Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 11:00 pm GMT

PDB ID	:	6TCL
EMDB ID	:	EMD-10461
Title	:	Photosystem I tetramer
Authors	:	Chen, M.; Perez-Boerema, A.; Li, S.; Amunts, A.
Deposited on	:	2019-11-06
Resolution	:	3.20 Å(reported)

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:

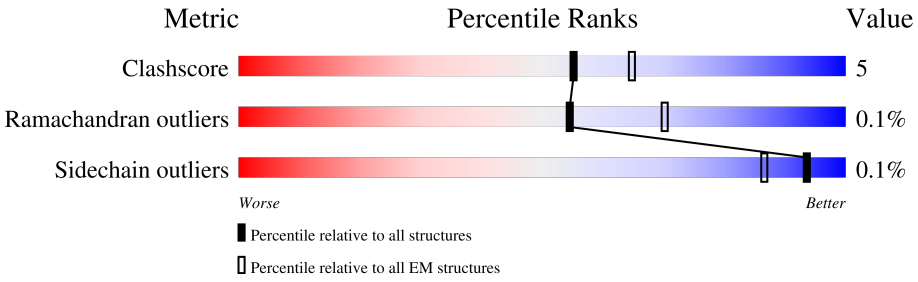
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	A	740	90% 10%
1	A1	740	89% 11%
1	A2	740	87% 13%
1	AA	740	91% 9%
2	B	739	87% 13%
2	B1	739	86% 14%
2	B2	739	86% 14%
2	BB	739	85% 15%

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Mol	Chain	Length	Quality of chain
3	C	80	6% 86% 14%
3	C1	80	5% 84% 15%
3	C2	80	6% 88% 11%
3	CC	80	6% 84% 16%
4	D	134	93% 7%
4	D1	134	94% 6%
4	D2	134	91% 9%
4	DD	134	94% 6%
5	E1	60	5% 92% 8%
5	E2	60	92% 8%
6	F	139	92% 8%
6	F1	139	90% 10%
6	FF	139	88% 12%
7	I	31	94% 6%
7	I1	31	97%
7	II	31	97%
8	J	48	83% 6% 10%
8	J1	48	81% 8% 10%
8	J2	48	79% 10% 10%
8	JJ	48	77% 12% 10%
9	K	74	68% 14% 19%
9	K1	74	96%
9	KK	74	72% 9% 19%
10	L1	166	89% 11%
11	M	31	84% 16%

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Mol	Chain	Length	Quality of chain
11	M1	31	10% 94% 6%
11	M2	31	10% 97%
11	MM	31	94% 6%
12	X	39	8% 95% 5%
12	X1	39	10% 92% 8%
12	X2	39	8% 90% 10%
12	XX	39	8% 97%
13	F2	137	85% 13%
14	I2	33	94% 6%
15	K2	73	88% 12%
16	L2	167	89% 10%
17	E	63	90% 10%
17	EE	63	87% 13%
18	L	154	95% 5%
18	LL	154	94% 6%

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
19	CLA	A	801	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	852	X	-	-	-
19	CLA	A1	801	X	-	-	-
19	CLA	A1	803	X	-	-	-
19	CLA	A1	804	X	-	-	-
19	CLA	A1	806	X	-	-	-
19	CLA	A1	807	X	-	-	-
19	CLA	A1	808	X	-	-	-
19	CLA	A1	809	X	-	-	-
19	CLA	A1	810	X	-	-	-
19	CLA	A1	811	X	-	-	-
19	CLA	A1	812	X	-	-	-
19	CLA	A1	813	X	-	-	-
19	CLA	A1	814	X	-	-	-
19	CLA	A1	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A1	816	X	-	-	-
19	CLA	A1	817	X	-	-	-
19	CLA	A1	818	X	-	-	-
19	CLA	A1	820	X	-	-	-
19	CLA	A1	821	X	-	-	-
19	CLA	A1	822	X	-	-	-
19	CLA	A1	823	X	-	-	-
19	CLA	A1	824	X	-	-	-
19	CLA	A1	825	X	-	-	-
19	CLA	A1	826	X	-	-	-
19	CLA	A1	827	X	-	-	-
19	CLA	A1	828	X	-	-	-
19	CLA	A1	829	X	-	-	-
19	CLA	A1	830	X	-	-	-
19	CLA	A1	831	X	-	-	-
19	CLA	A1	832	X	-	-	-
19	CLA	A1	833	X	-	-	-
19	CLA	A1	834	X	-	-	-
19	CLA	A1	835	X	-	-	-
19	CLA	A1	836	X	-	-	-
19	CLA	A1	837	X	-	-	-
19	CLA	A1	838	X	-	-	-
19	CLA	A1	839	X	-	-	-
19	CLA	A1	840	X	-	-	-
19	CLA	A1	841	X	-	-	-
19	CLA	A1	842	X	-	-	-
19	CLA	A1	844	X	-	-	-
19	CLA	A1	852	X	-	-	-
19	CLA	A2	801	X	-	-	-
19	CLA	A2	802	X	-	-	-
19	CLA	A2	804	X	-	-	-
19	CLA	A2	805	X	-	-	-
19	CLA	A2	806	X	-	-	-
19	CLA	A2	807	X	-	-	-
19	CLA	A2	808	X	-	-	-
19	CLA	A2	809	X	-	-	-
19	CLA	A2	810	X	-	-	-
19	CLA	A2	811	X	-	-	-
19	CLA	A2	812	X	-	-	-
19	CLA	A2	813	X	-	-	-
19	CLA	A2	814	X	-	-	-
19	CLA	A2	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A2	816	X	-	-	-
19	CLA	A2	817	X	-	-	-
19	CLA	A2	818	X	-	-	-
19	CLA	A2	819	X	-	-	-
19	CLA	A2	820	X	-	-	-
19	CLA	A2	821	X	-	-	-
19	CLA	A2	822	X	-	-	-
19	CLA	A2	823	X	-	-	-
19	CLA	A2	824	X	-	-	-
19	CLA	A2	825	X	-	-	-
19	CLA	A2	826	X	-	-	-
19	CLA	A2	827	X	-	-	-
19	CLA	A2	828	X	-	-	-
19	CLA	A2	829	X	-	-	-
19	CLA	A2	830	X	-	-	-
19	CLA	A2	831	X	-	-	-
19	CLA	A2	832	X	-	-	-
19	CLA	A2	833	X	-	-	-
19	CLA	A2	834	X	-	-	-
19	CLA	A2	835	X	-	-	-
19	CLA	A2	837	X	-	-	-
19	CLA	A2	838	X	-	-	-
19	CLA	A2	839	X	-	-	-
19	CLA	A2	840	X	-	-	-
19	CLA	A2	841	X	-	-	-
19	CLA	A2	842	X	-	-	-
19	CLA	A2	844	X	-	-	-
19	CLA	A2	852	X	-	-	-
19	CLA	AA	801	X	-	-	-
19	CLA	AA	804	X	-	-	-
19	CLA	AA	805	X	-	-	-
19	CLA	AA	806	X	-	-	-
19	CLA	AA	807	X	-	-	-
19	CLA	AA	808	X	-	-	-
19	CLA	AA	809	X	-	-	-
19	CLA	AA	810	X	-	-	-
19	CLA	AA	811	X	-	-	-
19	CLA	AA	812	X	-	-	-
19	CLA	AA	813	X	-	-	-
19	CLA	AA	814	X	-	-	-
19	CLA	AA	815	X	-	-	-
19	CLA	AA	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	AA	817	X	-	-	-
19	CLA	AA	818	X	-	-	-
19	CLA	AA	819	X	-	-	-
19	CLA	AA	820	X	-	-	-
19	CLA	AA	821	X	-	-	-
19	CLA	AA	823	X	-	-	-
19	CLA	AA	824	X	-	-	-
19	CLA	AA	825	X	-	-	-
19	CLA	AA	826	X	-	-	-
19	CLA	AA	827	X	-	-	-
19	CLA	AA	828	X	-	-	-
19	CLA	AA	829	X	-	-	-
19	CLA	AA	830	X	-	-	-
19	CLA	AA	831	X	-	-	-
19	CLA	AA	832	X	-	-	-
19	CLA	AA	833	X	-	-	-
19	CLA	AA	834	X	-	-	-
19	CLA	AA	835	X	-	-	-
19	CLA	AA	836	X	-	-	-
19	CLA	AA	837	X	-	-	-
19	CLA	AA	838	X	-	-	-
19	CLA	AA	839	X	-	-	-
19	CLA	AA	840	X	-	-	-
19	CLA	AA	841	X	-	-	-
19	CLA	AA	842	X	-	-	-
19	CLA	AA	843	X	-	-	-
19	CLA	AA	845	X	-	-	-
19	CLA	AA	853	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	B	854	X	-	-	-
19	CLA	B	858	X	-	-	-
19	CLA	B	859	X	-	-	-
19	CLA	B	860	X	-	-	-
19	CLA	B1	801	X	-	-	-
19	CLA	B1	802	X	-	-	-
19	CLA	B1	803	X	-	-	-
19	CLA	B1	804	X	-	-	-
19	CLA	B1	805	X	-	-	-
19	CLA	B1	806	X	-	-	-
19	CLA	B1	807	X	-	-	-
19	CLA	B1	808	X	-	-	-
19	CLA	B1	809	X	-	-	-
19	CLA	B1	810	X	-	-	-
19	CLA	B1	811	X	-	-	-
19	CLA	B1	812	X	-	-	-
19	CLA	B1	813	X	-	-	-
19	CLA	B1	814	X	-	-	-
19	CLA	B1	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B1	816	X	-	-	-
19	CLA	B1	817	X	-	-	-
19	CLA	B1	818	X	-	-	-
19	CLA	B1	819	X	-	-	-
19	CLA	B1	820	X	-	-	-
19	CLA	B1	821	X	-	-	-
19	CLA	B1	822	X	-	-	-
19	CLA	B1	823	X	-	-	-
19	CLA	B1	824	X	-	-	-
19	CLA	B1	825	X	-	-	-
19	CLA	B1	826	X	-	-	-
19	CLA	B1	827	X	-	-	-
19	CLA	B1	828	X	-	-	-
19	CLA	B1	829	X	-	-	-
19	CLA	B1	830	X	-	-	-
19	CLA	B1	831	X	-	-	-
19	CLA	B1	832	X	-	-	-
19	CLA	B1	833	X	-	-	-
19	CLA	B1	834	X	-	-	-
19	CLA	B1	835	X	-	-	-
19	CLA	B1	836	X	-	-	-
19	CLA	B1	845	X	-	-	-
19	CLA	B1	848	X	-	-	-
19	CLA	B1	849	X	-	-	-
19	CLA	B1	850	X	-	-	-
19	CLA	B2	801	X	-	-	-
19	CLA	B2	802	X	-	-	-
19	CLA	B2	803	X	-	-	-
19	CLA	B2	804	X	-	-	-
19	CLA	B2	805	X	-	-	-
19	CLA	B2	806	X	-	-	-
19	CLA	B2	807	X	-	-	-
19	CLA	B2	808	X	-	-	-
19	CLA	B2	809	X	-	-	-
19	CLA	B2	810	X	-	-	-
19	CLA	B2	811	X	-	-	-
19	CLA	B2	812	X	-	-	-
19	CLA	B2	813	X	-	-	-
19	CLA	B2	814	X	-	-	-
19	CLA	B2	815	X	-	-	-
19	CLA	B2	816	X	-	-	-
19	CLA	B2	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B2	818	X	-	-	-
19	CLA	B2	819	X	-	-	-
19	CLA	B2	820	X	-	-	-
19	CLA	B2	821	X	-	-	-
19	CLA	B2	822	X	-	-	-
19	CLA	B2	823	X	-	-	-
19	CLA	B2	824	X	-	-	-
19	CLA	B2	825	X	-	-	-
19	CLA	B2	826	X	-	-	-
19	CLA	B2	827	X	-	-	-
19	CLA	B2	828	X	-	-	-
19	CLA	B2	829	X	-	-	-
19	CLA	B2	830	X	-	-	-
19	CLA	B2	831	X	-	-	-
19	CLA	B2	832	X	-	-	-
19	CLA	B2	834	X	-	-	-
19	CLA	B2	835	X	-	-	-
19	CLA	B2	836	X	-	-	-
19	CLA	B2	837	X	-	-	-
19	CLA	B2	846	X	-	-	-
19	CLA	B2	849	X	-	-	-
19	CLA	B2	850	X	-	-	-
19	CLA	B2	851	X	-	-	-
19	CLA	B2	852	X	-	-	-
19	CLA	BB	801	X	-	-	-
19	CLA	BB	802	X	-	-	-
19	CLA	BB	803	X	-	-	-
19	CLA	BB	804	X	-	-	-
19	CLA	BB	805	X	-	-	-
19	CLA	BB	806	X	-	-	-
19	CLA	BB	807	X	-	-	-
19	CLA	BB	808	X	-	-	-
19	CLA	BB	809	X	-	-	-
19	CLA	BB	810	X	-	-	-
19	CLA	BB	811	X	-	-	-
19	CLA	BB	812	X	-	-	-
19	CLA	BB	813	X	-	-	-
19	CLA	BB	814	X	-	-	-
19	CLA	BB	815	X	-	-	-
19	CLA	BB	816	X	-	-	-
19	CLA	BB	817	X	-	-	-
19	CLA	BB	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	BB	819	X	-	-	-
19	CLA	BB	820	X	-	-	-
19	CLA	BB	821	X	-	-	-
19	CLA	BB	822	X	-	-	-
19	CLA	BB	823	X	-	-	-
19	CLA	BB	824	X	-	-	-
19	CLA	BB	825	X	-	-	-
19	CLA	BB	826	X	-	-	-
19	CLA	BB	827	X	-	-	-
19	CLA	BB	828	X	-	-	-
19	CLA	BB	829	X	-	-	-
19	CLA	BB	830	X	-	-	-
19	CLA	BB	831	X	-	-	-
19	CLA	BB	833	X	-	-	-
19	CLA	BB	834	X	-	-	-
19	CLA	BB	835	X	-	-	-
19	CLA	BB	836	X	-	-	-
19	CLA	BB	845	X	-	-	-
19	CLA	BB	852	X	-	-	-
19	CLA	BB	855	X	-	-	-
19	CLA	BB	856	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F1	301	X	-	-	-
19	CLA	F1	302	X	-	-	-
19	CLA	F1	305	X	-	-	-
19	CLA	F2	301	X	-	-	-
19	CLA	F2	302	X	-	-	-
19	CLA	FF	301	X	-	-	-
19	CLA	FF	302	X	-	-	-
19	CLA	FF	305	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	J1	101	X	-	-	-
19	CLA	J1	103	X	-	-	-
19	CLA	J2	101	X	-	-	-
19	CLA	J2	103	X	-	-	-
19	CLA	JJ	101	X	-	-	-
19	CLA	JJ	103	X	-	-	-
19	CLA	K	101	X	-	-	-
19	CLA	K	102	X	-	-	-
19	CLA	K1	102	X	-	-	-
19	CLA	K1	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	K1	105	X	-	-	-
19	CLA	K2	102	X	-	-	-
19	CLA	K2	104	X	-	-	-
19	CLA	KK	101	X	-	-	-
19	CLA	KK	102	X	-	-	-
19	CLA	L	202	X	-	-	-
19	CLA	L	203	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L1	205	X	-	-	-
19	CLA	L1	206	X	-	-	-
19	CLA	L1	207	X	-	-	-
19	CLA	L2	204	X	-	-	-
19	CLA	L2	205	X	-	-	-
19	CLA	L2	206	X	-	-	-
19	CLA	LL	201	X	-	-	-
19	CLA	LL	202	X	-	-	-
19	CLA	LL	203	X	-	-	-
19	CLA	X	101	X	-	-	-
19	CLA	X1	101	X	-	-	-
19	CLA	X2	101	X	-	-	-
19	CLA	XX	101	X	-	-	-
20	CL0	A	803	X	-	-	-
20	CL0	A1	802	X	-	-	-
20	CL0	A2	803	X	-	-	-
20	CL0	AA	803	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 199181 atoms, of which 99577 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	A1	740	Total	C	H	N	O	S	0	0
			11478	3809	5672	1000	976	21		
1	A2	740	Total	C	H	N	O	S	0	0
			11486	3809	5680	1000	976	21		
1	A	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		
1	AA	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B1	739	Total	C	H	N	O	S	0	0
			11579	3905	5660	990	1006	18		
2	B2	739	Total	C	H	N	O	S	0	0
			11581	3905	5662	990	1006	18		
2	B	739	Total	C	H	N	O	S	0	0
			11586	3905	5667	990	1006	18		
2	BB	739	Total	C	H	N	O	S	0	0
			11595	3905	5676	990	1006	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C1	80	Total	C	H	N	O	S	0	0
			1183	367	584	103	118	11		
3	C2	80	Total	C	H	N	O	S	0	0
			1179	367	580	103	118	11		
3	C	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		
3	CC	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D1	134	Total	C	H	N	O	S	0	0
			2073	664	1037	178	193	1		
4	D2	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	D	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	DD	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	60	Total	C	H	N	O	0	0
			958	308	477	83	90		
5	E2	60	Total	C	H	N	O	0	0
			958	308	477	83	90		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F1	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		
6	F	139	Total	C	H	N	O	S	0	0
			2111	678	1051	179	201	2		
6	FF	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I1	31	Total	C	H	N	O	0	0
			508	177	255	35	41		
7	I	31	Total	C	H	N	O	0	0
			508	177	255	35	41		
7	II	31	Total	C	H	N	O	0	0
			508	177	255	35	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J1	43	Total	C	H	N	O	0	0
			701	237	355	52	57		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J2	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	J	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	JJ	43	Total	C	H	N	O	0	0
			700	237	354	52	57		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K1	74	Total	C	H	N	O	S	0	0
			1091	356	555	87	92	1		
9	K	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		
9	KK	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L1	166	Total	C	H	N	O	S	0	0
			2483	810	1239	213	220	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M1	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M2	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	MM	31	Total	C	H	N	O	0	0
			496	160	256	37	43		

