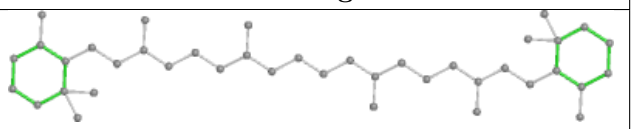
Bond lengths



Bond angles

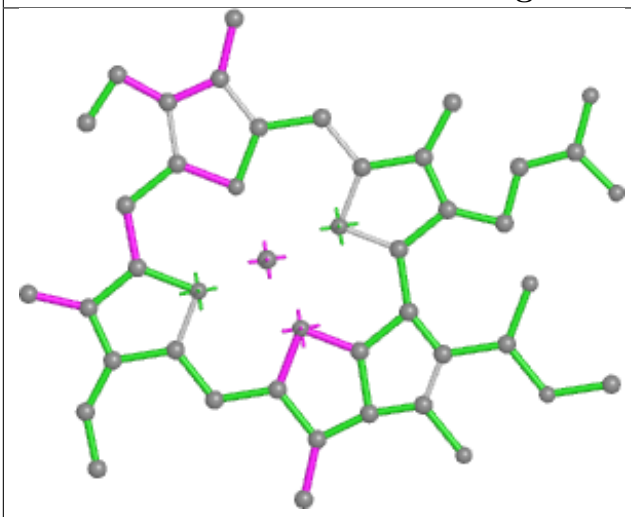


Torsions

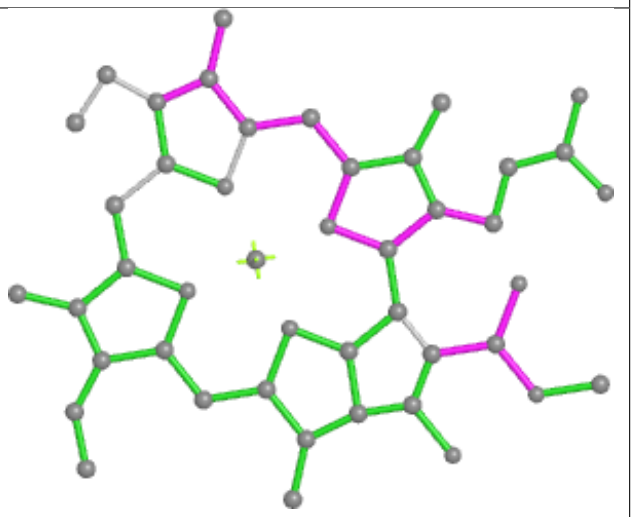


Rings

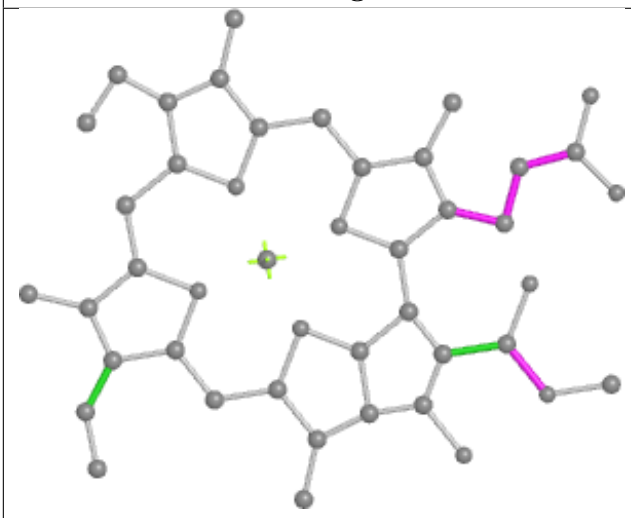
Ligand CLA aB 835



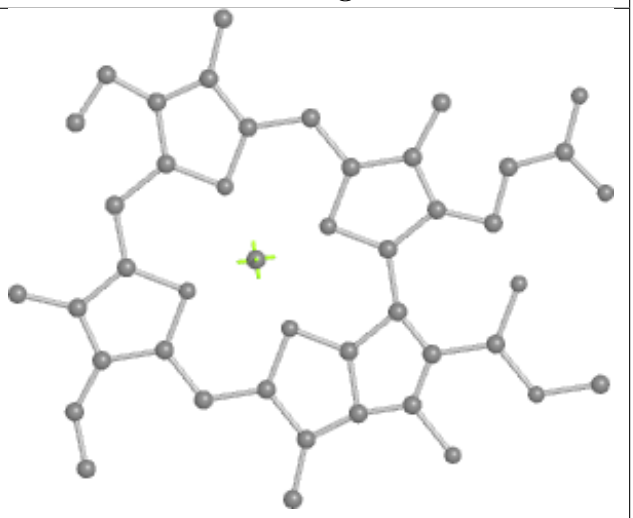
Bond lengths



Bond angles

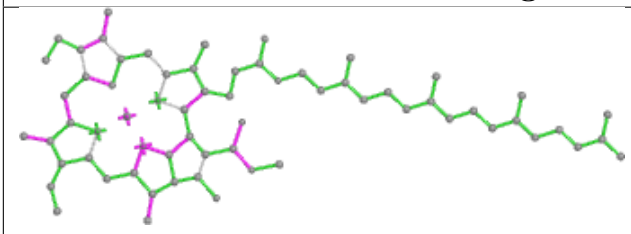


Torsions

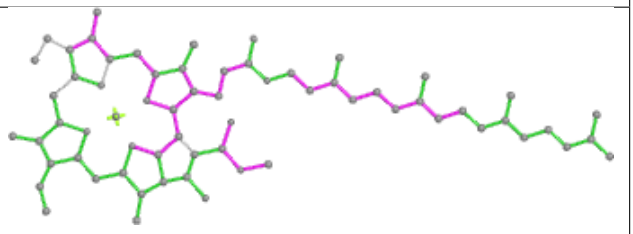


Rings

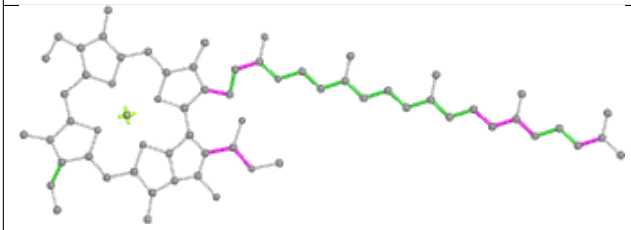
Ligand CLA a4 421



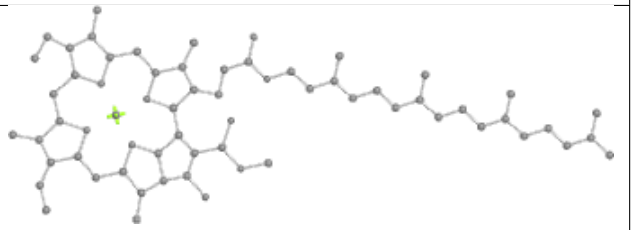
Bond lengths



Bond angles

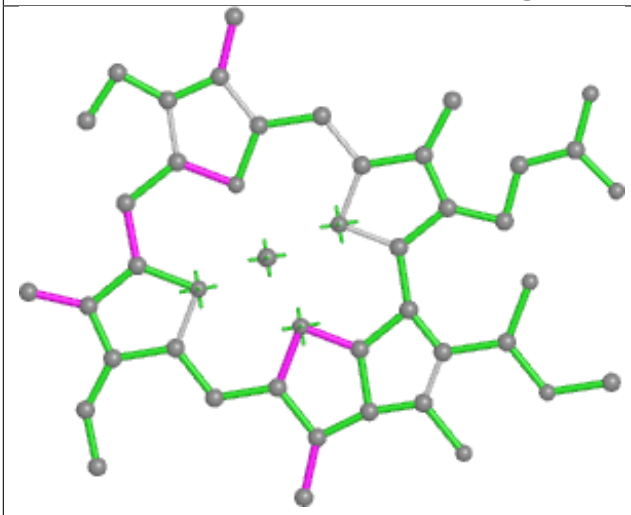


Torsions

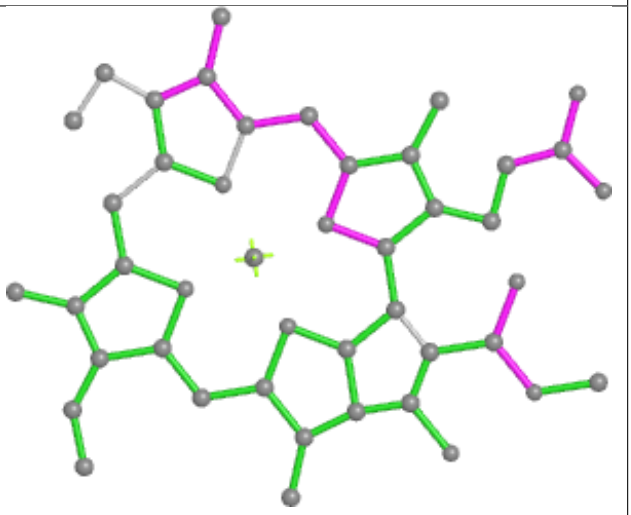


Rings

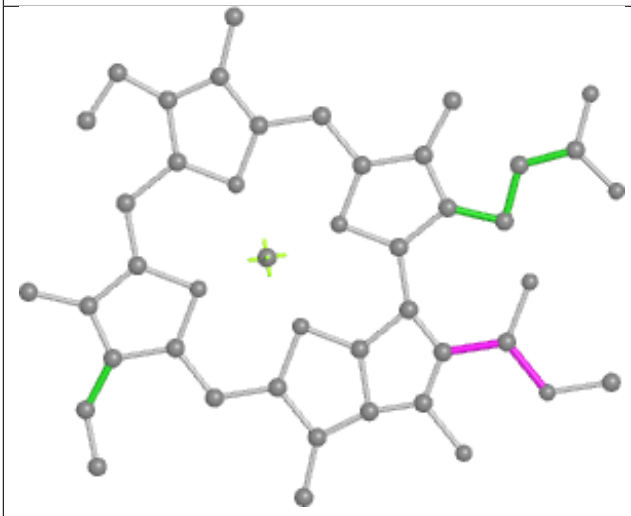
Ligand CLA b5 406