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X1	39	Total	C	H	N	O	0	0
			627	212	318	49	48		
12	X2	39	Total	C	H	N	O	0	0
			627	212	318	49	48		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	39	Total	C	H	N	O	0	0
			628	212	319	49	48		
12	XX	39	Total	C	H	N	O	0	0
			628	212	319	49	48		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	F2	137	Total	C	H	N	O	S	0	0
			2087	670	1040	177	198	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I2	33	Total	C	H	N	O	0	0
			536	186	268	37	45		

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K2	73	Total	C	H	N	O	S	0	0
			1081	353	550	86	91	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L2	167	Total	C	H	N	O	S	0	0
			2498	815	1245	215	222	1		

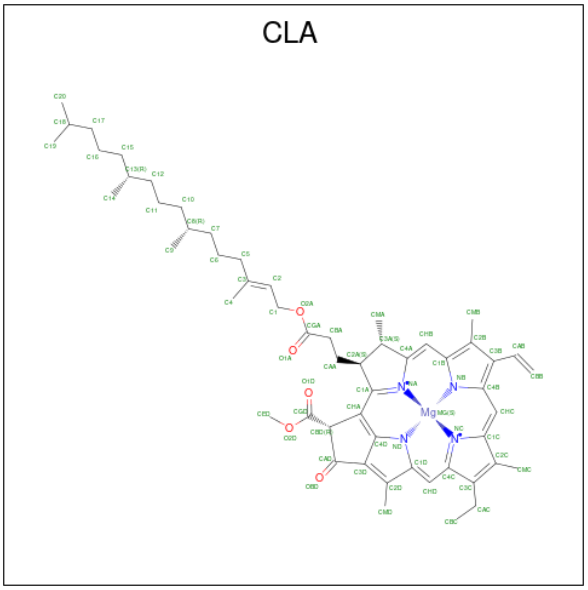
- Molecule 17 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	63	Total	C	H	N	O	0	0
			994	321	492	86	95		
17	EE	63	Total	C	H	N	O	0	0
			994	321	492	86	95		

- Molecule 18 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	154	Total	C	H	N	O	S	0	0
			2309	758	1153	196	201	1		
18	LL	154	Total	C	H	N	O	S	0	0
			2310	758	1154	196	201	1		

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	J1	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	J1	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	

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Mol	Chain	Residues	Atoms						AltConf
19	X1	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	F2	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	F2	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	J2	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	J2	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	K2	1	Total	C	H	Mg	N	O	0
			147	68	61	2	8	8	
19	K2	1	Total	C	H	Mg	N	O	0
			147	68	61	2	8	8	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	X2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	F	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	F	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	J	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	J	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	K	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	K	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	L	1	Total	C	H	Mg	N	O	0
			389	161	198	3	12	15	
19	L	1	Total	C	H	Mg	N	O	0
			389	161	198	3	12	15	
19	L	1	Total	C	H	Mg	N	O	0
			389	161	198	3	12	15	

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Mol	Chain	Residues	Atoms						AltConf
19	X	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	AA	1	Total	C	H	Mg	N	O	0
			4683	1982	2279	43	172	207	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	

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Mol	Chain	Residues	Atoms						AltConf
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	
19	BB	1	Total	C	H	Mg	N	O	0
			4490	1885	2219	40	160	186	

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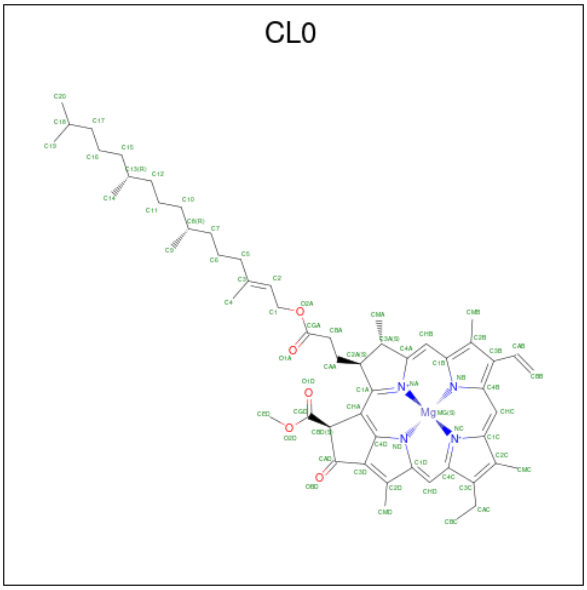
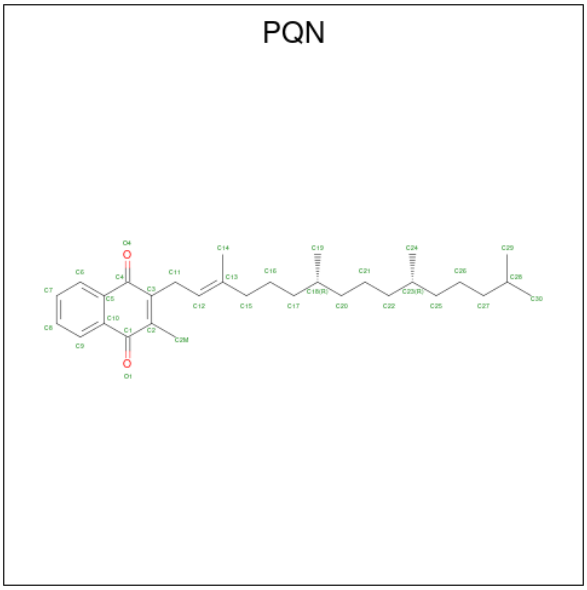
Mol	Chain	Residues	Atoms						AltConf
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	JJ	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	JJ	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	KK	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	KK	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	XX	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

- Molecule 20 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



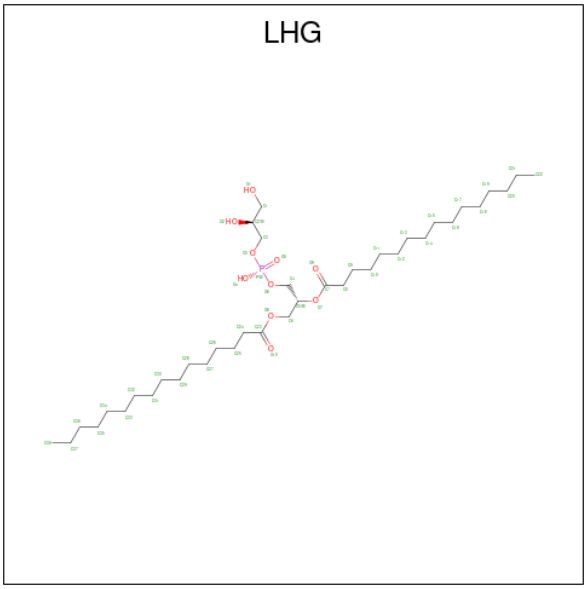
Mol	Chain	Residues	Atoms						AltConf
20	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				AltConf
21	A1	1	Total	C	H	O	0
			79	31	46	2	
21	B1	1	Total	C	H	O	0
			79	31	46	2	
21	A2	1	Total	C	H	O	0
			79	31	46	2	
21	B2	1	Total	C	H	O	0
			79	31	46	2	
21	A	1	Total	C	H	O	0
			79	31	46	2	
21	B	1	Total	C	H	O	0
			79	31	46	2	
21	AA	1	Total	C	H	O	0
			79	31	46	2	
21	BB	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	A1	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A1	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B1	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L1	1	Total	C	H	O	P	0
			68	22	35	10	1	
22	X1	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	X1	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	A2	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A2	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B2	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L2	1	Total	C	H	O	P	0
			74	24	39	10	1	
22	X2	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	X2	1	Total	C	H	O	P	0
			212	67	123	20	2	

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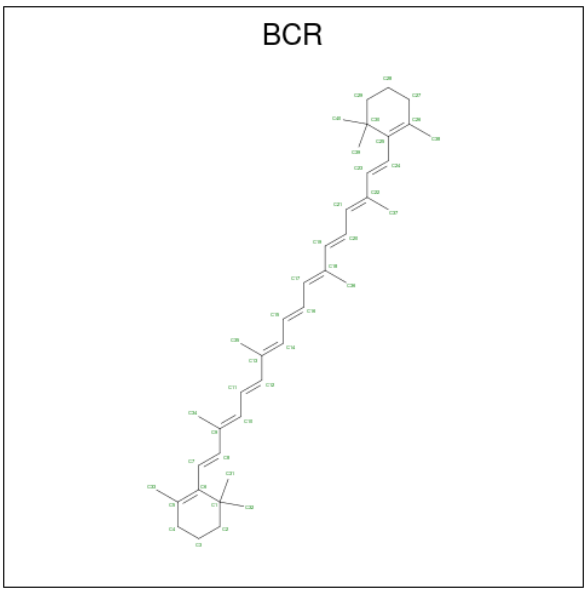
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	B	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	L	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	X	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	AA	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	AA	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	BB	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	BB	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	LL	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	XX	1	Total	C	H	O	P	0
			89	29	49	10	1	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			AltConf
23	A1	1	Total 572	C 239	H 333	0
23	A1	1	Total 572	C 239	H 333	0
23	A1	1	Total 572	C 239	H 333	0
23	A1	1	Total 572	C 239	H 333	0
23	A1	1	Total 572	C 239	H 333	0
23	A1	1	Total 572	C 239	H 333	0
23	B1	1	Total 480	C 200	H 280	0
23	B1	1	Total 480	C 200	H 280	0
23	B1	1	Total 480	C 200	H 280	0
23	B1	1	Total 480	C 200	H 280	0
23	B1	1	Total 480	C 200	H 280	0
23	F1	1	Total 283	C 120	H 163	0
23	F1	1	Total 283	C 120	H 163	0
23	F1	1	Total 283	C 120	H 163	0
23	I1	1	Total 96	C 40	H 56	0
23	J1	1	Total 192	C 80	H 112	0
23	J1	1	Total 192	C 80	H 112	0
23	K1	1	Total 192	C 80	H 112	0
23	K1	1	Total 192	C 80	H 112	0
23	L1	1	Total 288	C 120	H 168	0
23	L1	1	Total 288	C 120	H 168	0
23	L1	1	Total 288	C 120	H 168	0

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Mol	Chain	Residues	Atoms			AltConf
23	M1	1	Total 96	C 40	H 56	0
23	A2	1	Total 572	C 239	H 333	0
23	A2	1	Total 572	C 239	H 333	0
23	A2	1	Total 572	C 239	H 333	0
23	A2	1	Total 572	C 239	H 333	0
23	A2	1	Total 572	C 239	H 333	0
23	A2	1	Total 572	C 239	H 333	0
23	B2	1	Total 475	C 200	H 275	0
23	B2	1	Total 475	C 200	H 275	0
23	B2	1	Total 475	C 200	H 275	0
23	B2	1	Total 475	C 200	H 275	0
23	B2	1	Total 475	C 200	H 275	0
23	F2	1	Total 283	C 120	H 163	0
23	F2	1	Total 283	C 120	H 163	0
23	F2	1	Total 283	C 120	H 163	0
23	I2	1	Total 288	C 120	H 168	0
23	I2	1	Total 288	C 120	H 168	0
23	I2	1	Total 288	C 120	H 168	0
23	J2	1	Total 192	C 80	H 112	0
23	J2	1	Total 192	C 80	H 112	0
23	K2	1	Total 192	C 80	H 112	0

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Mol	Chain	Residues	Atoms	AltConf
23	K2	1	Total C H 192 80 112	0
23	L2	1	Total C H 96 40 56	0
23	M2	1	Total C H 96 40 56	0
23	A	1	Total C H 668 279 389	0
23	A	1	Total C H 668 279 389	0
23	A	1	Total C H 668 279 389	0
23	A	1	Total C H 668 279 389	0
23	A	1	Total C H 668 279 389	0
23	A	1	Total C H 668 279 389	0
23	A	1	Total C H 668 279 389	0
23	B	1	Total C H 576 240 336	0
23	B	1	Total C H 576 240 336	0
23	B	1	Total C H 576 240 336	0
23	B	1	Total C H 576 240 336	0
23	B	1	Total C H 576 240 336	0
23	B	1	Total C H 576 240 336	0
23	F	1	Total C H 283 120 163	0
23	F	1	Total C H 283 120 163	0
23	F	1	Total C H 283 120 163	0
23	I	1	Total C H 192 80 112	0
23	I	1	Total C H 192 80 112	0

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Mol	Chain	Residues	Atoms	AltConf
23	J	1	Total C H 192 80 112	0
23	J	1	Total C H 192 80 112	0
23	K	1	Total C H 96 40 56	0
23	L	1	Total C H 192 80 112	0
23	L	1	Total C H 192 80 112	0
23	M	1	Total C H 91 40 51	0
23	AA	1	Total C H 668 279 389	0
23	AA	1	Total C H 668 279 389	0
23	AA	1	Total C H 668 279 389	0
23	AA	1	Total C H 668 279 389	0
23	AA	1	Total C H 668 279 389	0
23	AA	1	Total C H 668 279 389	0
23	AA	1	Total C H 668 279 389	0
23	BB	1	Total C H 576 240 336	0
23	BB	1	Total C H 576 240 336	0
23	BB	1	Total C H 576 240 336	0
23	BB	1	Total C H 576 240 336	0
23	BB	1	Total C H 576 240 336	0
23	BB	1	Total C H 576 240 336	0
23	FF	1	Total C H 283 120 163	0
23	FF	1	Total C H 283 120 163	0

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Mol	Chain	Residues	Atoms			AltConf
23	FF	1	Total 283	C 120	H 163	0
23	II	1	Total 288	C 120	H 168	0
23	II	1	Total 288	C 120	H 168	0
23	II	1	Total 288	C 120	H 168	0
23	JJ	1	Total 192	C 80	H 112	0
23	JJ	1	Total 192	C 80	H 112	0
23	KK	1	Total 96	C 40	H 56	0
23	LL	1	Total 96	C 40	H 56	0
23	MM	1	Total 93	C 40	H 53	0

- Molecule 24 is a ligand with the chemical component id AJP but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for AJP. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

Mol	Chain	Residues	Atoms				AltConf
24	A1	1	Total 171	C 60	H 96	O 15	0
24	A1	1	Total 171	C 60	H 96	O 15	0
24	L1	1	Total 192	C 66	H 106	O 20	0
24	L1	1	Total 192	C 66	H 106	O 20	0
24	A2	1	Total 75	C 27	H 43	O 5	0
24	I2	1	Total 73	C 27	H 42	O 4	0
24	L2	1	Total 192	C 66	H 106	O 20	0
24	L2	1	Total 192	C 66	H 106	O 20	0
24	M2	1	Total 74	C 27	H 43	O 4	0

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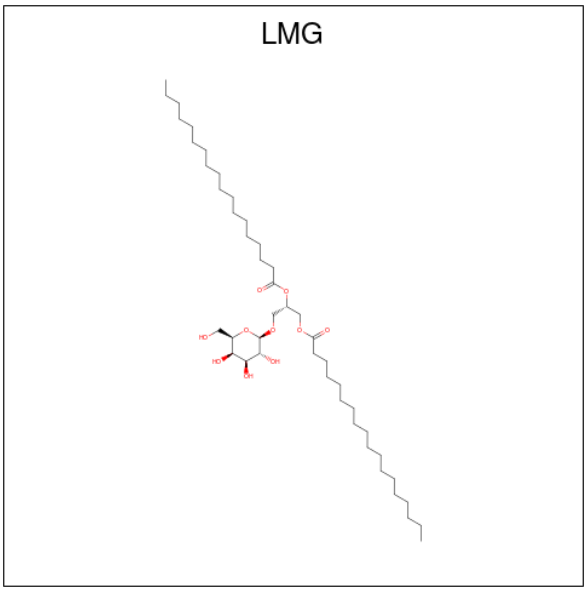
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	H	O	0
			153	56	88	9	
24	A	1	Total	C	H	O	0
			153	56	88	9	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	K	1	Total	C	H	O	0
			91	32	50	9	
24	L	1	Total	C	H	O	0
			147	54	85	8	
24	L	1	Total	C	H	O	0
			147	54	85	8	
24	AA	1	Total	C	H	O	0
			153	56	88	9	
24	AA	1	Total	C	H	O	0
			153	56	88	9	
24	BB	1	Total	C	H	O	0
			192	66	106	20	
24	BB	1	Total	C	H	O	0
			192	66	106	20	
24	KK	1	Total	C	H	O	0
			91	32	50	9	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
25	A1	1	Total	C	H	O	1
			152	48	84	20	
25	A1	1	Total	C	H	O	1
			152	48	84	20	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	I1	1	Total	C	H	O	0
			75	25	40	10	
25	K1	1	Total	C	H	O	1
			120	38	62	20	
25	K1	1	Total	C	H	O	1
			120	38	62	20	
25	L1	1	Total	C	H	O	1
			223	71	132	20	
25	L1	1	Total	C	H	O	0
			223	71	132	20	
25	A2	1	Total	C	H	O	1
			171	54	97	20	
25	A2	1	Total	C	H	O	1
			171	54	97	20	
25	B2	1	Total	C	H	O	0
			265	87	148	30	
25	B2	1	Total	C	H	O	0
			265	87	148	30	