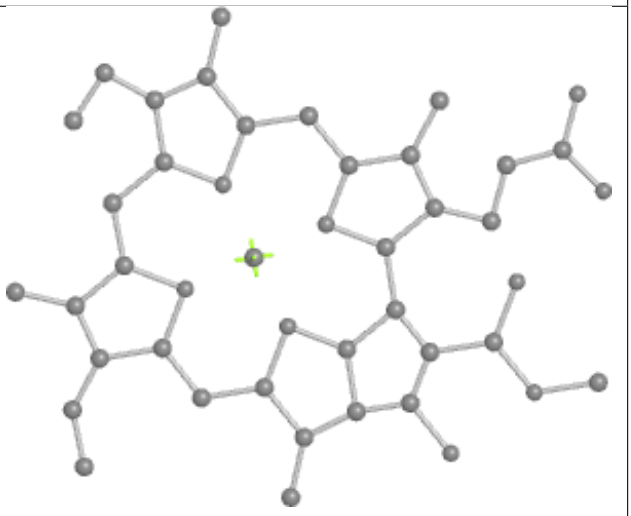
Bond lengths



Bond angles

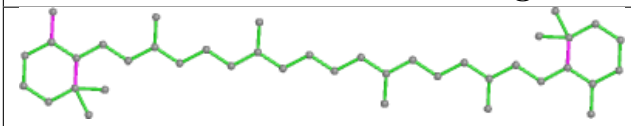


Torsions

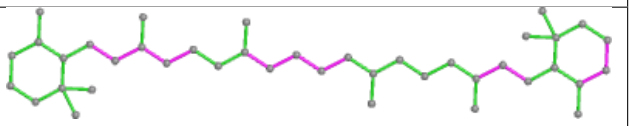


Rings

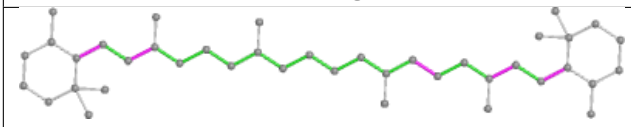
Ligand BCR aB 844



Bond lengths



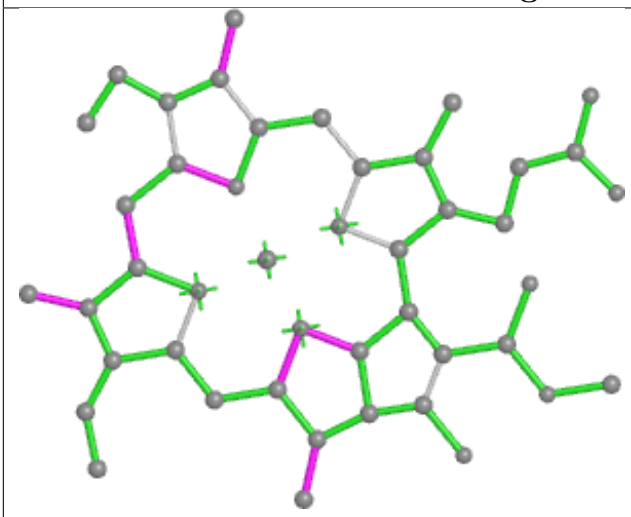
Bond angles



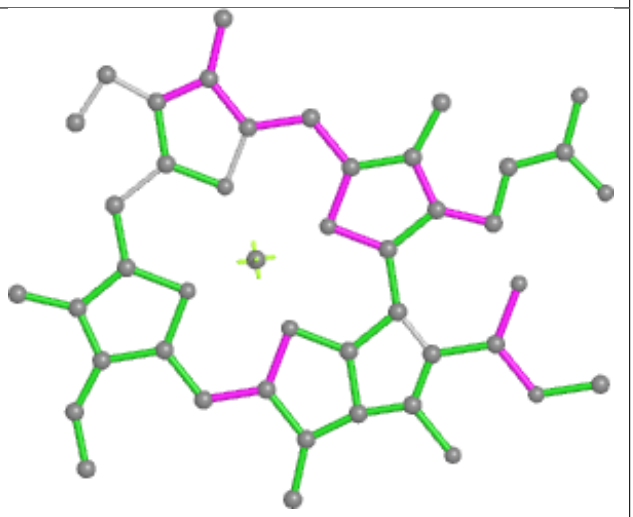
Torsions

Rings

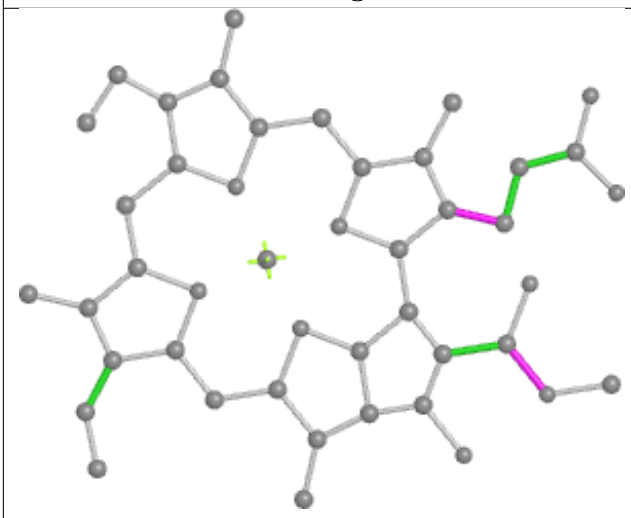
Ligand CLA c4 411



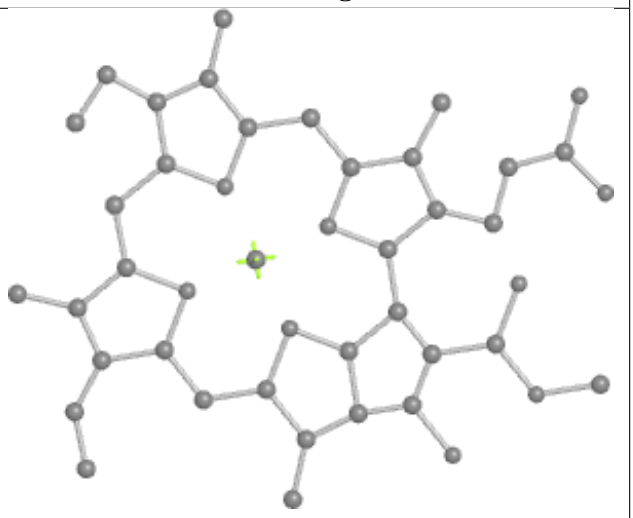
Bond lengths



Bond angles

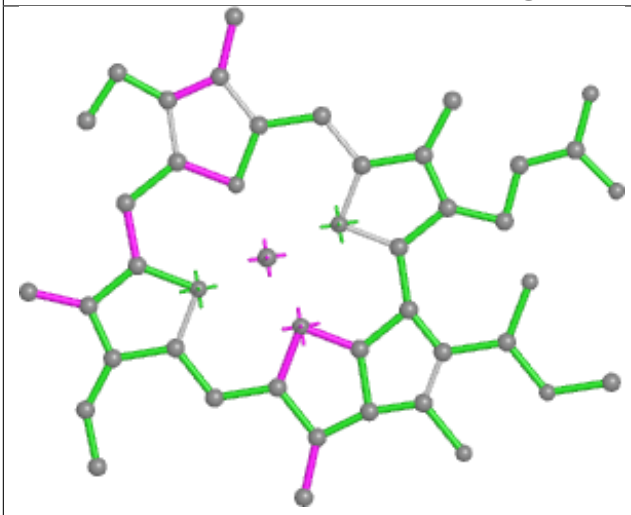


Torsions

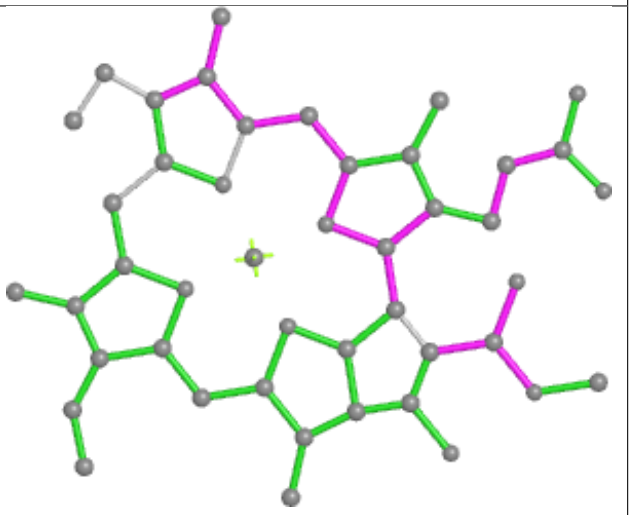


Rings

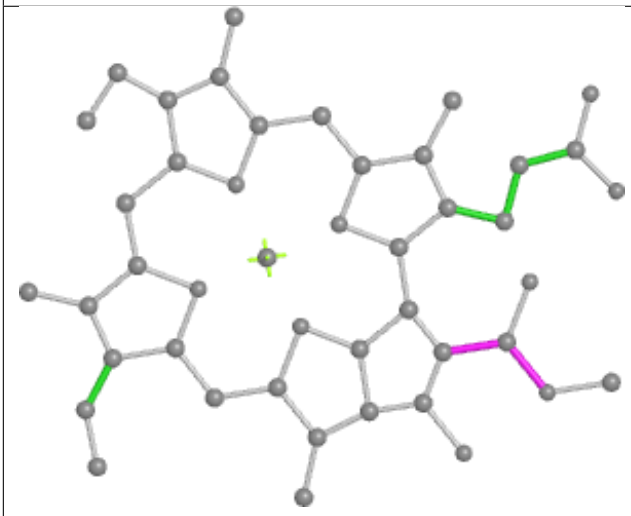
Ligand CLA cJ 101



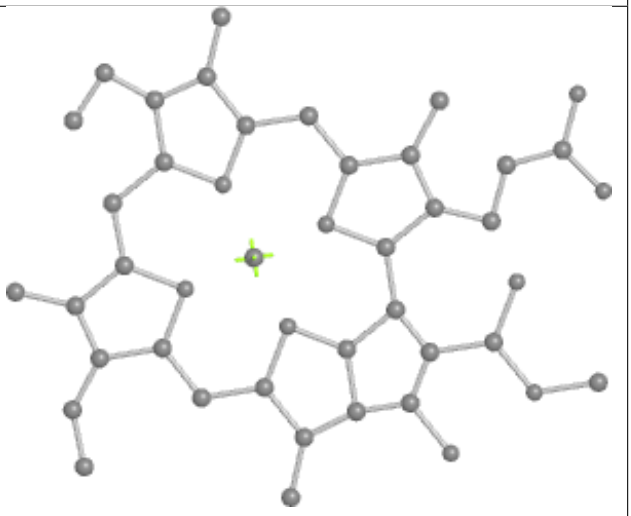
Bond lengths



Bond angles