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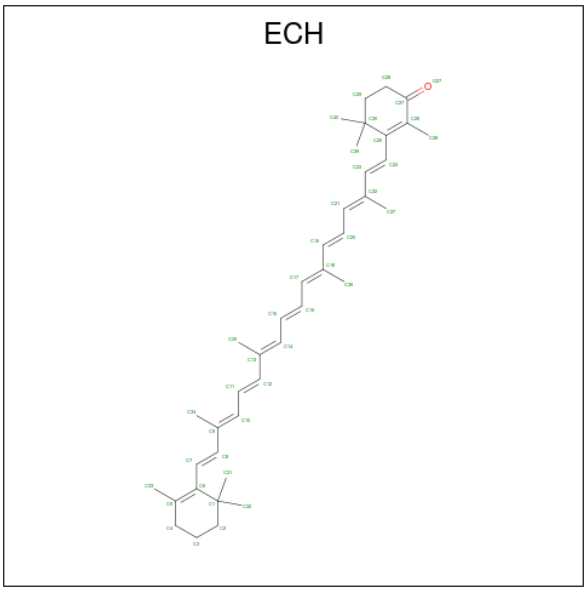
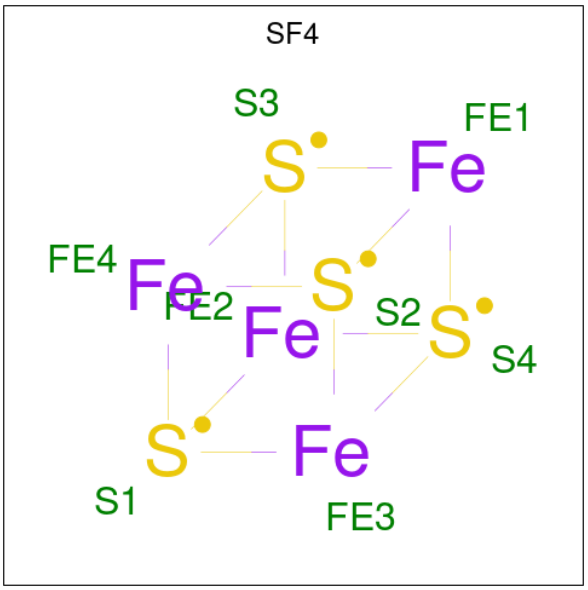
Mol	Chain	Residues	Atoms				AltConf
25	B2	1	Total	C	H	O	0
			265	87	148	30	
25	I2	1	Total	C	H	O	0
			75	25	40	10	
25	K2	1	Total	C	H	O	1
			114	36	58	20	
25	K2	1	Total	C	H	O	1
			114	36	58	20	
25	L2	1	Total	C	H	O	1
			82	26	46	10	
25	B	1	Total	C	H	O	0
			427	136	251	40	
25	B	1	Total	C	H	O	1
			427	136	251	40	
25	B	1	Total	C	H	O	0
			427	136	251	40	
25	B	1	Total	C	H	O	1
			427	136	251	40	
25	L	1	Total	C	H	O	1
			85	27	48	10	
25	M	1	Total	C	H	O	0
			105	36	59	10	
25	BB	1	Total	C	H	O	0
			289	92	167	30	
25	BB	1	Total	C	H	O	1
			289	92	167	30	
25	BB	1	Total	C	H	O	1
			289	92	167	30	
25	II	1	Total	C	H	O	1
			181	59	102	20	
25	II	1	Total	C	H	O	0
			181	59	102	20	

- Molecule 26 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



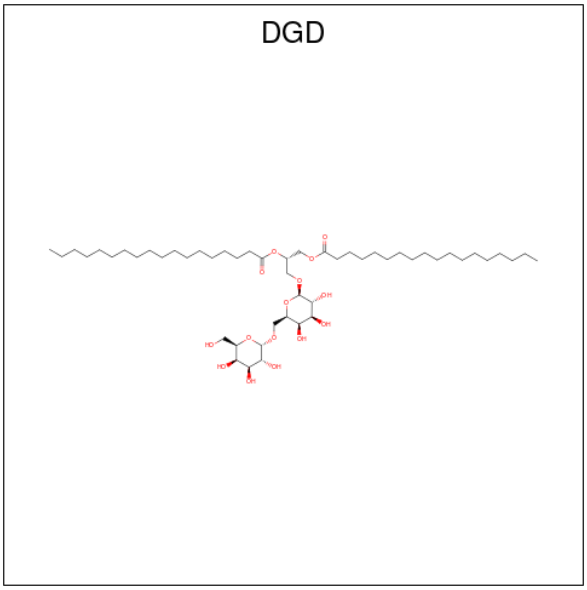
Mol	Chain	Residues	Atoms				AltConf
26	B1	1	Total	C	H	O	0
			95	40	54	1	
26	B2	1	Total	C	H	O	0
			95	40	54	1	
26	B	1	Total	C	H	O	0
			95	40	54	1	
26	BB	1	Total	C	H	O	0
			95	40	54	1	

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
27	B1	1	Total Fe S 8 4 4	0
27	C1	1	Total Fe S 16 8 8	0
27	C1	1	Total Fe S 16 8 8	0
27	B2	1	Total Fe S 8 4 4	0
27	C2	1	Total Fe S 16 8 8	0
27	C2	1	Total Fe S 16 8 8	0
27	B	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 16 8 8	0
27	C	1	Total Fe S 16 8 8	0
27	BB	1	Total Fe S 8 4 4	0
27	CC	1	Total Fe S 16 8 8	0
27	CC	1	Total Fe S 16 8 8	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	H	O	0
			88	27	46	15	
28	BB	1	Total	C	H	O	0
			88	27	46	15	

3 Residue-property plots (i)

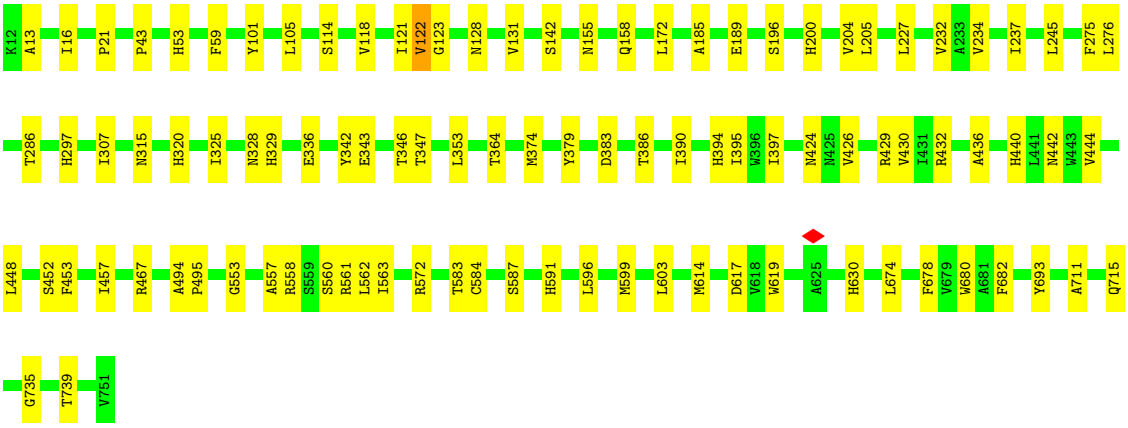
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 A1:

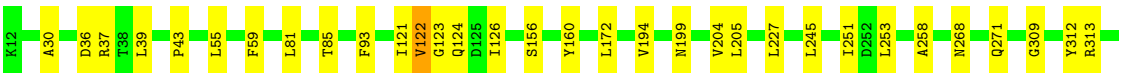
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

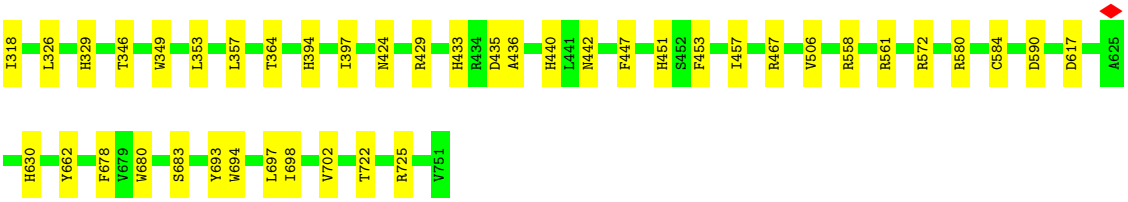
Chain A2:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

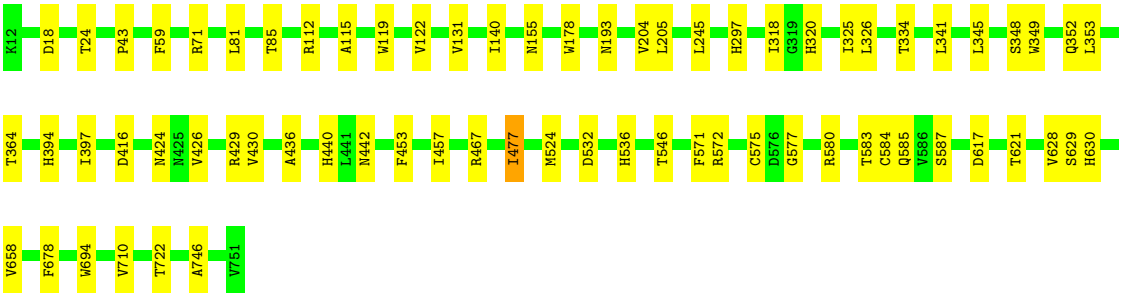
Chain A:





• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA:

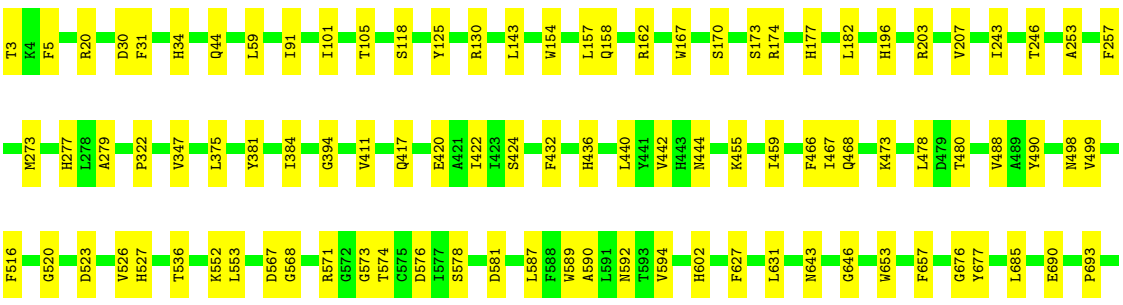


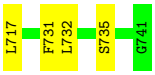
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B1:

• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

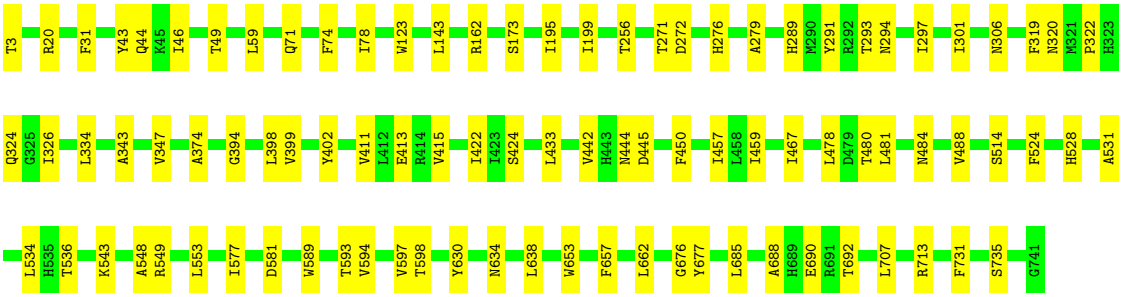
Chain B2:





• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B:

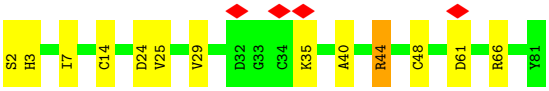


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain BB:

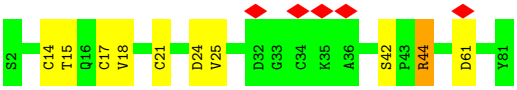
• Molecule 3: Photosystem I iron-sulfur center

Chain C1:



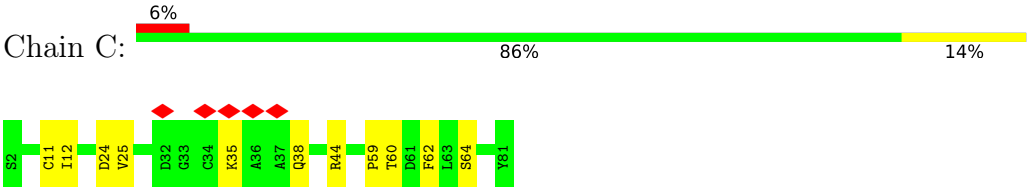
• Molecule 3: Photosystem I iron-sulfur center

Chain C2:



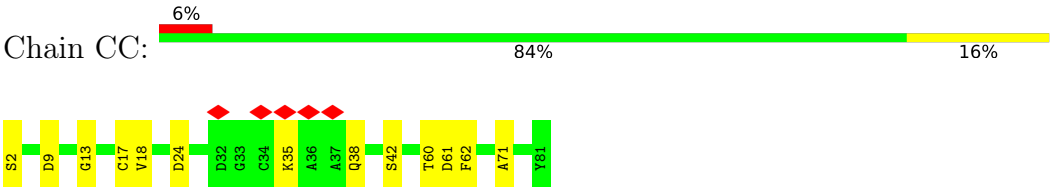
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



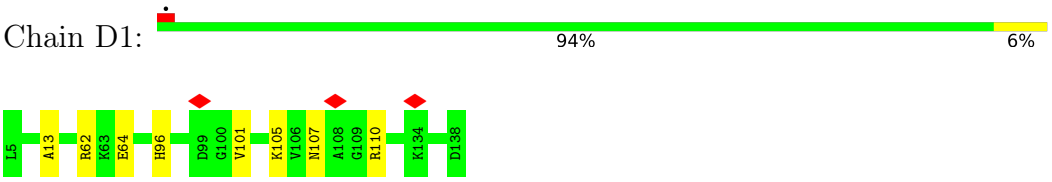
• Molecule 3: Photosystem I iron-sulfur center

Chain CC:



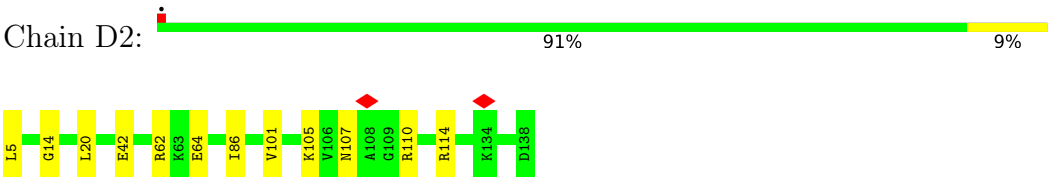
• Molecule 4: Photosystem I reaction center subunit II

Chain D1:



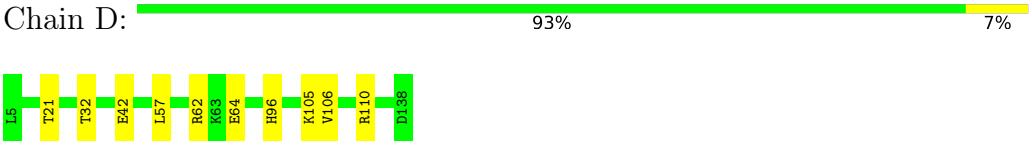
• Molecule 4: Photosystem I reaction center subunit II

Chain D2:



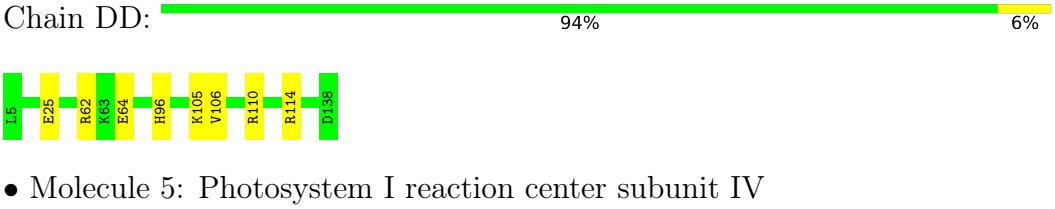
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



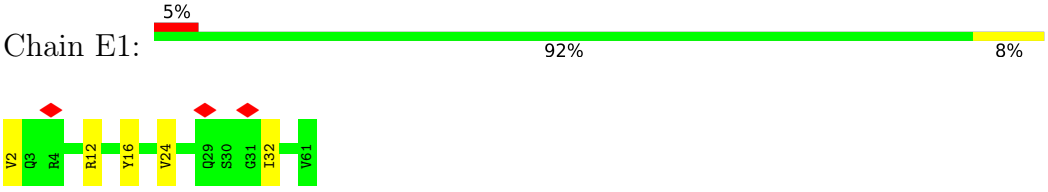
• Molecule 4: Photosystem I reaction center subunit II