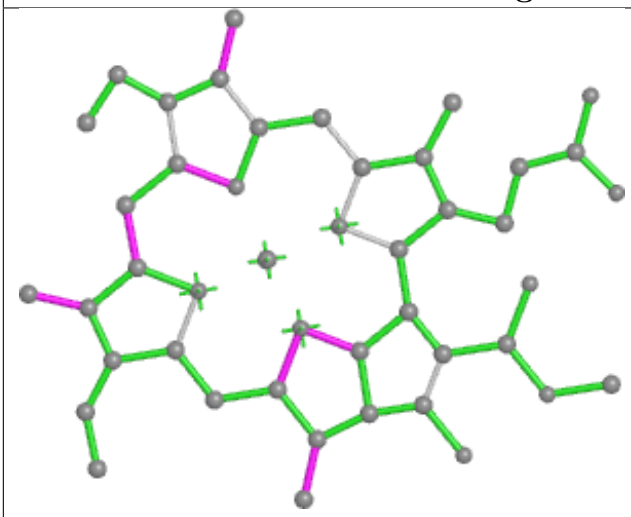


Torsions

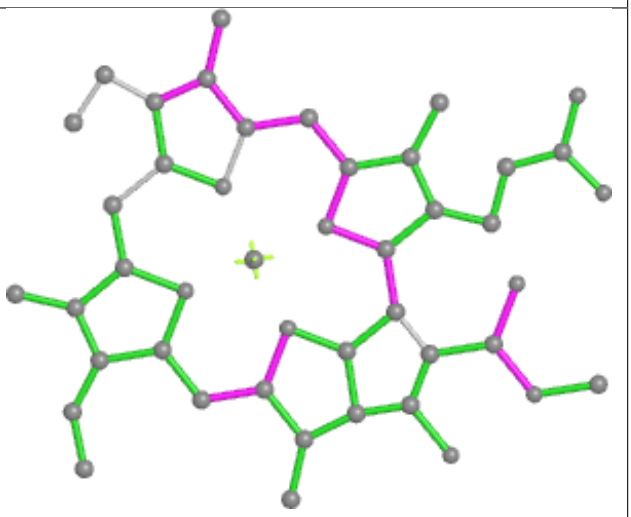


Rings

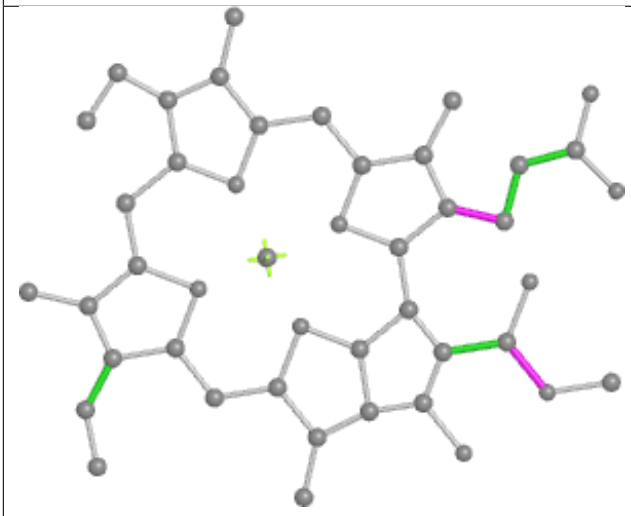
Ligand CLA aB 812



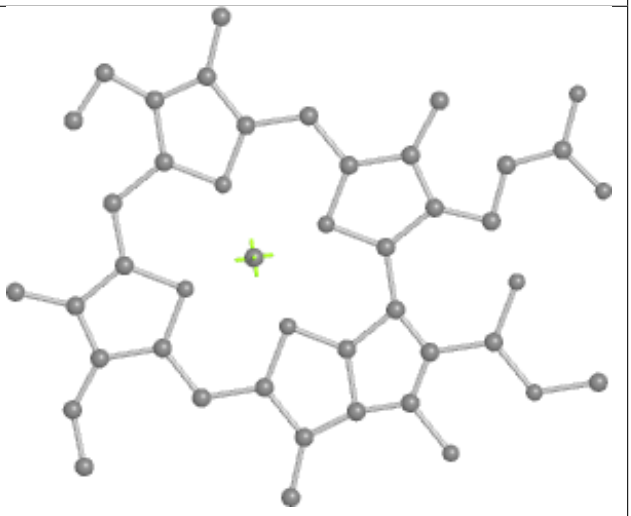
Bond lengths



Bond angles

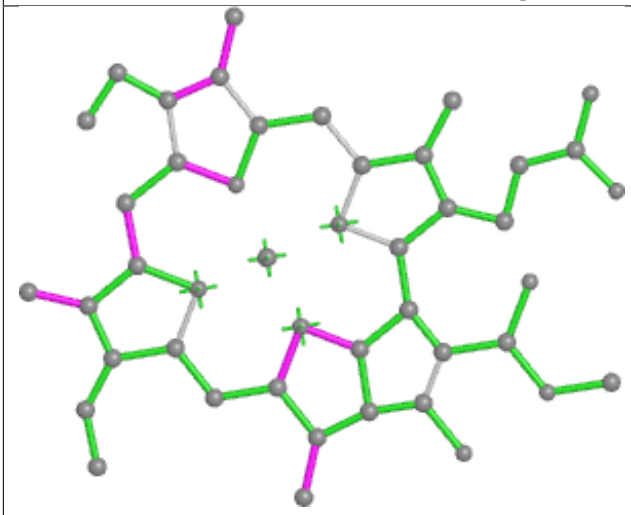


Torsions

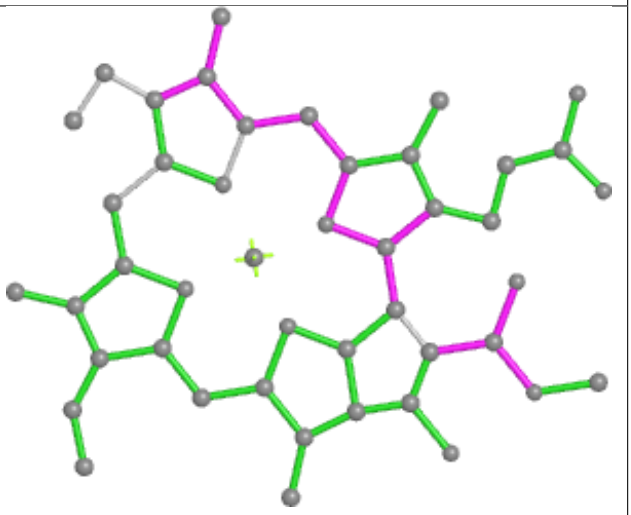


Rings

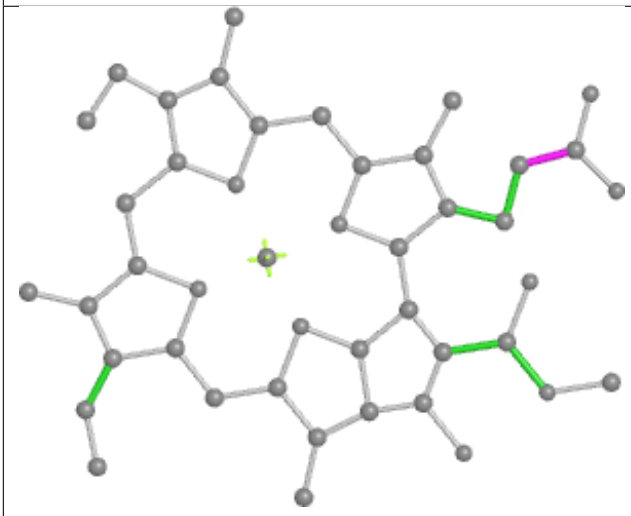
Ligand CLA bB 841



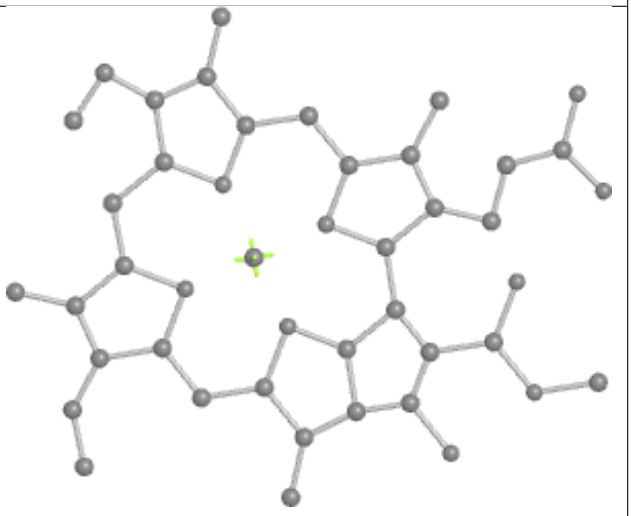
Bond lengths



Bond angles

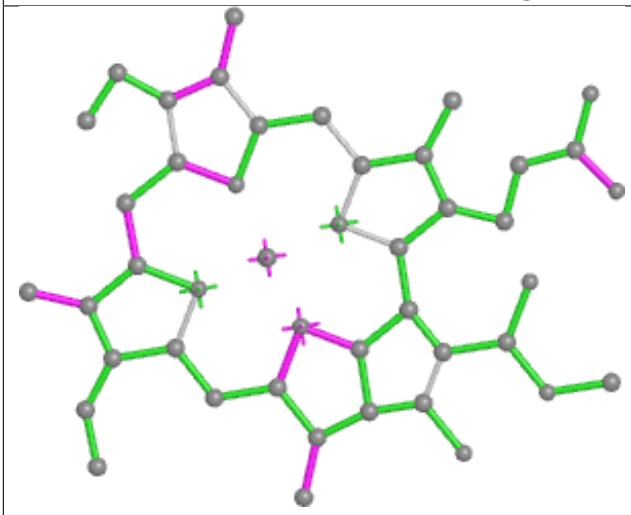


Torsions

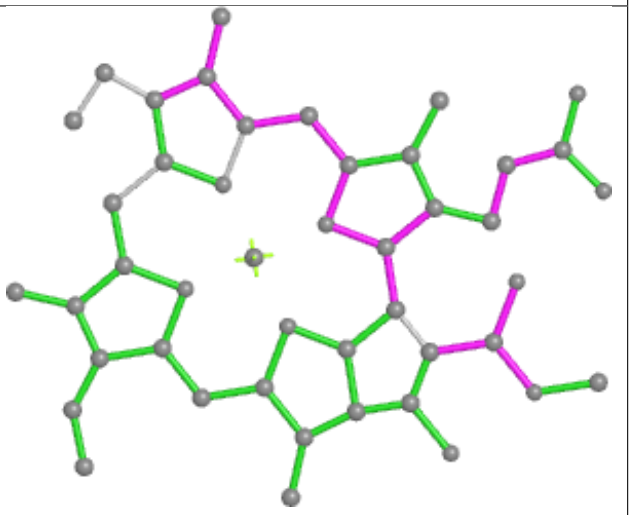


Rings

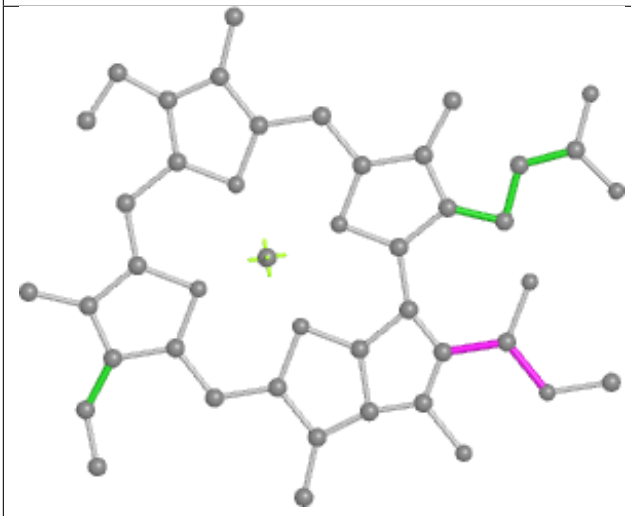
Ligand CLA bJ 101



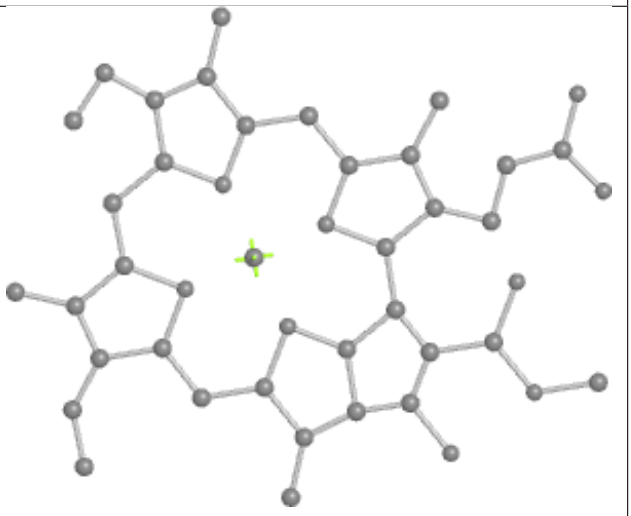
Bond lengths



Bond angles

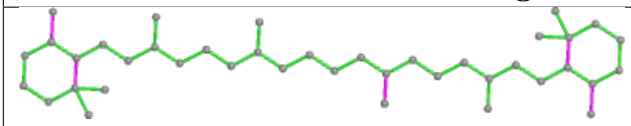


Torsions

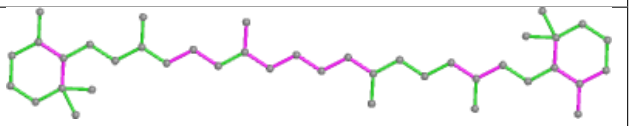


Rings

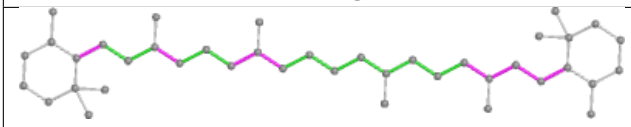
Ligand BCR cB 849



Bond lengths

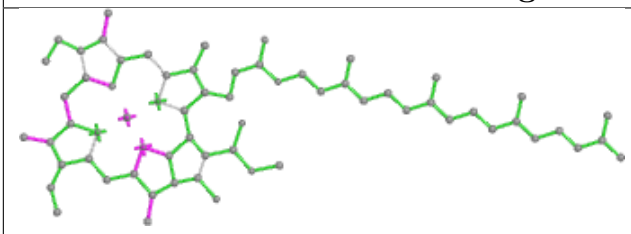
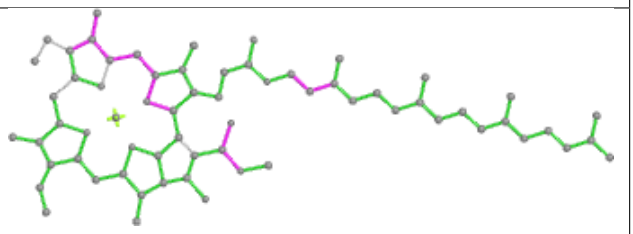
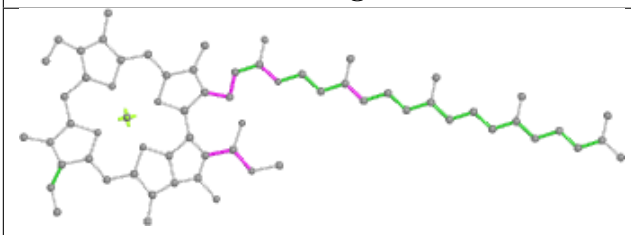
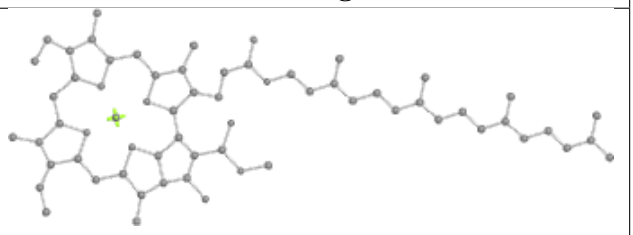


Bond angles



Torsions

Rings

Ligand CLA b4 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

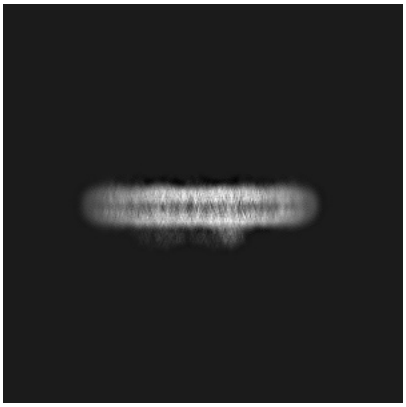
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9908. These allow visual inspection of the internal detail of the map and identification of artifacts.

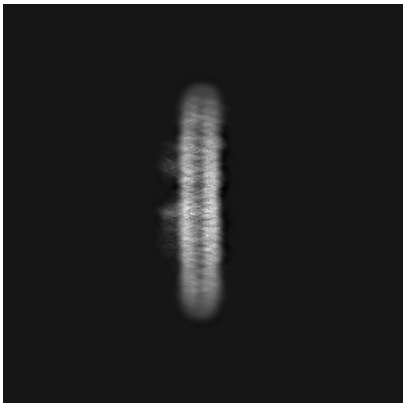
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