Chain DD:



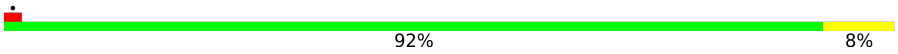
• Molecule 5: Photosystem I reaction center subunit IV

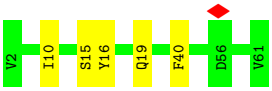
Chain E1:



• Molecule 5: Photosystem I reaction center subunit IV

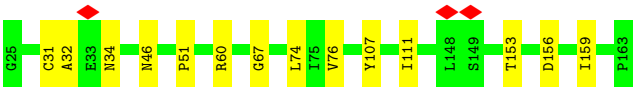
Chain E2:





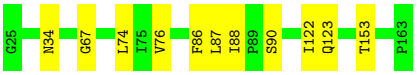
• Molecule 6: Photosystem I reaction center subunit III

Chain F1:



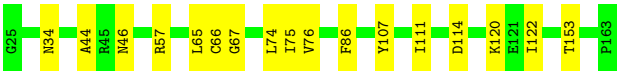
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



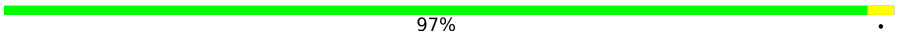
• Molecule 6: Photosystem I reaction center subunit III

Chain FF:



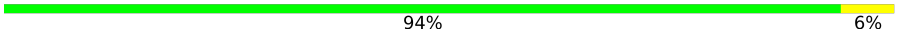
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:



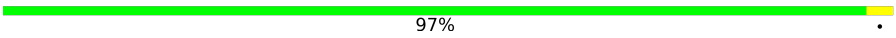
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



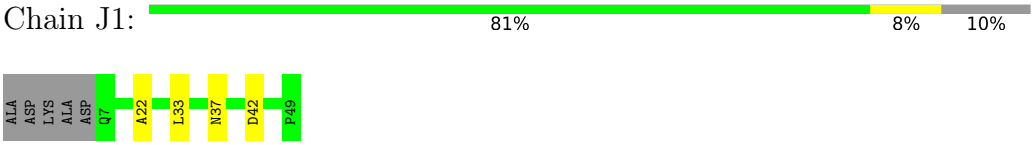
• Molecule 7: Photosystem I reaction center subunit VIII

Chain II:



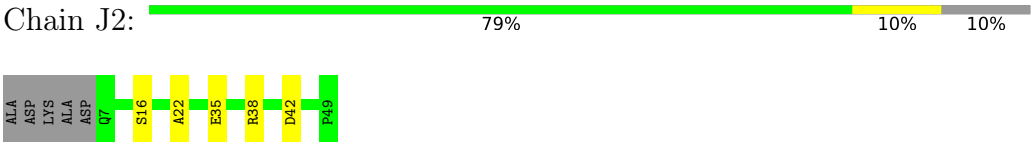
• Molecule 8: Photosystem I reaction center subunit IX

Chain J1:



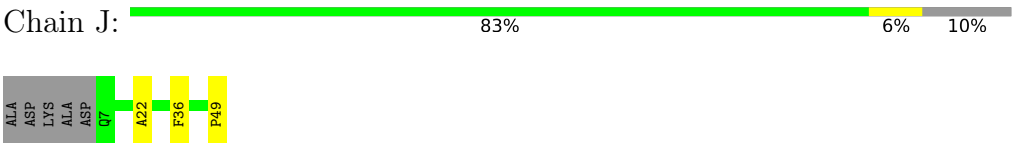
• Molecule 8: Photosystem I reaction center subunit IX

Chain J2:



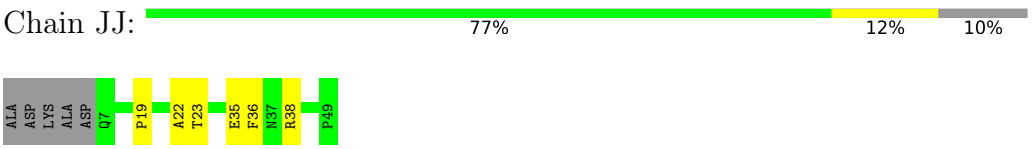
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



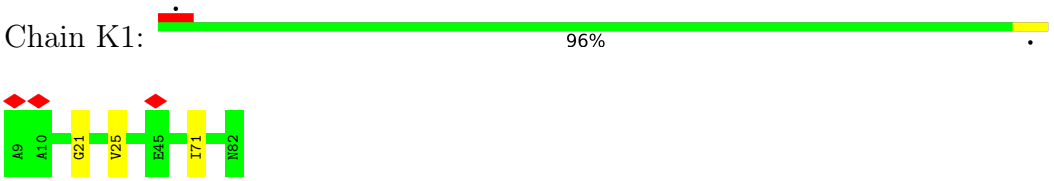
• Molecule 8: Photosystem I reaction center subunit IX

Chain JJ:



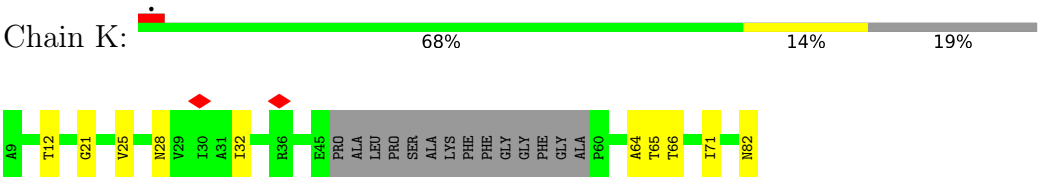
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K1:



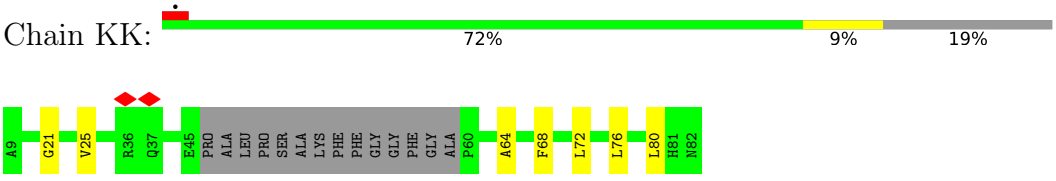
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:



• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain KK:

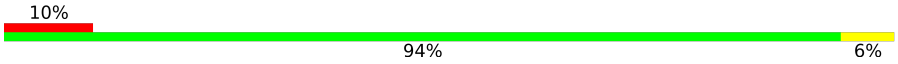


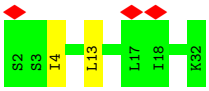
• Molecule 10: Photosystem I reaction center subunit XI

Chain L1:

• Molecule 11: Photosystem I reaction center subunit XII

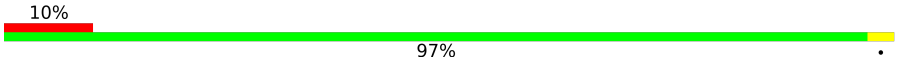
Chain M1:

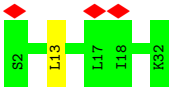




• Molecule 11: Photosystem I reaction center subunit XII

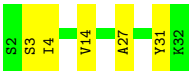
Chain M2:





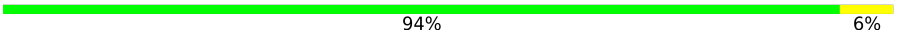
• Molecule 11: Photosystem I reaction center subunit XII

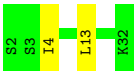
Chain M:



• Molecule 11: Photosystem I reaction center subunit XII

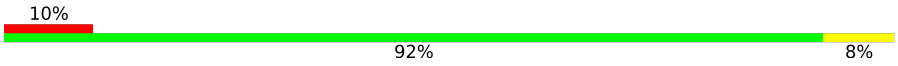
Chain MM:

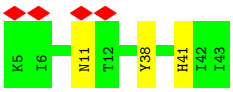




• Molecule 12: Photosystem I 4.8 kDa protein

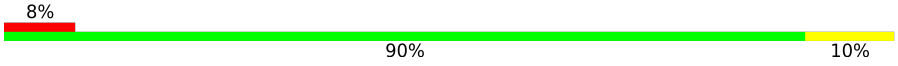
Chain X1:

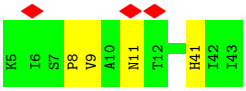




• Molecule 12: Photosystem I 4.8 kDa protein

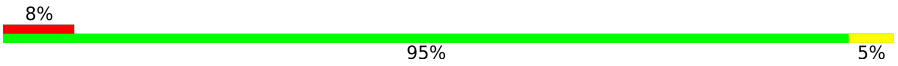
Chain X2:

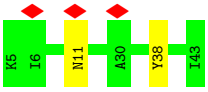




• Molecule 12: Photosystem I 4.8 kDa protein

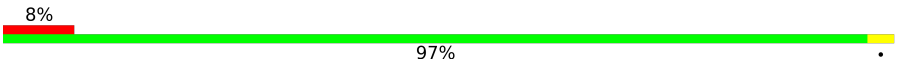
Chain X:

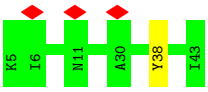




• Molecule 12: Photosystem I 4.8 kDa protein

Chain XX:



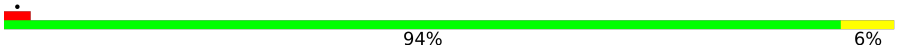


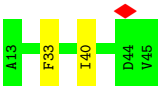
• Molecule 13: Photosystem I reaction center subunit III

Chain F2:

• Molecule 14: Photosystem I reaction center subunit VIII

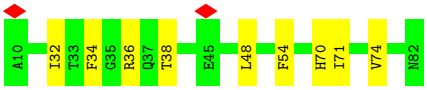
Chain I2:





• Molecule 15: Photosystem I reaction center subunit PsaK 1

Chain K2:

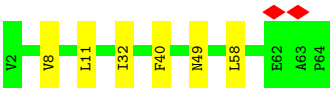


• Molecule 16: Photosystem I reaction center subunit XI

Chain L2:

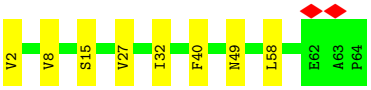
• Molecule 17: Photosystem I reaction center subunit IV

Chain E:



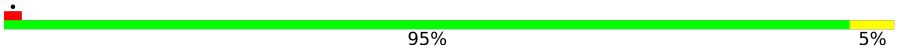
• Molecule 17: Photosystem I reaction center subunit IV

Chain EE:



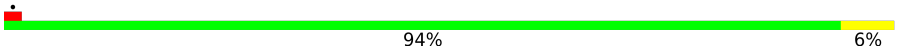
• Molecule 18: Photosystem I reaction center subunit XI

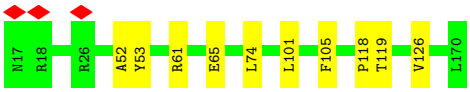
Chain L:



• Molecule 18: Photosystem I reaction center subunit XI

Chain LL:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.390	Depositor
Minimum map value	-1.168	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.434	Depositor
Map size (Å)	392.19998, 392.19998, 392.19998	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.29	0/6004	0.44	0/8193
1	A1	0.28	0/6004	0.45	0/8193
1	A2	0.29	0/6004	0.46	0/8193
1	AA	0.28	0/6004	0.44	0/8193
2	B	0.32	0/6143	0.46	0/8396
2	B1	0.29	0/6143	0.44	0/8396
2	B2	0.30	0/6143	0.44	0/8396
2	BB	0.32	0/6143	0.45	0/8396
3	C	0.28	0/609	0.52	0/826
3	C1	0.28	0/609	0.52	0/826
3	C2	0.28	0/609	0.49	0/826
3	CC	0.28	0/609	0.51	0/826
4	D	0.28	0/1060	0.52	0/1431
4	D1	0.27	0/1060	0.50	0/1431
4	D2	0.27	0/1060	0.53	0/1431
4	DD	0.28	0/1060	0.52	0/1431
5	E1	0.27	0/490	0.49	0/665
5	E2	0.30	0/490	0.47	0/665
6	F	0.28	0/1084	0.47	0/1475
6	F1	0.26	0/1084	0.46	0/1475
6	FF	0.27	0/1084	0.47	0/1475
7	I	0.29	0/262	0.41	0/358
7	I1	0.30	0/262	0.40	0/358
7	II	0.30	0/262	0.41	0/358
8	J	0.28	0/358	0.46	0/491
8	J1	0.27	0/358	0.43	0/491
8	J2	0.27	0/358	0.41	0/491
8	JJ	0.27	0/358	0.42	0/491
9	K	0.25	0/448	0.41	0/613
9	K1	0.27	0/551	0.45	0/755
9	KK	0.25	0/448	0.44	0/613
10	L1	0.30	0/1281	0.46	0/1756

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	M	0.26	0/244	0.37	0/334
11	M1	0.26	0/244	0.42	0/334
11	M2	0.25	0/244	0.41	0/334
11	MM	0.26	0/244	0.39	0/334
12	X	0.29	0/320	0.46	0/439
12	X1	0.27	0/320	0.43	0/439
12	X2	0.29	0/320	0.44	0/439
12	XX	0.29	0/320	0.44	0/439
13	F2	0.29	0/1070	0.52	0/1455
14	I2	0.30	0/277	0.42	0/379
15	K2	0.26	0/546	0.45	0/748
16	L2	0.31	0/1290	0.47	0/1768
17	E	0.29	0/512	0.49	0/696
17	EE	0.28	0/512	0.48	0/696
18	L	0.30	0/1191	0.47	0/1632
18	LL	0.30	0/1191	0.45	0/1632
All	All	0.29	0/73287	0.46	0/100012

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
13	F2	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	F2	158	GLU	Peptide
13	F2	159	ILE	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	A	5806	5677	5682	58	0
1	A1	5806	5672	5682	73	0
1	A2	5806	5680	5682	73	0
1	AA	5806	5677	5682	56	0
2	B	5919	5667	5677	73	0
2	B1	5919	5660	5677	82	0
2	B2	5919	5662	5677	79	0
2	BB	5919	5676	5677	89	0
3	C	599	582	585	8	0
3	C1	599	584	585	10	0
3	C2	599	580	585	6	0
3	CC	599	582	585	10	0
4	D	1036	1042	1042	9	0
4	D1	1036	1037	1042	7	0
4	D2	1036	1042	1042	10	0
4	DD	1036	1042	1042	7	0
5	E1	481	477	478	4	0
5	E2	481	477	478	7	0
6	F	1060	1051	1054	8	0
6	F1	1060	1052	1054	11	0
6	FF	1060	1052	1054	11	0
7	I	253	255	255	2	0
7	I1	253	255	255	1	0
7	II	253	255	255	1	0
8	J	346	355	355	3	0
8	J1	346	355	355	4	0
8	J2	346	355	355	5	0
8	JJ	346	354	355	5	0
9	K	439	461	461	6	0
9	K1	536	555	555	2	0
9	KK	439	461	461	4	0
10	L1	1244	1239	1242	16	0
11	M	240	256	256	5	0
11	M1	240	256	256	3	0
11	M2	240	256	256	1	0
11	MM	240	256	256	4	0
12	X	309	319	319	2	0
12	X1	309	318	319	4	0
12	X2	309	318	319	5	0
12	XX	309	319	319	1	0
13	F2	1047	1040	1042	15	0
14	I2	268	268	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K2	531	550	550	7	0
16	L2	1253	1245	1250	12	0
17	E	502	492	496	5	0
17	EE	502	492	496	6	0
18	L	1156	1153	1157	4	0
18	LL	1156	1154	1157	8	0
19	A	2339	2207	2215	48	0
19	A1	2394	2261	2275	59	0
19	A2	2375	2227	2236	47	0
19	AA	2404	2279	2287	43	0
19	B	2401	2357	2375	73	0
19	B1	2291	2253	2270	61	0
19	B2	2401	2358	2375	50	0
19	BB	2271	2219	2231	64	0
19	F	102	89	90	3	0
19	F1	147	122	123	5	0
19	F2	102	89	90	3	0
19	FF	167	161	162	6	0
19	J	82	58	58	4	0
19	J1	82	57	58	1	0
19	J2	82	58	58	2	0
19	JJ	82	57	58	1	0
19	K	91	65	66	0	0
19	K1	131	92	94	2	0
19	K2	86	61	62	1	0
19	KK	91	65	66	0	0
19	L	191	198	205	4	0
19	L1	191	202	205	5	0
19	L2	186	187	191	0	0
19	LL	168	155	164	7	0
19	X	45	32	33	0	0
19	X1	45	32	33	0	0
19	X2	45	32	33	1	0
19	XX	45	32	33	0	0
20	A	65	72	72	1	0
20	A1	65	72	71	3	0
20	A2	65	72	70	5	0
20	AA	65	72	71	1	0
21	A	33	46	46	3	0
21	A1	33	46	46	1	0
21	A2	33	46	46	1	0
21	AA	33	46	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	33	46	46	2	0
21	B1	33	46	46	0	0
21	B2	33	46	46	0	0
21	BB	33	46	46	2	0
22	A	87	122	123	3	0
22	A1	87	122	123	1	0
22	A2	87	122	123	2	0
22	AA	87	122	123	3	0
22	B	82	110	110	1	0
22	B1	33	36	36	1	0
22	B2	33	36	36	0	0
22	BB	82	110	110	0	0
22	L	34	42	38	0	0
22	L1	33	35	36	3	0
22	L2	35	39	40	2	0
22	LL	34	42	38	0	0
22	X	40	49	50	0	0
22	X1	89	123	124	0	0
22	X2	89	123	124	0	0
22	XX	40	49	50	0	0
23	A	279	389	389	7	0
23	A1	239	333	333	6	0
23	A2	239	333	333	7	0
23	AA	279	389	389	8	0
23	B	240	336	336	12	0
23	B1	200	280	280	7	0
23	B2	200	275	280	8	0
23	BB	240	336	336	10	0
23	F	120	163	168	8	0
23	F1	120	163	168	7	0
23	F2	120	163	168	7	0
23	FF	120	163	168	7	0
23	I	80	112	112	0	0
23	I1	40	56	56	1	0
23	I2	120	168	168	1	0
23	II	120	168	168	0	0
23	J	80	112	112	2	0
23	J1	80	112	112	2	0
23	J2	80	112	112	3	0
23	JJ	80	112	112	2	0
23	K	40	56	56	0	0
23	K1	80	112	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K2	80	112	112	3	0
23	KK	40	56	56	0	0
23	L	80	112	112	1	0
23	L1	120	168	168	0	0
23	L2	40	56	56	0	0
23	LL	40	56	56	1	0
23	M	40	51	56	2	0
23	M1	40	56	56	0	0
23	M2	40	56	56	0	0
23	MM	40	53	56	1	0
24	A	65	88	0	0	0
24	A1	75	96	0	0	0
24	A2	32	43	0	0	0
24	AA	65	88	0	0	0
24	B	129	159	0	1	0
24	BB	86	106	0	1	0
24	I2	31	42	0	0	0
24	K	41	50	0	0	0
24	KK	41	50	0	0	0
24	L	62	85	0	0	0
24	L1	86	106	0	1	0
24	L2	86	106	0	1	0
24	M2	31	43	0	0	0
25	A1	68	84	0	0	0
25	A2	74	97	0	0	0
25	B	176	251	172	0	0
25	B1	117	148	150	0	0
25	B2	117	148	150	0	0
25	BB	122	167	86	0	0
25	I1	35	40	40	0	0
25	I2	35	40	40	1	0
25	II	79	102	54	0	0
25	K1	58	62	0	0	0
25	K2	56	58	0	0	0
25	L	37	48	0	0	0
25	L1	91	132	86	1	0
25	L2	36	46	0	0	0
25	M	46	59	62	1	0
26	B	41	54	54	1	0
26	B1	41	54	54	1	0
26	B2	41	54	54	1	0
26	BB	41	54	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	8	0	0	0	0
27	B1	8	0	0	0	0
27	B2	8	0	0	0	0
27	BB	8	0	0	0	0
27	C	16	0	0	1	0
27	C1	16	0	0	1	0
27	C2	16	0	0	0	0
27	CC	16	0	0	0	0
28	B	42	46	42	1	0
28	BB	42	46	42	1	0
All	All	99604	99577	98156	1039	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 5.