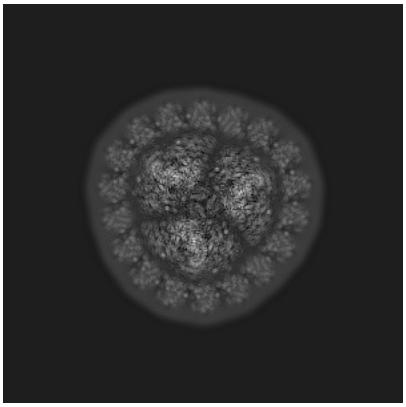
6.1.1 Primary map



X



Y

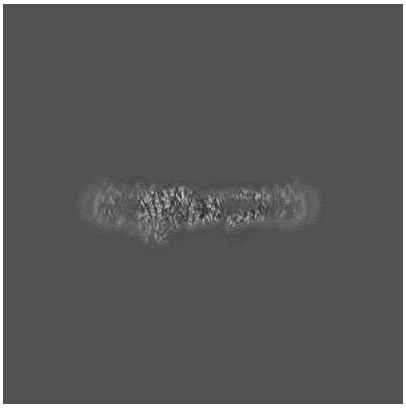


Z

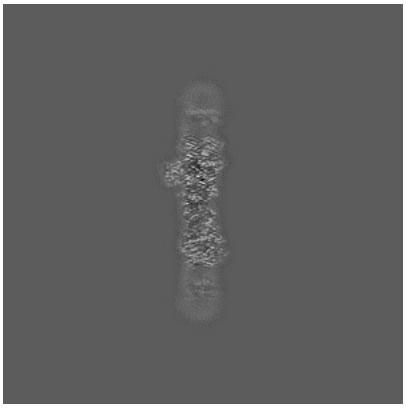
The images above show the map projected in three orthogonal directions.

6.2 Central slices

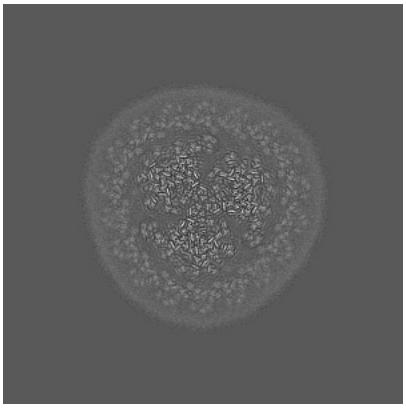
6.2.1 Primary map



X Index: 240



Y Index: 240

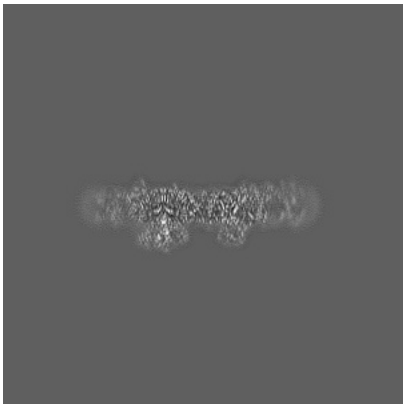


Z Index: 240

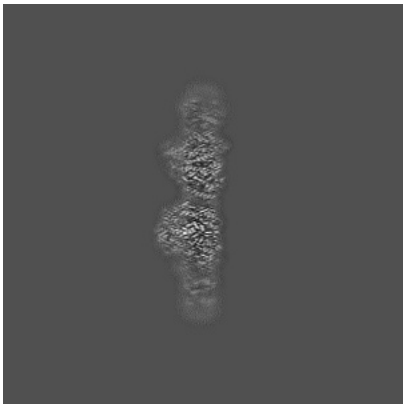
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

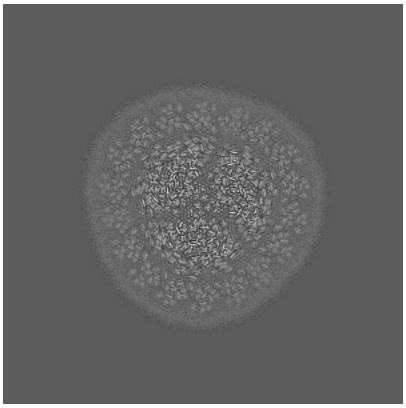
6.3.1 Primary map



X Index: 229



Y Index: 273

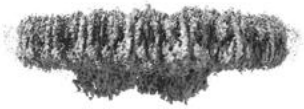


Z Index: 245

The images above show the largest variance slices of the map in three orthogonal directions.