All (1039) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:587:LEU:HD23	2:B2:717:LEU:HD21	1.55	0.88
2:B:553:LEU:HD23	2:B:577:ILE:HD11	1.56	0.86
19:B2:822:CLA:H93	23:B2:843:BCR:H333	1.57	0.84
19:B1:822:CLA:H93	23:B1:842:BCR:H333	1.58	0.83
2:B1:534:LEU:HD12	19:B1:834:CLA:HED3	1.63	0.81
2:B:415:VAL:HG11	23:B:842:BCR:H401	1.62	0.81
19:B:834:CLA:H93	19:B:835:CLA:HBC1	1.63	0.79
19:BB:833:CLA:H93	19:BB:834:CLA:HBC1	1.64	0.79
1:A:199:ASN:ND2	1:A:309:GLY:O	2.16	0.79
19:B:822:CLA:H93	23:B:843:BCR:H333	1.66	0.78
19:B1:833:CLA:H93	19:B1:834:CLA:HBC1	1.66	0.77
1:A1:199:ASN:ND2	1:A1:309:GLY:O	2.18	0.77
1:A2:572:ARG:NH1	22:A2:845:LHG:O10	2.20	0.75
6:F1:31:CYS:SG	6:F1:32:ALA:N	2.59	0.75
19:BB:822:CLA:H93	23:BB:842:BCR:H333	1.68	0.75
2:B1:587:LEU:HD12	2:B1:717:LEU:HD21	1.69	0.75
2:B2:490:TYR:O	2:B2:498:ASN:ND2	2.21	0.74
1:A:693:TYR:O	2:B:543:LYS:NZ	2.20	0.74
2:B1:490:TYR:O	2:B1:498:ASN:ND2	2.21	0.74
4:D:105:LYS:O	4:D:110:ARG:NH2	2.22	0.73
2:B2:44:GLN:OE1	2:B2:162:ARG:NH2	2.22	0.73
2:B2:473:LYS:NZ	2:B2:516:PHE:O	2.20	0.72
2:BB:44:GLN:OE1	2:BB:162:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:473:LYS:NZ	2:B1:516:PHE:O	2.20	0.72
1:A1:693:TYR:O	2:B1:543:LYS:NZ	2.21	0.71
2:B:402:TYR:OH	2:B:413:GLU:OE2	2.08	0.71
19:B:834:CLA:HBC3	19:B:834:CLA:HMC1	1.72	0.71
19:BB:833:CLA:HBC3	19:BB:833:CLA:HMC1	1.72	0.71
6:F1:46:ASN:ND2	6:F1:51:PRO:O	2.23	0.70
13:F2:31:CYS:SG	13:F2:32:ALA:N	2.64	0.70
1:A1:576:ASP:OD2	1:A1:580:ARG:NH2	2.24	0.70
1:A2:715:GLN:NE2	5:E2:16:TYR:OH	2.25	0.69
2:B2:567:ASP:OD2	2:B2:571:ARG:NH2	2.25	0.69
4:D1:62:ARG:NH2	4:D1:64:GLU:OE1	2.26	0.69
2:BB:377:THR:HG23	2:BB:598:THR:HG21	1.73	0.69
18:LL:61:ARG:NH2	18:LL:65:GLU:OE1	2.26	0.69
1:A1:333:PHE:O	1:A1:429:ARG:NH1	2.25	0.68
1:A2:735:GLY:O	1:A2:739:THR:OG1	2.10	0.68
19:BB:829:CLA:HMC1	19:BB:829:CLA:HBC2	1.75	0.68
2:BB:306:ASN:ND2	2:BB:324:GLN:O	2.27	0.68
1:A1:435:ASP:OD2	1:A1:561:ARG:NH2	2.26	0.68
19:B1:833:CLA:HBC2	19:B1:834:CLA:HBC3	1.76	0.68
3:C1:61:ASP:OD1	5:E1:12:ARG:NH1	2.26	0.68
1:AA:722:THR:OG1	22:AA:846:LHG:O5	2.12	0.68
16:L2:114:ASN:ND2	22:L2:208:LHG:O9	2.28	0.67
1:AA:575:CYS:O	1:AA:583:THR:OG1	2.08	0.67
19:B1:821:CLA:HMA2	19:B1:821:CLA:O2A	1.94	0.67
23:A1:851:BCR:H362	19:A1:852:CLA:H43	1.77	0.67
1:A:722:THR:OG1	22:A:845:LHG:O5	2.13	0.67
23:A:851:BCR:H362	19:A:852:CLA:H43	1.76	0.67
4:D:62:ARG:NH2	4:D:64:GLU:OE1	2.27	0.67
19:B2:821:CLA:O2A	19:B2:821:CLA:HMA2	1.95	0.67
16:L2:11:LEU:O	16:L2:17:ASN:ND2	2.27	0.67
5:E2:19:GLN:NE2	13:F2:153:THR:O	2.28	0.67
19:A1:844:CLA:OBD	10:L1:18:ARG:NH2	2.28	0.67
1:A1:383:ASP:OD2	1:A1:386:THR:OG1	2.11	0.66
2:B1:409:GLY:N	2:B1:413:GLU:OE1	2.28	0.66
19:B:821:CLA:HMA2	19:B:821:CLA:O2A	1.95	0.66
2:B1:693:PRO:O	10:L1:53:TYR:OH	2.13	0.66
19:B1:832:CLA:CGD	19:B1:833:CLA:HMB1	2.26	0.66
19:B:834:CLA:HBB2	19:B:835:CLA:HED2	1.78	0.66
19:B2:834:CLA:HMC1	19:B2:834:CLA:HBC3	1.77	0.66
4:D2:62:ARG:NH2	4:D2:64:GLU:OE1	2.29	0.66
19:B:806:CLA:H18	25:M:102:LMG:H392	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BB:832:CLA:CGD	19:BB:833:CLA:HMB1	2.26	0.66
2:B2:384:ILE:CG2	2:B2:590:ALA:HB1	2.25	0.65
19:AA:804:CLA:O1A	2:BB:532:LEU:HD11	1.96	0.65
1:A1:571:PHE:O	1:A1:587:SER:OG	2.14	0.65
1:A2:329:HIS:O	22:A2:846:LHG:O2	2.10	0.65
2:B2:432:PHE:O	2:B2:436:HIS:ND1	2.29	0.65
19:BB:821:CLA:O2A	19:BB:821:CLA:HMA2	1.95	0.65
1:AA:580:ARG:NH1	4:DD:64:GLU:OE2	2.30	0.65
19:B:833:CLA:CGD	19:B:834:CLA:HMB1	2.27	0.65
3:C:64:SER:OG	27:C:102:SF4:S2	2.50	0.65
19:BB:833:CLA:HBC2	19:BB:834:CLA:HBC3	1.78	0.65
2:B1:236:ASN:ND2	2:B1:252:THR:OG1	2.22	0.65
3:C2:61:ASP:OD2	5:E2:15:SER:OG	2.09	0.65
1:A2:383:ASP:OD2	1:A2:386:THR:OG1	2.12	0.65
2:B1:432:PHE:O	2:B1:436:HIS:ND1	2.29	0.64
2:BB:490:TYR:O	2:BB:498:ASN:ND2	2.31	0.64
19:B1:833:CLA:HBC3	19:B1:833:CLA:HMC1	1.79	0.64
23:A2:851:BCR:H362	19:A2:852:CLA:H43	1.78	0.64
2:B:690:GLU:OE2	4:D:21:THR:OG1	2.16	0.64
3:CC:9:ASP:OD1	3:CC:35:LYS:NZ	2.31	0.64
2:B2:693:PRO:O	16:L2:53:TYR:OH	2.14	0.64
1:AA:621:THR:OG1	1:AA:629:SER:OG	2.15	0.64
3:C:25:VAL:HG23	3:C:44:ARG:O	1.99	0.63
3:C2:25:VAL:HG23	3:C2:44:ARG:O	1.99	0.63
2:B2:552:LYS:NZ	5:E2:15:SER:O	2.32	0.63
1:A1:691:ARG:N	2:B1:575:CYS:SG	2.70	0.63
1:A2:205:LEU:HD11	19:A2:815:CLA:H42	1.80	0.63
19:AA:843:CLA:H202	19:BB:835:CLA:H192	1.81	0.63
1:A1:467:ARG:NH2	19:A1:835:CLA:O1D	2.32	0.63
13:F2:124:LEU:O	8:J2:16:SER:OG	2.16	0.63
1:AA:397:ILE:HD13	19:AA:830:CLA:HBC3	1.79	0.63
1:A1:585:GLN:OE1	2:B1:674:TRP:N	2.32	0.62
1:AA:205:LEU:HD11	19:AA:815:CLA:H42	1.81	0.62
1:A1:277:THR:OG1	1:A1:293:ASP:OD1	2.17	0.62
1:A2:680:TRP:NE1	20:A2:803:CL0:O1A	2.32	0.62
2:BB:467:ILE:HD11	19:BB:832:CLA:H43	1.81	0.62
2:B2:440:LEU:O	2:B2:444:ASN:ND2	2.32	0.62
4:D2:101:VAL:HG11	4:D2:107:ASN:HB2	1.81	0.62
23:F2:305:BCR:H311	23:F2:305:BCR:HC8	1.82	0.62
1:A:122:VAL:HG11	19:B:830:CLA:HMD1	1.82	0.62
2:B:480:THR:O	2:B:484:ASN:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A1:852:CLA:HMB3	19:B1:848:CLA:H191	1.81	0.62
19:B:834:CLA:HBC2	19:B:835:CLA:HBC3	1.81	0.62
19:B:833:CLA:HED2	19:B:834:CLA:HBB1	1.81	0.62
2:BB:324:GLN:NE2	2:BB:408:LYS:O	2.33	0.62
1:A1:122:VAL:HG11	19:B1:829:CLA:HMD1	1.81	0.61
3:C1:25:VAL:HG23	3:C1:44:ARG:O	1.99	0.61
19:A2:830:CLA:HMC1	19:A2:830:CLA:HBC2	1.80	0.61
2:B1:384:ILE:HG23	2:B1:590:ALA:HB1	1.83	0.61
2:B:306:ASN:ND2	2:B:324:GLN:O	2.33	0.61
4:D1:105:LYS:O	4:D1:110:ARG:NH1	2.33	0.61
1:A:580:ARG:NH2	4:D:64:GLU:OE2	2.33	0.61
9:K:12:THR:OG1	9:K:82:ASN:O	2.16	0.61
2:BB:273:MET:O	2:BB:277:HIS:ND1	2.26	0.61
3:C2:21:CYS:SG	3:C2:24:ASP:N	2.73	0.61
2:B:326:ILE:HG21	19:B:820:CLA:HMD3	1.83	0.61
2:B:692:THR:HG21	19:B:860:CLA:HMA2	1.82	0.61
4:D:21:THR:HG21	18:L:121:LEU:HD11	1.83	0.61
1:AA:348:SER:OG	1:AA:416:ASP:OD2	2.15	0.61
1:A1:329:HIS:O	22:A1:846:LHG:O2	2.10	0.60
2:B:593:THR:O	2:B:597:VAL:HG23	2.00	0.60
1:A1:205:LEU:HD11	19:A1:814:CLA:H42	1.82	0.60
2:B1:723:GLY:O	2:B1:727:THR:HG22	2.01	0.60
1:A2:155:ASN:ND2	1:A2:158:GLN:OE1	2.34	0.60
19:B:801:CLA:H12	11:M:27:ALA:HB1	1.82	0.60
19:B1:832:CLA:O2D	19:B1:833:CLA:HMB1	2.00	0.60
2:BB:634:ASN:OD1	2:BB:739:LYS:NZ	2.35	0.60
1:A1:707:LYS:NZ	6:F1:156:ASP:OD1	2.30	0.60
1:A:436:ALA:O	1:A:440:HIS:ND1	2.34	0.60
19:B1:832:CLA:HED2	19:B1:833:CLA:CBB	2.32	0.60
2:B1:44:GLN:OE1	2:B1:162:ARG:NH2	2.35	0.60
2:B2:568:GLY:O	2:B2:574:THR:OG1	2.19	0.60
23:BB:841:BCR:H311	23:BB:841:BCR:H343	1.84	0.60
19:B:834:CLA:HAB	19:B:835:CLA:CGD	2.32	0.59
23:B:842:BCR:H311	23:B:842:BCR:H343	1.84	0.59
2:B2:203:ARG:NH2	2:B2:253:ALA:O	2.34	0.59
1:A:205:LEU:HD11	19:A:815:CLA:H42	1.83	0.59
1:AA:318:ILE:HG23	19:AA:822:CLA:HED1	1.84	0.59
6:FF:107:TYR:CZ	6:FF:111:ILE:HD11	2.37	0.59
19:B2:829:CLA:H142	23:F2:303:BCR:H333	1.83	0.59
13:F2:107:TYR:CZ	13:F2:111:ILE:HD11	2.38	0.59
2:B:279:ALA:HA	19:B:813:CLA:HMC3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:674:LEU:HD11	2:B2:627:PHE:CZ	2.38	0.59
5:E2:19:GLN:NE2	13:F2:157:SER:OG	2.36	0.59
2:BB:432:PHE:O	2:BB:436:HIS:ND1	2.35	0.59
2:B1:440:LEU:O	2:B1:444:ASN:ND2	2.36	0.59
4:D2:105:LYS:O	4:D2:110:ARG:NH2	2.34	0.59
1:A1:363:LEU:HD21	19:A1:828:CLA:H43	1.85	0.59
15:K2:34:PHE:O	15:K2:38:THR:OG1	2.15	0.59
2:BB:619:ASN:OD1	2:BB:622:TYR:OH	2.12	0.59
23:F1:306:BCR:HC8	23:F1:306:BCR:H311	1.84	0.59
16:L2:110:SER:O	16:L2:114:ASN:ND2	2.35	0.59
1:A1:345:LEU:HD23	1:A1:352:GLN:OE1	2.03	0.58
1:A1:442:ASN:ND2	2:B1:685:LEU:HD21	2.18	0.58
2:B:31:PHE:CD2	19:B:802:CLA:HMC2	2.38	0.58
8:JJ:35:GLU:OE1	8:JJ:38:ARG:NE	2.35	0.58
6:F1:60:ARG:NH2	8:J1:42:ASP:O	2.36	0.58
19:A:852:CLA:HMB3	19:B:854:CLA:H191	1.84	0.58
2:B:433:LEU:HD11	19:B:834:CLA:HMC3	1.85	0.58
19:B:833:CLA:HED2	19:B:834:CLA:CBB	2.34	0.58
1:AA:245:LEU:HD21	19:AA:818:CLA:HBC1	1.85	0.58
2:B:459:ILE:HD11	2:B:524:PHE:CE1	2.38	0.58
19:B:810:CLA:H143	19:B:815:CLA:H42	1.85	0.58
2:B:467:ILE:HD11	19:B:833:CLA:H43	1.85	0.58
1:AA:572:ARG:NH1	22:AA:846:LHG:O10	2.36	0.58
19:BB:833:CLA:HAB	19:BB:834:CLA:CGD	2.33	0.58
19:B1:828:CLA:H142	23:F1:303:BCR:H333	1.86	0.58
19:BB:832:CLA:O2D	19:BB:833:CLA:HMB1	2.03	0.58
19:B1:833:CLA:O1D	6:F1:76:VAL:HG13	2.03	0.58
8:J2:35:GLU:OE2	8:J2:38:ARG:NH2	2.36	0.58
16:L2:53:TYR:CD2	16:L2:126:VAL:HG21	2.38	0.57
2:BB:459:ILE:HG22	6:FF:74:LEU:HB2	1.87	0.57
2:B1:243:ILE:O	2:B1:246:THR:OG1	2.17	0.57
2:BB:293:THR:HG21	19:BB:817:CLA:OBD	2.05	0.57
23:FF:306:BCR:HC8	23:FF:306:BCR:H311	1.85	0.57
2:B1:467:ILE:HD11	19:B1:832:CLA:H43	1.86	0.57
2:B:3:THR:OG1	2:B:20:ARG:NH2	2.38	0.57
13:F2:34:ASN:ND2	13:F2:67:GLY:O	2.36	0.57
19:LL:203:CLA:HMC1	19:LL:203:CLA:HBC3	1.86	0.57
1:A2:121:ILE:O	1:A2:123:GLY:N	2.37	0.57
1:AA:424:ASN:OD1	1:AA:429:ARG:NH2	2.37	0.57
1:AA:436:ALA:O	1:AA:440:HIS:ND1	2.37	0.57
2:B2:527:HIS:HB3	19:B2:833:CLA:HED1	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:F:305:BCR:HC8	23:F:305:BCR:H311	1.85	0.57