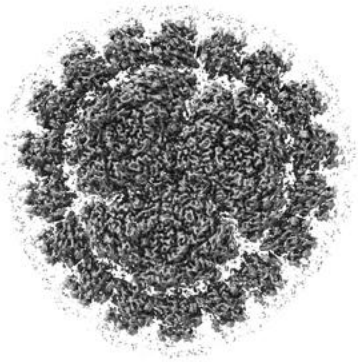
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

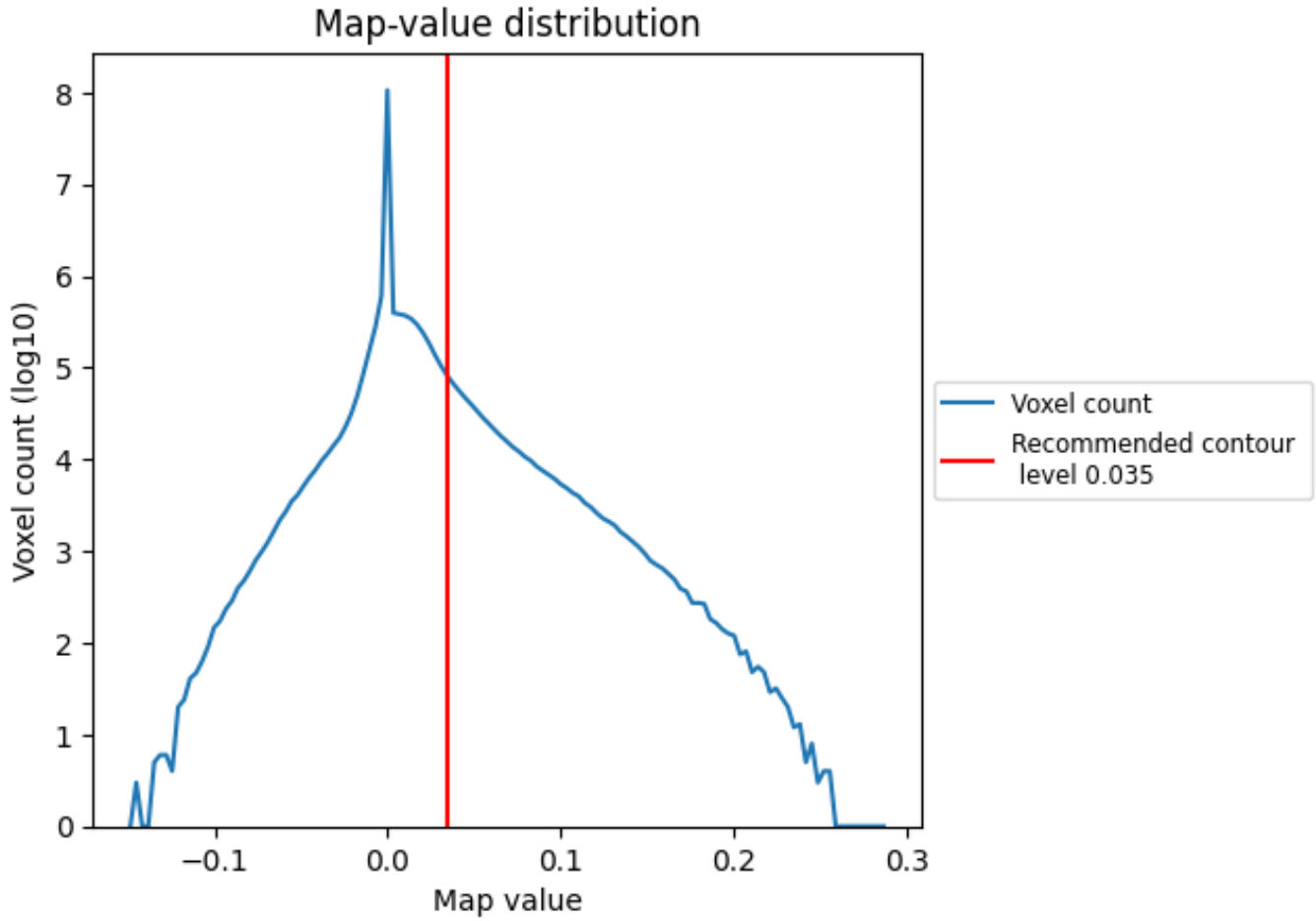
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

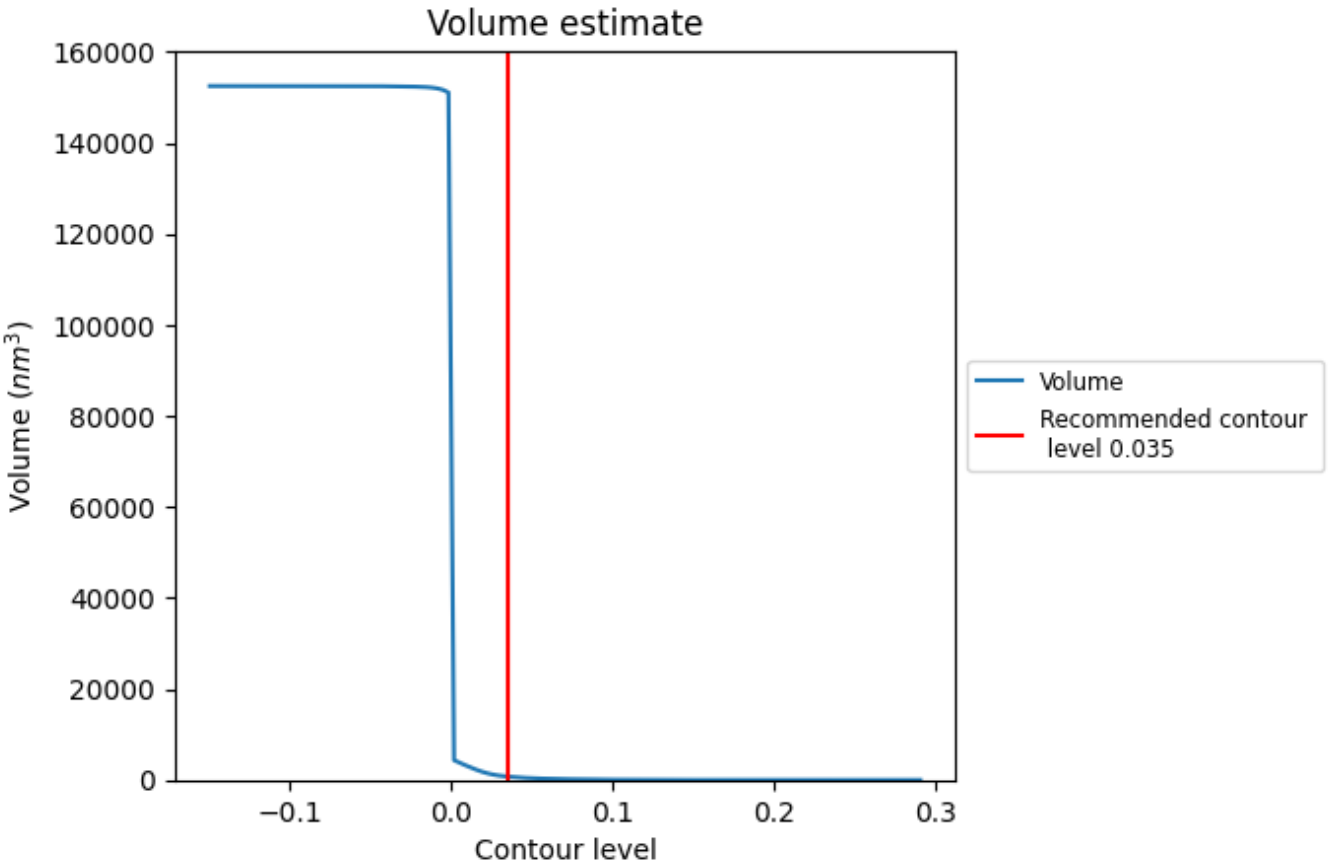
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