4:DD:62:ARG:NH2	4:DD:64:GLU:OE1	2.37	0.57
17:EE:8:VAL:CG1	17:EE:58:LEU:HD22	2.34	0.57
2:B2:467:ILE:HD11	19:B2:833:CLA:H43	1.85	0.57
19:B2:836:CLA:H192	19:B2:852:CLA:H202	1.85	0.57
1:A:442:ASN:ND2	2:B:685:LEU:HD21	2.20	0.57
2:B:195:ILE:HA	2:B:199:ILE:HD12	1.87	0.57
2:BB:433:LEU:HD11	19:BB:833:CLA:HMC3	1.87	0.57
19:BB:810:CLA:H143	19:BB:815:CLA:H42	1.84	0.57
19:B:833:CLA:O2D	19:B:834:CLA:HMB1	2.05	0.57
2:B1:469:ALA:O	2:B1:483:SER:OG	2.21	0.56
1:A:572:ARG:NH1	22:A:845:LHG:O10	2.37	0.56
20:A2:803:CL0:CBB	2:B2:631:LEU:HD13	2.35	0.56
2:BB:723:GLY:O	2:BB:727:THR:HG22	2.05	0.56
2:B1:69:ALA:HB1	11:M1:4:ILE:HD11	1.86	0.56
19:B1:833:CLA:HBB2	19:B1:834:CLA:HED2	1.87	0.56
1:A2:424:ASN:OD1	1:A2:429:ARG:NH2	2.38	0.56
1:A2:599:MET:O	1:A2:603:LEU:HD23	2.05	0.56
3:C:38:GLN:HB3	4:D:106:VAL:HG21	1.86	0.56
1:A1:14:ARG:NH2	1:A1:16:ILE:HD11	2.21	0.56
6:F1:107:TYR:CZ	6:F1:111:ILE:HD11	2.41	0.56
19:K1:105:CLA:HMC1	19:K1:105:CLA:HBC2	1.87	0.56
1:A1:401:LEU:HD21	19:A1:807:CLA:H142	1.88	0.56
2:B2:573:GLY:O	2:B2:574:THR:OG1	2.23	0.56
19:B:836:CLA:H192	19:B:860:CLA:H202	1.85	0.56
1:AA:442:ASN:ND2	2:BB:685:LEU:HD21	2.21	0.56
19:BB:832:CLA:HED2	19:BB:833:CLA:CBB	2.35	0.56
2:B1:727:THR:HG23	19:B1:848:CLA:O1D	2.06	0.56
1:A2:307:ILE:HG12	23:K2:105:BCR:H362	1.87	0.56
23:AA:852:BCR:H362	19:AA:853:CLA:H43	1.87	0.56
2:BB:424:SER:OG	19:BB:856:CLA:HED3	2.06	0.56
1:A1:617:ASP:O	1:A1:630:HIS:NE2	2.39	0.56
2:B1:455:LYS:NZ	8:J1:42:ASP:OD1	2.29	0.56
10:L1:118:PRO:O	10:L1:119:THR:HG23	2.06	0.56
1:A2:142:SER:O	1:A2:390:ILE:HD11	2.05	0.56
2:B1:31:PHE:CD2	19:B1:802:CLA:HMC2	2.41	0.56
19:A2:820:CLA:CMD	19:A2:821:CLA:H202	2.36	0.56
2:B2:455:LYS:NZ	8:J2:42:ASP:OD2	2.23	0.56
2:B:424:SER:OG	19:B:859:CLA:HED3	2.06	0.56
1:A2:328:ASN:OD1	19:A2:825:CLA:HED3	2.06	0.56
2:B2:381:TYR:CE1	2:B2:594:VAL:HG11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HG23	19:A:822:CLA:HED1	1.88	0.56
2:BB:31:PHE:CD2	19:BB:802:CLA:HMC2	2.41	0.56
2:B2:31:PHE:CD2	19:B2:802:CLA:HMC2	2.41	0.55
1:A:43:PRO:HG3	6:F:122:ILE:HD12	1.87	0.55
1:A:245:LEU:HD21	19:A:818:CLA:HBC1	1.89	0.55
1:A:617:ASP:O	1:A:630:HIS:NE2	2.39	0.55
2:BB:459:ILE:HD11	2:BB:524:PHE:CE1	2.41	0.55
19:F1:301:CLA:H43	19:F1:302:CLA:CBC	2.36	0.55
1:A2:227:LEU:O	1:A2:232:VAL:HG22	2.05	0.55
1:A2:343:GLU:O	1:A2:347:THR:OG1	2.12	0.55
19:B2:811:CLA:H43	26:B2:841:ECH:H36A	1.88	0.55
2:B:322:PRO:O	2:B:411:VAL:HG23	2.07	0.55
2:B:123:TRP:CZ2	19:B:810:CLA:H191	2.41	0.55
19:B:811:CLA:H43	26:B:841:ECH:H36A	1.89	0.55
19:B1:804:CLA:HMD2	11:M1:13:LEU:HD21	1.89	0.55
16:L2:61:ARG:NH2	16:L2:65:GLU:OE1	2.39	0.55
1:A:397:ILE:HD13	19:A:830:CLA:HBC3	1.88	0.55
1:A:467:ARG:NH2	19:A:836:CLA:O1D	2.40	0.55
8:JJ:19:PRO:O	8:JJ:23:THR:HG23	2.05	0.55
2:B:320:ASN:ND2	22:B:852:LHG:O4	2.39	0.55
2:B1:5:PHE:CD1	7:I1:40:ILE:HG22	2.42	0.55
19:B1:833:CLA:HAB	19:B1:834:CLA:CGD	2.37	0.55
1:A1:363:LEU:CD2	19:A1:828:CLA:H43	2.35	0.55
19:A1:842:CLA:H202	19:B1:835:CLA:H192	1.88	0.55
19:AA:801:CLA:OBD	2:BB:677:TYR:OH	2.15	0.55
2:B1:320:ASN:ND2	22:B1:847:LHG:O4	2.39	0.55
5:E2:10:ILE:HD11	5:E2:40:PHE:HZ	1.72	0.55
19:BB:833:CLA:HBB2	19:BB:834:CLA:HED2	1.88	0.55
19:A:804:CLA:H193	19:A:852:CLA:H192	1.88	0.55
1:AA:617:ASP:O	1:AA:630:HIS:NE2	2.40	0.55
19:B1:833:CLA:H42	23:F1:303:BCR:H392	1.89	0.54
2:B2:417:GLN:OE1	12:X2:11:ASN:ND2	2.40	0.54
19:AA:853:CLA:HMB3	19:BB:852:CLA:H191	1.89	0.54
2:BB:508:ILE:HG23	2:BB:509:ASN:OD1	2.07	0.54
2:B1:520:GLY:N	2:B1:523:ASP:OD2	2.41	0.54
19:B2:826:CLA:H41	19:B2:826:CLA:C7	2.37	0.54
2:BB:663:VAL:HG22	19:BB:836:CLA:HMB3	1.89	0.54
1:A1:715:GLN:NE2	5:E1:16:TYR:OH	2.40	0.54
2:B2:173:SER:O	2:B2:177:HIS:ND1	2.40	0.54
9:K:32:ILE:HA	9:K:65:THR:HG21	1.88	0.54
11:MM:13:LEU:HB3	23:MM:101:BCR:H371	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:322:PRO:O	2:B1:411:VAL:HG13	2.08	0.54
2:B:291:TYR:HE1	2:B:301:ILE:HD11	1.72	0.54
2:BB:69:ALA:CB	11:MM:4:ILE:HD11	2.38	0.54
19:B1:826:CLA:H41	19:B1:826:CLA:C7	2.37	0.54
23:A2:851:BCR:H362	19:A2:852:CLA:C4	2.38	0.54
19:F2:301:CLA:H43	19:F2:302:CLA:CBC	2.37	0.54
19:F:301:CLA:H42	8:J:22:ALA:HA	1.90	0.54
19:B1:811:CLA:H43	26:B1:840:ECH:H36A	1.87	0.54
25:L1:210:LMG:H161	2:BB:297:ILE:HD12	1.88	0.54
23:A2:851:BCR:H403	23:A2:851:BCR:H23C	1.90	0.54
2:B1:478:LEU:O	12:X1:41:HIS:NE2	2.41	0.54
2:B2:322:PRO:O	2:B2:411:VAL:HG13	2.08	0.54
2:B2:553:LEU:HD21	2:B2:574:THR:HG22	1.89	0.54
1:AA:345:LEU:HD22	1:AA:352:GLN:OE1	2.07	0.54
1:A1:386:THR:HG22	1:A1:390:ILE:HD12	1.90	0.54
22:L1:211:LHG:HC61	19:L:202:CLA:HBC1	1.90	0.54
1:A2:122:VAL:HG11	19:B2:830:CLA:HMD1	1.89	0.54
2:B2:417:GLN:NE2	12:X2:8:PRO:O	2.41	0.54
23:B2:842:BCR:H382	23:B2:843:BCR:H21C	1.90	0.54
19:A:852:CLA:HMD3	19:B:854:CLA:O1A	2.08	0.54
19:BB:826:CLA:H41	19:BB:826:CLA:C7	2.38	0.54
19:B2:849:CLA:HMB3	19:B2:850:CLA:OBD	2.07	0.54
1:A1:691:ARG:NH1	2:B1:573:GLY:O	2.41	0.53
2:B1:459:ILE:HD11	2:B1:524:PHE:CE1	2.43	0.53
1:AA:397:ILE:CD1	19:AA:830:CLA:HBC3	2.38	0.53
6:FF:44:ALA:O	6:FF:57:ARG:NH2	2.41	0.53
1:A2:275:PHE:O	1:A2:276:LEU:HD12	2.09	0.53
15:K2:32:ILE:HG12	19:K2:104:CLA:HBA2	1.91	0.53
19:A:805:CLA:C15	23:J:102:BCR:H353	2.38	0.53
3:CC:24:ASP:OD2	4:DD:96:HIS:ND1	2.41	0.53
19:A2:804:CLA:HMC2	19:A2:852:CLA:CAC	2.38	0.53
1:AA:467:ARG:NH2	19:AA:836:CLA:O1D	2.41	0.53
17:EE:8:VAL:HG11	17:EE:58:LEU:HD22	1.90	0.53
19:B:837:CLA:HBC2	19:B:837:CLA:HHD	1.91	0.53
2:BB:289:HIS:CE1	23:BB:838:BCR:H363	2.43	0.53
19:LL:201:CLA:H92	19:LL:201:CLA:C4	2.38	0.53
1:A2:678:PHE:CD2	23:A2:851:BCR:H363	2.43	0.53
2:B2:578:SER:N	2:B2:581:ASP:OD2	2.41	0.53
2:B:581:ASP:OD1	2:B:713:ARG:NH1	2.41	0.53
2:B:731:PHE:O	2:B:735:SER:OG	2.10	0.53
1:A1:121:ILE:O	1:A1:123:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:347:VAL:HB	19:B2:823:CLA:H43	1.89	0.53
22:L2:208:LHG:HC92	19:LL:201:CLA:HMD2	1.91	0.53
1:A:678:PHE:CD2	23:A:851:BCR:H363	2.44	0.53
20:A:803:CL0:H13	19:A:852:CLA:OBD	2.08	0.53
2:B:688:ALA:O	2:B:692:THR:HG23	2.09	0.53
10:L1:8:SER:OG	10:L1:14:ASP:OD1	2.27	0.53
19:AA:804:CLA:H193	19:AA:853:CLA:H192	1.91	0.53
19:BB:832:CLA:HED2	19:BB:833:CLA:HBB1	1.91	0.53
5:E1:2:VAL:HG21	5:E1:24:VAL:HG21	1.91	0.53
1:AA:353:LEU:HB2	19:AA:807:CLA:HMD3	1.91	0.53
2:B1:123:TRP:CZ2	19:B1:810:CLA:H191	2.44	0.53
25:I2:105:LMG:O5	25:I2:105:LMG:O4	2.14	0.53
1:AA:546:THR:HG21	19:AA:828:CLA:HBC3	1.91	0.53
1:A1:245:LEU:HD21	19:A1:817:CLA:HBC1	1.91	0.52
2:B2:424:SER:OG	19:B2:851:CLA:HED3	2.09	0.52
9:K1:71:ILE:HD11	23:K1:106:BCR:C36	2.39	0.52
1:A2:442:ASN:HD22	2:B2:685:LEU:HD21	1.74	0.52
2:B2:170:SER:OG	19:B2:810:CLA:HBC1	2.10	0.52
19:A:804:CLA:HMC2	19:A:852:CLA:CAC	2.40	0.52
17:E:8:VAL:CG2	17:E:58:LEU:HD22	2.38	0.52
2:BB:553:LEU:HD21	2:BB:574:THR:HG22	1.91	0.52
6:FF:76:VAL:HG12	6:FF:86:PHE:HB2	1.90	0.52
2:B1:248:GLN:N	2:B1:248:GLN:OE1	2.43	0.52
19:A:822:CLA:HMA2	9:K:64:ALA:HB2	1.92	0.52
2:B:459:ILE:HG22	6:F:74:LEU:HB2	1.91	0.52
19:B:834:CLA:H42	23:F:303:BCR:H392	1.91	0.52
19:LL:201:CLA:H92	19:LL:201:CLA:C3	2.40	0.52
1:A:172:LEU:HD11	19:A:812:CLA:HBC1	1.90	0.52
1:A1:14:ARG:HH21	1:A1:16:ILE:HD11	1.75	0.52
23:B1:841:BCR:H343	23:B1:841:BCR:H311	1.90	0.52
2:B:488:VAL:HG12	19:B:832:CLA:HMD3	1.92	0.52
1:A1:59:PHE:CD2	19:A1:806:CLA:HMC2	2.45	0.52
2:B:347:VAL:HB	19:B:823:CLA:H43	1.91	0.52
19:A2:805:CLA:C15	23:J2:102:BCR:H353	2.39	0.52
2:B2:384:ILE:HG21	2:B2:590:ALA:HB1	1.91	0.52
13:F2:157:SER:HB3	12:X2:9:VAL:HG11	1.90	0.52
1:A1:587:SER:O	1:A1:591:HIS:ND1	2.42	0.52
23:A1:851:BCR:H403	23:A1:851:BCR:H23C	1.91	0.52
2:BB:693:PRO:O	18:LL:53:TYR:OH	2.19	0.52
3:CC:38:GLN:HB3	4:DD:106:VAL:HG21	1.91	0.52
1:A1:67:GLU:N	1:A1:67:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:193:ASN:OD1	19:AA:815:CLA:HBC1	2.09	0.52
1:A:251:ILE:HD11	1:A:258:ALA:HB2	1.91	0.51
2:BB:279:ALA:HA	19:BB:813:CLA:HMC3	1.92	0.51
19:BB:828:CLA:O1A	6:FF:153:THR:HG21	2.10	0.51
19:A2:852:CLA:H42	2:B2:442:VAL:HG22	1.91	0.51
19:F:301:CLA:H43	19:F:302:CLA:CBC	2.41	0.51
2:BB:340:TRP:CH2	23:BB:841:BCR:H372	2.46	0.51
23:F1:306:BCR:H382	23:F1:306:BCR:H371	1.92	0.51
19:A2:816:CLA:CHC	23:A2:847:BCR:H352	2.40	0.51
4:D2:5:LEU:CD1	4:D2:86:ILE:HD11	2.40	0.51
19:AA:853:CLA:HMD3	19:BB:852:CLA:O1A	2.10	0.51
18:LL:74:LEU:HD13	18:LL:101:LEU:HD22	1.91	0.51
1:A1:357:LEU:HD11	1:A1:401:LEU:HD22	1.92	0.51
1:A1:561:ARG:O	4:D1:62:ARG:NH1	2.43	0.51
19:A1:801:CLA:OBD	2:B1:677:TYR:OH	2.27	0.51
1:A2:682:PHE:HZ	19:A2:842:CLA:HBC2	1.76	0.51
1:AA:678:PHE:CD2	23:AA:852:BCR:H363	2.45	0.51
2:B2:478:LEU:HB3	2:B2:480:THR:HG23	1.93	0.51
2:B2:520:GLY:N	2:B2:523:ASP:OD2	2.42	0.51
1:A:194:VAL:HG21	1:A:346:THR:HG22	1.92	0.51
19:BB:826:CLA:H41	19:BB:826:CLA:H72	1.93	0.51
1:A2:114:SER:HB3	1:A2:131:VAL:HG21	1.91	0.51
1:A2:286:THR:HG22	1:A2:379:TYR:CE2	2.45	0.51
2:B2:488:VAL:HG12	19:B2:832:CLA:HMD3	1.93	0.51
19:A:852:CLA:H41	19:A:852:CLA:H71	1.93	0.51