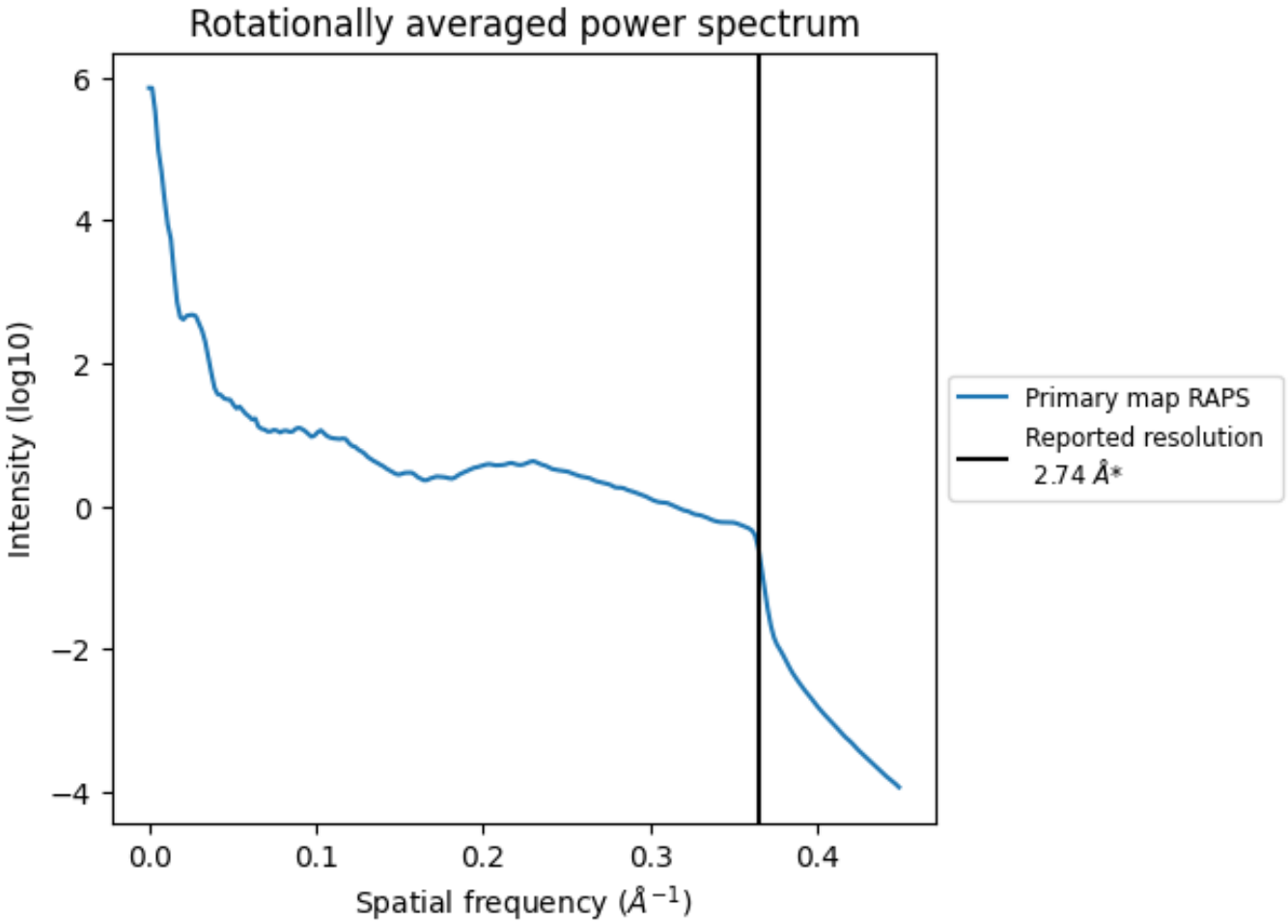
7.2 Volume estimate



The volume at the recommended contour level is 747 nm^3; this corresponds to an approximate mass of 675 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

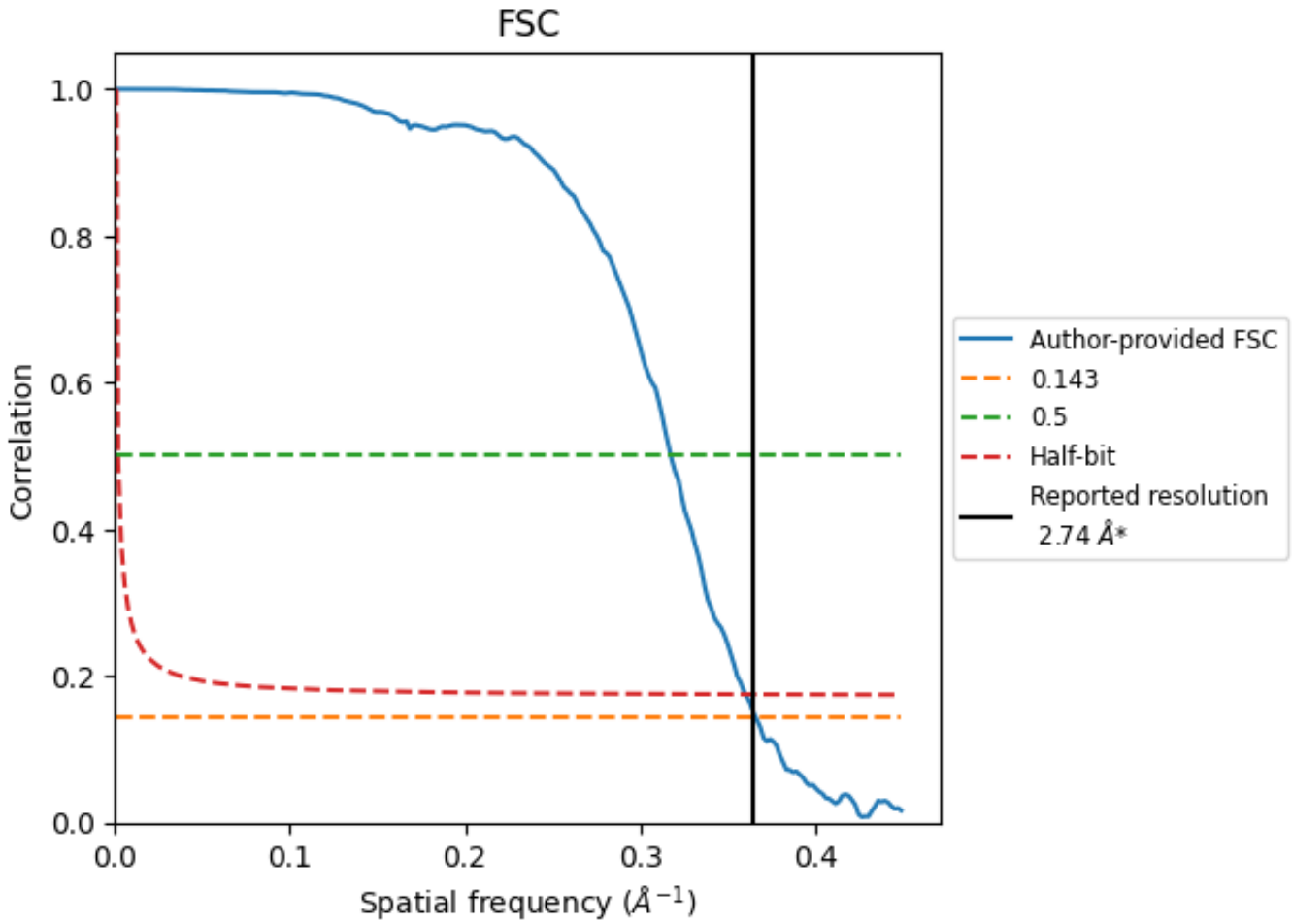


*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8.2 Resolution estimates (i)

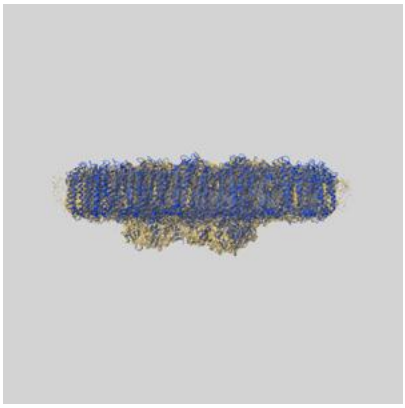
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.15	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

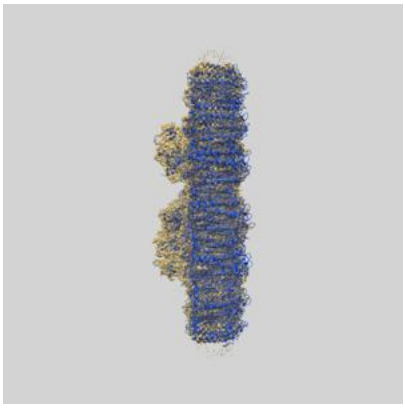
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9908 and PDB model 6K33. Per-residue inclusion information can be found in section 3 on page 64.