19:B:828:CLA:HBC3	23:F:303:BCR:H362	1.91	0.51
19:AA:805:CLA:C15	23:JJ:102:BCR:H353	2.40	0.51
2:BB:727:THR:HG23	19:BB:852:CLA:O1D	2.10	0.51
19:B1:848:CLA:HMB3	19:B1:849:CLA:OBD	2.11	0.51
1:A2:374:MET:CE	19:A2:829:CLA:HMC2	2.41	0.51
2:B2:466:PHE:HD1	2:B2:480:THR:HG21	1.76	0.51
2:B2:552:LYS:NZ	13:F2:158:GLU:OE1	2.42	0.51
2:B:467:ILE:CD1	19:B:831:CLA:HMC3	2.41	0.51
2:BB:653:TRP:O	2:BB:657:PHE:N	2.43	0.51
2:B1:236:ASN:HD21	2:B1:252:THR:HG1	1.54	0.51
1:A2:467:ARG:NH2	19:A2:836:CLA:O1D	2.43	0.51
4:D:32:THR:HG22	4:D:57:LEU:HD13	1.92	0.51
1:AA:453:PHE:CZ	1:AA:457:ILE:HD11	2.46	0.51
2:BB:326:ILE:HG21	19:BB:820:CLA:HMD3	1.93	0.51
17:EE:40:PHE:O	17:EE:49:ASN:ND2	2.41	0.51
19:A1:820:CLA:HBB1	19:A1:820:CLA:HMB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:587:SER:O	1:A2:591:HIS:ND1	2.44	0.51
2:B2:422:ILE:HG23	19:B2:835:CLA:CBB	2.41	0.51
2:B2:478:LEU:O	12:X2:41:HIS:NE2	2.44	0.51
2:B:44:GLN:OE1	2:B:162:ARG:NH2	2.44	0.51
19:A1:804:CLA:C15	23:J1:102:BCR:H353	2.40	0.50
2:B1:352:VAL:HG22	19:B1:815:CLA:C2	2.41	0.50
19:B:830:CLA:H42	8:J:36:PHE:CE2	2.45	0.50
1:AA:297:HIS:NE2	19:AA:821:CLA:HMB3	2.26	0.50
19:A1:805:CLA:HMA2	19:A1:812:CLA:HMD2	1.93	0.50
2:B1:461:PRO:HG2	2:B1:519:ILE:HD12	1.93	0.50
19:A:816:CLA:CHC	23:A:847:BCR:H352	2.41	0.50
2:BB:126:THR:CG2	2:BB:270:LEU:HD21	2.41	0.50
6:FF:34:ASN:ND2	6:FF:67:GLY:O	2.45	0.50
19:A1:803:CLA:HMC2	19:A1:852:CLA:CAC	2.41	0.50
19:A1:852:CLA:HMD3	19:B1:848:CLA:O1A	2.11	0.50
1:A2:353:LEU:HB2	19:A2:807:CLA:HMD3	1.94	0.50
1:A2:693:TYR:N	2:B2:576:ASP:O	2.45	0.50
1:A:353:LEU:HB2	19:A:807:CLA:HMD3	1.93	0.50
23:A:854:BCR:H361	23:A:854:BCR:H21C	1.92	0.50
1:AA:571:PHE:O	1:AA:587:SER:OG	2.29	0.50
1:A1:353:LEU:HB2	19:A1:806:CLA:HMD3	1.94	0.50
2:B1:420:GLU:N	2:B1:420:GLU:OE1	2.45	0.50
1:A2:245:LEU:HD21	19:A2:818:CLA:HBC1	1.93	0.50
15:K2:71:ILE:HD11	23:K2:105:BCR:C36	2.41	0.50
1:A:680:TRP:O	1:A:683:SER:OG	2.25	0.50
1:AA:204:VAL:HG11	19:AA:815:CLA:CBB	2.42	0.50
19:B2:820:CLA:HBC2	19:B2:820:CLA:HHD	1.93	0.50
3:CC:35:LYS:HA	17:EE:32:ILE:HG22	1.94	0.50
1:A1:204:VAL:HG11	19:A1:814:CLA:CBB	2.42	0.50
19:A2:833:CLA:HMA1	19:A2:834:CLA:O1D	2.12	0.50
18:L:17:ASN:OD1	18:L:18:ARG:N	2.44	0.50
19:B:854:CLA:HMB3	19:B:858:CLA:OBD	2.11	0.50
19:BB:828:CLA:HBC3	23:FF:303:BCR:H362	1.93	0.50
19:A:810:CLA:H43	19:A:830:CLA:HMD2	1.94	0.50
2:BB:592:ASN:OD1	19:BB:852:CLA:H42	2.11	0.50
19:A1:832:CLA:HMA1	19:A1:833:CLA:O1D	2.12	0.49
1:A2:297:HIS:HE1	19:A2:821:CLA:HMB3	1.76	0.49
1:A2:614:MET:O	1:A2:619:TRP:N	2.41	0.49
2:B2:157:LEU:O	2:B2:162:ARG:NE	2.43	0.49
23:F2:305:BCR:H382	23:F2:305:BCR:H371	1.94	0.49
2:B1:736:THR:O	2:B1:740:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:455:LYS:NZ	19:B2:830:CLA:OBD	2.39	0.49
19:B:828:CLA:O1A	6:F:153:THR:HG21	2.13	0.49
2:B1:556:ASP:OD1	3:C1:66:ARG:NH2	2.45	0.49
1:A2:320:HIS:CB	1:A2:325:ILE:HD11	2.43	0.49
19:B2:829:CLA:HMC3	23:F2:305:BCR:C34	2.43	0.49
23:AA:852:BCR:H403	23:AA:852:BCR:H23C	1.93	0.49
2:BB:523:ASP:O	2:BB:527:HIS:ND1	2.44	0.49
3:CC:61:ASP:OD2	17:EE:15:SER:OG	2.15	0.49
1:A1:436:ALA:O	1:A1:440:HIS:ND1	2.45	0.49
2:B1:445:ASP:OD1	2:B1:623:LEU:N	2.44	0.49
2:B2:154:TRP:O	2:B2:158:GLN:NE2	2.43	0.49
19:B2:804:CLA:HMD2	11:M2:13:LEU:HD21	1.94	0.49
19:A2:802:CLA:H3A	23:K2:103:BCR:H362	1.94	0.49
2:B2:257:PHE:HD2	2:B2:499:VAL:HG23	1.76	0.49
2:B2:422:ILE:HG23	19:B2:835:CLA:HBB2	1.94	0.49
1:A:364:THR:HG22	1:A:394:HIS:HB3	1.93	0.49
19:AA:804:CLA:HMC2	19:AA:853:CLA:CAC	2.42	0.49
19:BB:833:CLA:H42	23:FF:303:BCR:H392	1.94	0.49
3:CC:42:SER:O	4:DD:114:ARG:NH1	2.46	0.49
1:A2:711:ALA:O	13:F2:108:LEU:HD21	2.13	0.49
19:A2:821:CLA:HBB1	19:A2:821:CLA:HMB1	1.94	0.49
2:B:662:LEU:HD12	19:B:858:CLA:O1A	2.13	0.49
6:F:34:ASN:ND2	6:F:67:GLY:O	2.44	0.49
19:L:202:CLA:H92	19:L:202:CLA:C4	2.43	0.49
2:B1:347:VAL:HB	19:B1:823:CLA:H43	1.95	0.49
2:B1:480:THR:OG1	2:B1:481:LEU:N	2.46	0.49
3:C1:29:VAL:HG12	4:D1:110:ARG:HB3	1.94	0.49
2:B2:690:GLU:OE1	4:D2:20:LEU:HD22	2.13	0.49
19:AA:816:CLA:CHC	23:AA:848:BCR:H352	2.42	0.49
1:A:121:ILE:O	1:A:123:GLY:N	2.45	0.49
19:B:826:CLA:H41	19:B:826:CLA:C7	2.42	0.49
10:L1:68:MET:HE1	19:L1:205:CLA:HED2	1.95	0.49
2:B:334:LEU:HD22	19:B:802:CLA:H201	1.94	0.49
1:AA:364:THR:HG22	1:AA:394:HIS:HB3	1.95	0.49
1:A2:245:LEU:CD2	19:A2:818:CLA:HBC1	2.43	0.49
1:A2:617:ASP:O	1:A2:630:HIS:NE2	2.46	0.49
1:A:30:ALA:O	6:F:123:GLN:NE2	2.45	0.49
23:A:851:BCR:H23C	23:A:851:BCR:H403	1.93	0.49
19:B:820:CLA:HBC3	19:B:820:CLA:HHD	1.94	0.49
19:BB:828:CLA:CBB	19:FF:305:CLA:H202	2.43	0.49
1:A1:307:ILE:HG12	23:K1:106:BCR:H362	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:806:CLA:HMA2	19:A2:813:CLA:HMD2	1.95	0.48
19:BB:856:CLA:HMC3	19:FF:301:CLA:C4D	2.43	0.48
1:A1:297:HIS:HE1	19:A1:820:CLA:HMB3	1.78	0.48
19:B1:827:CLA:O1D	12:X1:11:ASN:ND2	2.46	0.48
19:B:859:CLA:HMC3	19:F:301:CLA:C4D	2.43	0.48
1:A1:245:LEU:CD2	19:A1:817:CLA:HBC1	2.44	0.48
1:A1:710:VAL:HG12	1:A1:710:VAL:O	2.13	0.48
19:A1:815:CLA:CHC	23:A1:847:BCR:H352	2.43	0.48
13:F2:46:ASN:ND2	13:F2:51:PRO:O	2.46	0.48
19:B:854:CLA:HMB3	19:B:858:CLA:CAD	2.43	0.48
9:K:28:ASN:HD21	9:K:66:THR:HG22	1.79	0.48
1:AA:18:ASP:OD2	1:AA:71:ARG:NH2	2.43	0.48
2:BB:32:GLU:OE1	2:BB:335:HIS:NE2	2.43	0.48
2:BB:384:ILE:HG23	2:BB:590:ALA:HB1	1.94	0.48
19:F1:301:CLA:H42	8:J1:22:ALA:HA	1.95	0.48
1:A2:204:VAL:HG11	19:A2:815:CLA:CBB	2.44	0.48
16:L2:152:GLY:O	16:L2:156:VAL:HG23	2.13	0.48
19:B:828:CLA:CBB	19:B:829:CLA:H202	2.43	0.48
19:AA:820:CLA:CMD	19:AA:821:CLA:H202	2.43	0.48
19:BB:833:CLA:C9	19:BB:834:CLA:HBC1	2.40	0.48
19:B2:828:CLA:CBB	19:B2:829:CLA:H202	2.43	0.48
19:F2:301:CLA:H42	8:J2:22:ALA:HA	1.96	0.48
19:A:820:CLA:CMD	19:A:821:CLA:H202	2.43	0.48
1:AA:326:LEU:HD23	19:AA:826:CLA:O1D	2.14	0.48
1:A1:337:GLY:C	1:A1:426:VAL:HG23	2.34	0.48
23:B1:841:BCR:H343	23:B1:841:BCR:C31	2.43	0.48
1:AA:24:THR:HG21	1:AA:178:TRP:HE1	1.77	0.48
1:AA:710:VAL:HG12	1:AA:710:VAL:O	2.13	0.48
3:CC:60:THR:OG1	3:CC:62:PHE:O	2.27	0.48
1:A1:299:LEU:HD13	19:A1:816:CLA:HMC1	1.95	0.48
2:B:272:ASP:O	2:B:276:HIS:N	2.47	0.48
3:C:60:THR:OG1	3:C:62:PHE:O	2.32	0.48
2:B:297:ILE:CG2	19:B:818:CLA:HMD1	2.43	0.48
2:BB:216:ALA:HA	19:BB:812:CLA:HED1	1.95	0.48
6:FF:66:CYS:SG	6:FF:67:GLY:N	2.86	0.48
20:A1:802:CL0:CAB	19:A1:852:CLA:HED1	2.43	0.48
19:K1:103:CLA:H3A	23:K1:104:BCR:H362	1.95	0.48
1:A2:562:LEU:HD21	1:A2:583:THR:HG22	1.95	0.48
19:A2:806:CLA:HBC2	19:A2:832:CLA:H43	1.96	0.48
1:AA:122:VAL:HG21	19:BB:829:CLA:HMD1	1.96	0.48
1:AA:524:MET:CE	1:AA:628:VAL:HG11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:828:CLA:HED2	19:AA:828:CLA:OBD	2.14	0.48
18:LL:61:ARG:NH1	19:LL:201:CLA:O2D	2.47	0.48
2:B1:459:ILE:HG22	6:F1:74:LEU:HB2	1.95	0.48
2:B1:460:GLU:OE2	2:B1:465:GLN:NE2	2.45	0.48
3:C1:2:SER:OG	3:C1:3:HIS:N	2.46	0.48
19:B2:834:CLA:H42	23:F2:303:BCR:H392	1.96	0.48
1:A:122:VAL:CG1	19:B:830:CLA:HMD1	2.43	0.48
9:KK:21:GLY:O	9:KK:25:VAL:HG23	2.14	0.48
1:A1:447:PHE:O	1:A1:451:HIS:ND1	2.45	0.47
20:A1:802:CL0:H13	19:A1:852:CLA:OBD	2.14	0.47
19:A1:839:CLA:H91	19:L1:206:CLA:H192	1.96	0.47
1:A:326:LEU:HD23	19:A:826:CLA:O1D	2.14	0.47
21:A:843:PQN:H211	19:B:859:CLA:HBC1	1.96	0.47
2:B:594:VAL:O	2:B:598:THR:OG1	2.17	0.47
6:F:76:VAL:HG12	6:F:86:PHE:HB2	1.96	0.47
2:B1:124:TRP:HA	2:B1:127:ILE:HD12	1.95	0.47
2:B1:531:ALA:HB2	19:B1:833:CLA:HBB1	1.96	0.47
10:L1:68:MET:CE	19:L1:205:CLA:HED2	2.43	0.47
19:B:833:CLA:O1D	19:B:834:CLA:HMB1	2.13	0.47
19:AA:830:CLA:HBB1	19:AA:830:CLA:HMB1	1.96	0.47
28:BB:854:DGD:HO2D	28:BB:854:DGD:C1A	2.27	0.47
3:C1:14:CYS:N	27:C1:102:SF4:S1	2.87	0.47
2:B2:394:GLY:HA2	23:B2:843:BCR:H393	1.95	0.47
19:A:801:CLA:OBD	2:B:677:TYR:OH	2.22	0.47
2:B:481:LEU:HD21	12:X:38:TYR:CD1	2.49	0.47
1:AA:585:GLN:OE1	2:BB:674:TRP:N	2.41	0.47
1:A1:114:SER:HB3	1:A1:131:VAL:HG21	1.94	0.47
2:B1:123:TRP:NE1	2:B1:127:ILE:HD11	2.29	0.47
1:A2:561:ARG:O	4:D2:62:ARG:NH1	2.47	0.47
9:K:21:GLY:O	9:K:25:VAL:HG23	2.14	0.47
2:BB:123:TRP:CZ2	19:BB:810:CLA:H191	2.49	0.47
19:A1:852:CLA:H42	2:B1:442:VAL:HG22	1.96	0.47
2:B1:343:ALA:HB2	23:B1:842:BCR:H372	1.96	0.47
1:A2:101:TYR:O	1:A2:105:LEU:HD23	2.13	0.47
1:A:156:SER:O	1:A:160:TYR:N	2.47	0.47
1:A:435:ASP:OD2	1:A:561:ARG:NH2	2.47	0.47
4:DD:105:LYS:O	4:DD:110:ARG:NH2	2.47	0.47
19:A1:834:CLA:H93	19:B1:836:CLA:H142	1.96	0.47
2:B1:126:THR:CG2	2:B1:270:LEU:HD21	2.45	0.47
23:F1:306:BCR:H381	19:J1:103:CLA:HBC3	1.96	0.47
2:B2:3:THR:OG1	2:B2:20:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ILE:CG2	19:B:820:CLA:HMD3	2.45	0.47
19:BB:804:CLA:HAA2	19:BB:806:CLA:HED1	1.96	0.47
19:BB:811:CLA:H43	26:BB:840:ECH:H36A	1.97	0.47
17:EE:2:VAL:O	17:EE:27:VAL:HG21	2.13	0.47
1:A1:114:SER:CB	1:A1:131:VAL:HG21	2.45	0.47
19:A1:841:CLA:H41	19:A1:841:CLA:H71	1.97	0.47
2:B1:157:LEU:O	2:B1:162:ARG:NE	2.43	0.47
2:B1:394:GLY:HA2	23:B1:842:BCR:H393	1.97	0.47