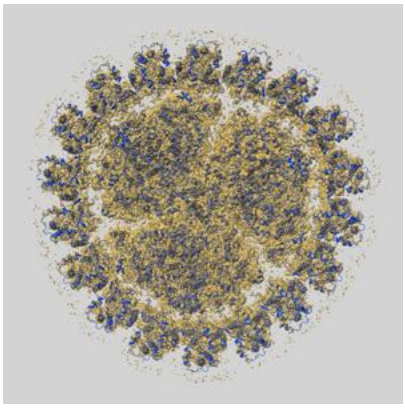
9.1 Map-model overlay



X



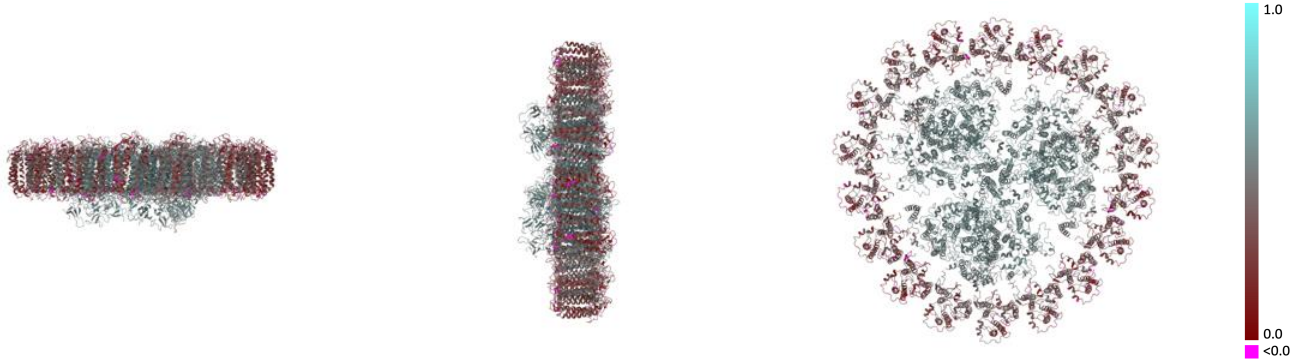
Y



Z

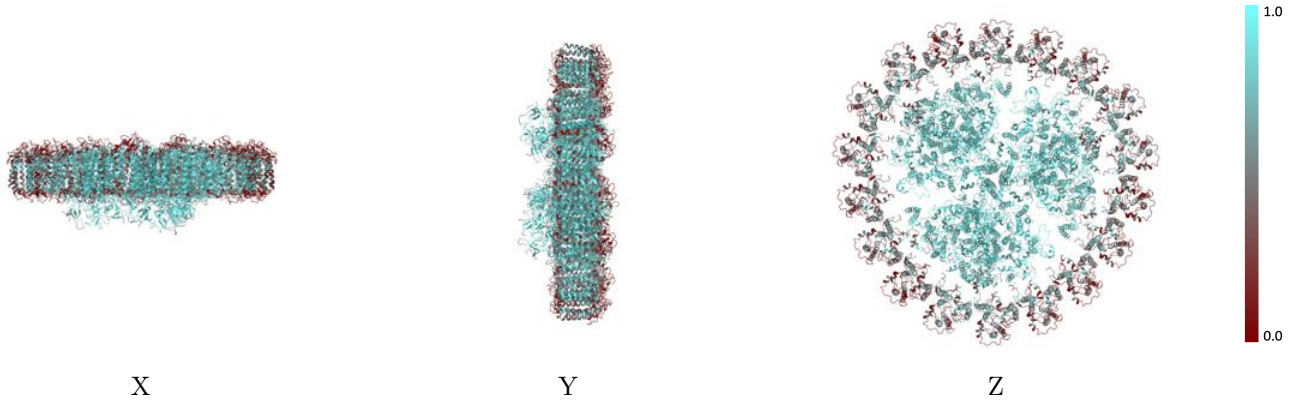
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



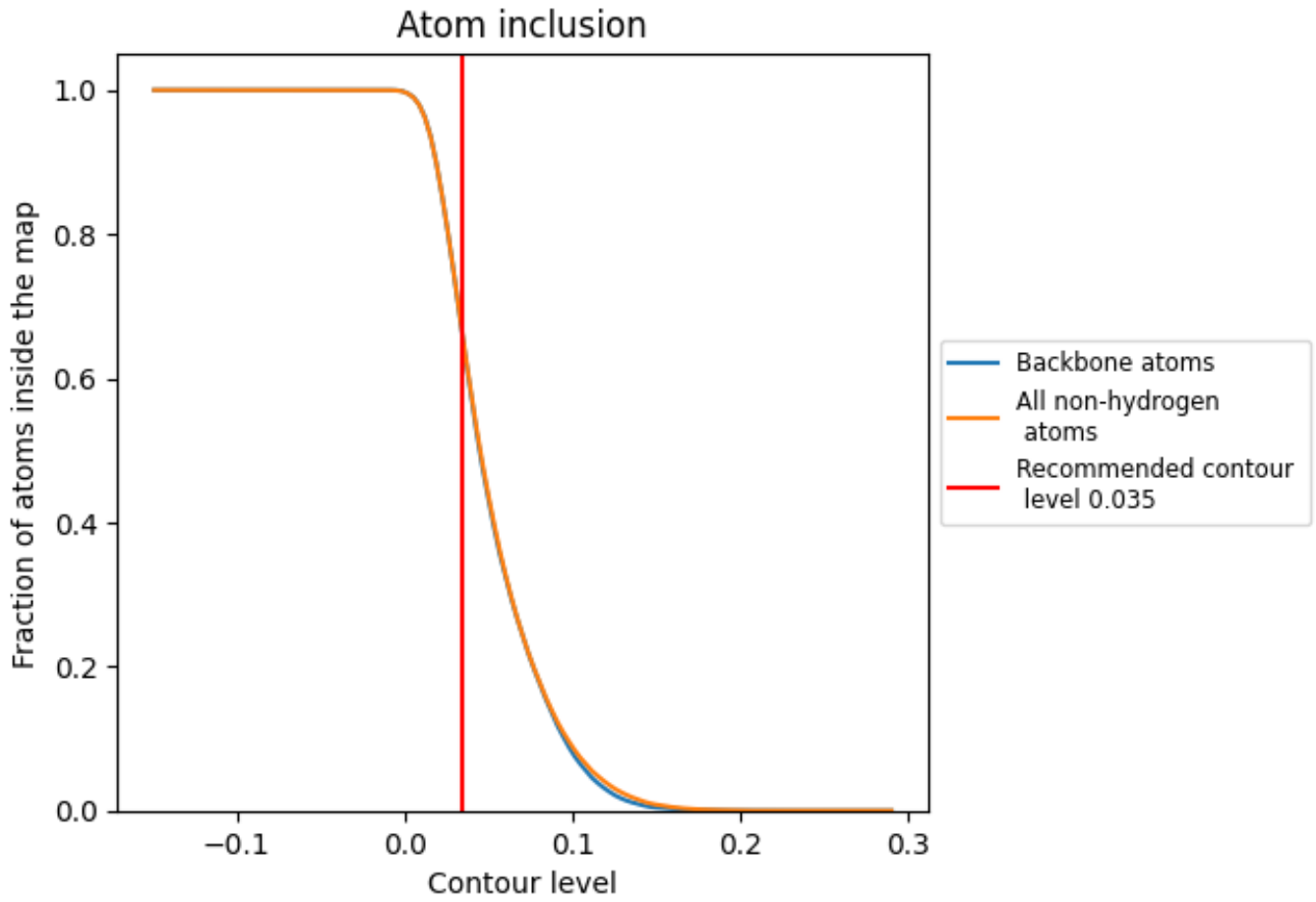
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6564	0.4450
a1	0.4049	0.2890
a2	0.3808	0.2690
a3	0.5045	0.3620
a4	0.4841	0.3610
a5	0.4288	0.3390
a6	0.3746	0.2970
aA	0.8720	0.5710
aB	0.8888	0.5690
aC	0.9200	0.5550
aD	0.8207	0.5560
aE	0.7723	0.5160
aF	0.7102	0.4700
aI	0.8897	0.5860
aJ	0.8030	0.5310
aK	0.8062	0.4710
aL	0.8836	0.5870
aM	0.8014	0.5490
aX	0.8247	0.5250
b1	0.4026	0.2870
b2	0.3721	0.2590
b3	0.4952	0.3600
b4	0.4810	0.3600
b5	0.4325	0.3380
b6	0.3713	0.2950
bA	0.8710	0.5680
bB	0.8898	0.5680
bC	0.9150	0.5500
bD	0.8216	0.5470
bE	0.7647	0.5100
bF	0.7367	0.5110
bI	0.9019	0.5940
bJ	0.8311	0.5420
bK	0.8193	0.4930
bL	0.8760	0.5850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
bM	0.7906	0.5420
bX	0.8247	0.5140
c1	0.4118	0.2890
c2	0.3679	0.2650
c3	0.4977	0.3590
c4	0.4880	0.3590
c5	0.4313	0.3390
c6	0.3714	0.2990
cA	0.8720	0.5700
cB	0.8872	0.5670
cC	0.9167	0.5510
cD	0.8245	0.5510
cE	0.7818	0.5150
cF	0.6930	0.4520
cI	0.8939	0.5930
cJ	0.8193	0.5400
cK	0.8304	0.4940
cL	0.8880	0.5900
cM	0.8087	0.5490
cX	0.8351	0.5280