19:B1:828:CLA:H202	19:F1:305:CLA:CBB	2.44	0.47
19:A2:804:CLA:HMC2	19:A2:852:CLA:HAC1	1.96	0.47
19:A2:831:CLA:H92	19:A2:831:CLA:HMD2	1.97	0.47
2:B2:273:MET:O	2:B2:277:HIS:ND1	2.46	0.47
3:C2:17:CYS:SG	3:C2:18:VAL:N	2.87	0.47
2:B:297:ILE:HG22	19:B:818:CLA:HMD1	1.96	0.47
2:BB:126:THR:HG23	2:BB:270:LEU:HD21	1.97	0.47
2:B1:488:VAL:HG12	19:B1:831:CLA:HMD3	1.97	0.47
1:A2:596:LEU:HD21	19:A2:832:CLA:HBC1	1.97	0.47
19:A2:852:CLA:HMB3	19:B2:849:CLA:H191	1.96	0.47
2:B2:91:ILE:HG22	19:B2:806:CLA:OBD	2.14	0.47
3:C:24:ASP:OD2	4:D:96:HIS:ND1	2.48	0.47
1:AA:349:TRP:HE3	19:AA:807:CLA:HMD2	1.80	0.47
2:B1:59:LEU:HD23	2:B1:143:LEU:HD23	1.95	0.47
2:B1:123:TRP:CE2	2:B1:127:ILE:HD11	2.50	0.47
10:L1:148:ILE:HD11	18:L:64:LEU:HD21	1.96	0.47
1:A2:59:PHE:CD2	19:A2:807:CLA:HMC2	2.50	0.47
19:A:828:CLA:OBD	19:A:828:CLA:HED2	2.15	0.47
19:AA:821:CLA:HBB1	19:AA:821:CLA:HMB1	1.97	0.47
2:BB:59:LEU:HD23	2:BB:143:LEU:HD23	1.97	0.47
2:BB:69:ALA:HB3	11:MM:4:ILE:HD11	1.97	0.47
2:B:71:GLN:NE2	19:B:804:CLA:O1D	2.47	0.47
6:F:87:LEU:O	6:F:90:SER:OG	2.13	0.47
23:AA:855:BCR:H21C	23:AA:855:BCR:H361	1.97	0.47
3:CC:2:SER:OG	3:CC:71:ALA:O	2.22	0.47
1:A2:432:ARG:NH1	4:D2:14:GLY:O	2.46	0.46
19:A2:842:CLA:H71	19:A2:842:CLA:H41	1.97	0.46
1:A:121:ILE:HG22	1:A:124:GLN:HE21	1.80	0.46
1:A2:16:ILE:HD11	1:A2:189:GLU:HB2	1.97	0.46
15:K2:70:HIS:O	15:K2:74:VAL:HG23	2.16	0.46
3:C:35:LYS:HA	17:E:32:ILE:HG22	1.97	0.46
19:BB:829:CLA:H42	8:JJ:36:PHE:CE2	2.50	0.46
1:A1:337:GLY:O	1:A1:426:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:59:LEU:HD23	2:B2:143:LEU:HD23	1.97	0.46
2:BB:319:PHE:CD2	19:BB:820:CLA:HMA1	2.51	0.46
2:BB:523:ASP:OD1	2:BB:600:TYR:OH	2.20	0.46
19:B1:804:CLA:HAA2	19:B1:806:CLA:HED1	1.97	0.46
19:B1:807:CLA:H141	19:B1:807:CLA:H162	1.72	0.46
15:K2:48:LEU:HD23	15:K2:54:PHE:CG	2.50	0.46
19:B:826:CLA:H41	19:B:826:CLA:H72	1.96	0.46
8:J:49:PRO:HB3	19:J:103:CLA:HED1	1.96	0.46
1:AA:119:TRP:HE1	23:AA:854:BCR:H332	1.80	0.46
2:B2:125:TYR:O	2:B2:130:ARG:NH1	2.48	0.46
2:B2:420:GLU:OE1	2:B2:420:GLU:N	2.49	0.46
2:B2:526:VAL:HG23	19:B2:849:CLA:H141	1.97	0.46
1:A:59:PHE:CD2	19:A:807:CLA:HMC2	2.51	0.46
2:B:256:THR:HG1	2:B:271:THR:HG1	1.56	0.46
19:B:836:CLA:HAB	21:B:838:PQN:H192	1.98	0.46
19:BB:820:CLA:HBC3	19:BB:820:CLA:HHD	1.96	0.46
2:B1:170:SER:OG	19:B1:810:CLA:HBC1	2.14	0.46
2:B2:118:SER:O	2:B2:375:LEU:HD21	2.16	0.46
19:BB:820:CLA:O1A	23:BB:841:BCR:H352	2.15	0.46
2:B1:526:VAL:HG23	19:B1:848:CLA:H141	1.96	0.46
2:B2:174:ARG:HB2	19:B2:810:CLA:HBC2	1.96	0.46
1:AA:694:TRP:CZ2	21:AA:844:PQN:H2M3	2.50	0.46
1:A2:114:SER:CB	1:A2:131:VAL:HG21	2.46	0.46
1:A:349:TRP:HE3	19:A:807:CLA:HMD2	1.81	0.46
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.51	0.46
1:AA:155:ASN:N	1:AA:155:ASN:OD1	2.49	0.46
1:A1:15:VAL:HG11	19:A1:811:CLA:CBA	2.46	0.46
19:B1:833:CLA:C9	19:B1:834:CLA:HBC1	2.43	0.46
6:F1:153:THR:HG21	19:F1:305:CLA:O1A	2.16	0.46
1:A1:122:VAL:CG1	19:B1:829:CLA:HMD1	2.46	0.46
19:A2:801:CLA:OBD	2:B2:677:TYR:OH	2.27	0.46
19:A:806:CLA:HBC2	19:A:832:CLA:H43	1.96	0.46
2:B:524:PHE:O	2:B:528:HIS:ND1	2.48	0.46
2:BB:533:GLY:HA3	2:BB:593:THR:HG22	1.96	0.46
1:A1:678:PHE:CD2	23:A1:851:BCR:H363	2.51	0.45
1:A2:678:PHE:CG	23:A2:851:BCR:H363	2.51	0.45
5:E2:10:ILE:HD11	5:E2:40:PHE:CZ	2.51	0.45
19:A:852:CLA:HMB3	19:B:854:CLA:C19	2.45	0.45
19:B:837:CLA:HMB2	23:B:844:BCR:C12	2.46	0.45
7:I:39:TYR:HH	11:M:31:TYR:HH	1.58	0.45
1:AA:426:VAL:O	1:AA:430:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:352:VAL:CG2	19:BB:815:CLA:H43	2.46	0.45
6:FF:65:LEU:HD12	6:FF:75:ILE:HD12	1.98	0.45
19:A1:803:CLA:H193	19:A1:852:CLA:H192	1.99	0.45
2:B1:174:ARG:HB2	19:B1:810:CLA:HBC2	1.98	0.45
19:B1:828:CLA:HMC3	23:F1:306:BCR:C34	2.46	0.45
8:J1:33:LEU:O	8:J1:37:ASN:ND2	2.48	0.45
1:A2:43:PRO:HG3	13:F2:122:ILE:HD12	1.98	0.45
19:A:830:CLA:HMC1	19:A:830:CLA:HBC2	1.99	0.45
19:B:827:CLA:O1D	12:X:11:ASN:ND2	2.49	0.45
19:A2:828:CLA:HAB	23:A2:850:BCR:H311	1.99	0.45
2:B2:101:ILE:O	2:B2:105:THR:HG23	2.16	0.45
16:L2:27:ASP:OD1	16:L2:29:GLN:NE2	2.49	0.45
1:AA:59:PHE:CD2	19:AA:807:CLA:HMC2	2.51	0.45
19:AA:806:CLA:HBC2	19:AA:832:CLA:H43	1.98	0.45
2:BB:343:ALA:HB2	23:BB:842:BCR:H372	1.97	0.45
1:A2:122:VAL:CG1	19:B2:830:CLA:HMD1	2.47	0.45
23:F2:305:BCR:H15C	23:F2:305:BCR:H351	1.79	0.45
1:A:227:LEU:HD21	1:A:253:LEU:HD11	1.99	0.45
19:B:829:CLA:HMC3	23:F:305:BCR:C34	2.47	0.45
17:E:40:PHE:O	17:E:49:ASN:ND2	2.49	0.45
1:A1:389:CYS:HB3	19:A1:829:CLA:HMA1	1.99	0.45
10:L1:126:VAL:HG13	10:L1:126:VAL:O	2.16	0.45
1:A2:172:LEU:HD11	19:A2:812:CLA:HBC1	1.98	0.45
1:A2:584:CYS:O	2:B2:676:GLY:N	2.49	0.45
2:B2:279:ALA:HA	19:B2:813:CLA:HMC3	1.99	0.45
11:M:14:VAL:HG23	23:M:101:BCR:H391	1.98	0.45
21:AA:844:PQN:H211	19:BB:856:CLA:HBC1	1.98	0.45
19:BB:835:CLA:HAB	21:BB:837:PQN:H192	1.99	0.45
19:A1:830:CLA:H92	19:A1:830:CLA:HMD2	1.99	0.45
23:B2:842:BCR:H331	23:B2:842:BCR:HC8	1.99	0.45
23:B:842:BCR:H343	23:B:842:BCR:C31	2.46	0.45
2:BB:58:PHE:HD1	2:BB:142:LEU:HD22	1.81	0.45
23:BB:841:BCR:H343	23:BB:841:BCR:C31	2.45	0.45
19:FF:305:CLA:HMC3	23:FF:306:BCR:C34	2.47	0.45
2:B1:381:TYR:HB3	19:B1:824:CLA:HMC3	1.99	0.45
1:A2:560:SER:N	1:A2:563:ILE:O	2.49	0.45
1:A:268:ASN:ND2	1:A:271:GLN:OE1	2.50	0.45
19:A:806:CLA:HMA2	19:A:813:CLA:HMD2	1.97	0.45
19:A:852:CLA:H42	2:B:442:VAL:HG22	1.99	0.45
18:LL:118:PRO:O	18:LL:119:THR:HG23	2.17	0.45
2:B1:279:ALA:HA	19:B1:813:CLA:HMC3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:25:VAL:HG21	3:C1:48:CYS:HB2	1.98	0.45
10:L1:114:ASN:ND2	22:L1:211:LHG:O9	2.50	0.45
19:A2:852:CLA:H41	19:A2:852:CLA:H71	1.99	0.45
16:L2:118:PRO:O	16:L2:119:THR:HG23	2.17	0.45
19:AA:805:CLA:CGA	19:AA:842:CLA:H43	2.47	0.45
23:AA:852:BCR:H362	19:AA:853:CLA:C4	2.46	0.45
9:K1:21:GLY:O	9:K1:25:VAL:HG23	2.17	0.45
19:A2:844:CLA:OBD	16:L2:18:ARG:NH2	2.50	0.45
2:B2:468:GLN:OE1	19:B2:833:CLA:HMB1	2.17	0.45
1:A:204:VAL:HG11	19:A:815:CLA:CBB	2.47	0.45
17:E:8:VAL:HG21	17:E:58:LEU:HD22	1.98	0.45
2:BB:69:ALA:HB1	11:MM:4:ILE:HD11	1.99	0.45
2:BB:384:ILE:HD11	2:BB:594:VAL:HB	1.98	0.45
1:A1:336:GLU:OE1	1:A1:336:GLU:N	2.49	0.44
1:A1:553:GLY:O	1:A1:557:ALA:HB2	2.17	0.44
2:B2:5:PHE:CD1	14:I2:40:ILE:HG22	2.52	0.44
23:F:305:BCR:C28	19:J:103:CLA:HMD3	2.47	0.44
2:BB:101:ILE:O	2:BB:105:THR:HG23	2.17	0.44
2:BB:347:VAL:HB	19:BB:823:CLA:H43	1.99	0.44
2:BB:707:LEU:N	21:BB:837:PQN:O4	2.47	0.44
2:B2:59:LEU:CD2	2:B2:143:LEU:HD23	2.47	0.44
19:A:804:CLA:HMC2	19:A:852:CLA:HAC1	1.99	0.44
17:E:11:LEU:HD12	17:E:11:LEU:O	2.17	0.44
1:AA:43:PRO:HG3	6:FF:122:ILE:HD12	1.97	0.44
1:AA:658:VAL:HG22	1:AA:746:ALA:HB3	1.99	0.44
2:BB:76:GLN:N	2:BB:76:GLN:OE1	2.50	0.44
19:A1:803:CLA:HMC2	19:A1:852:CLA:HAC1	2.00	0.44
2:B1:424:SER:OG	19:B1:850:CLA:HED3	2.17	0.44
23:B2:842:BCR:H331	23:B2:842:BCR:C8	2.46	0.44
13:F2:107:TYR:CE2	13:F2:111:ILE:HD11	2.53	0.44
1:A:429:ARG:O	1:A:433:HIS:ND1	2.51	0.44
19:A:842:CLA:H41	19:A:842:CLA:H71	2.00	0.44
23:A:851:BCR:H362	19:A:852:CLA:C4	2.45	0.44
2:B:173:SER:HA	2:B:293:THR:HG22	1.99	0.44
19:B:804:CLA:HAA2	19:B:806:CLA:HED1	1.98	0.44
19:B:811:CLA:HMB1	19:B:811:CLA:HBB1	2.00	0.44
2:BB:492:ALA:HB3	2:BB:495:ASN:O	2.17	0.44
2:B2:243:ILE:O	2:B2:246:THR:OG1	2.33	0.44
2:BB:428:TRP:HZ3	19:BB:834:CLA:HBC2	1.82	0.44
2:BB:481:LEU:HD21	12:XX:38:TYR:CD1	2.52	0.44
1:A1:589:TRP:NE1	19:A1:831:CLA:HMD1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:453:PHE:CZ	1:A2:457:ILE:HD11	2.53	0.44
8:J2:38:ARG:HH11	23:J2:104:BCR:H311	1.82	0.44
2:B:398:LEU:O	2:B:549:ARG:NH1	2.50	0.44
23:B:839:BCR:HC8	23:B:839:BCR:H311	1.98	0.44
6:F:88:ILE:HG12	19:J:103:CLA:HMB3	1.99	0.44
23:F:305:BCR:H381	19:J:103:CLA:HBC3	1.98	0.44
19:A2:815:CLA:HBB1	19:A2:815:CLA:HMB1	1.99	0.44
19:A2:842:CLA:H93	21:A2:843:PQN:H293	2.00	0.44
2:B2:587:LEU:HD23	2:B2:717:LEU:CD2	2.38	0.44
3:C2:14:CYS:O	3:C2:15:THR:OG1	2.23	0.44
4:D2:5:LEU:HD11	4:D2:86:ILE:HD11	1.99	0.44
1:AA:577:GLY:O	1:AA:583:THR:OG1	2.35	0.44
19:A1:827:CLA:HAB	23:A1:850:BCR:H311	1.98	0.44
19:A1:852:CLA:H41	19:A1:852:CLA:H71	2.00	0.44
1:A2:397:ILE:HD13	19:A2:830:CLA:HBC3	1.99	0.44
19:B:806:CLA:H203	23:L:205:BCR:C31	2.47	0.44
19:B:822:CLA:H143	19:B:832:CLA:HBB2	2.00	0.44
2:BB:715:VAL:O	2:BB:719:HIS:ND1	2.50	0.44
23:BB:838:BCR:HC8	23:BB:838:BCR:H311	1.98	0.44
15:K2:48:LEU:HD23	15:K2:54:PHE:CD2	2.53	0.44
2:B:289:HIS:CE1	23:B:839:BCR:H363	2.53	0.44
1:A1:16:ILE:HG21	1:A1:187:LYS:HD3	2.00	0.44
1:A1:432:ARG:NH1	4:D1:13:ALA:HB3	2.33	0.44
2:B1:69:ALA:CB	11:M1:4:ILE:HD11	2.47	0.44
2:B1:675:ARG:O	2:B1:678:TRP:N	2.46	0.44
19:B1:814:CLA:HMD2	19:B1:815:CLA:H202	2.00	0.44
19:B1:850:CLA:C14	19:F1:301:CLA:HED2	2.48	0.44
6:F1:76:VAL:O	6:F1:76:VAL:HG22	2.17	0.44
1:A2:101:TYR:CZ	1:A2:105:LEU:HD21	2.53	0.44
2:BB:157:LEU:O	2:BB:162:ARG:NE	2.45	0.44
19:A1:804:CLA:CGA	19:A1:841:CLA:H43	2.48	0.43
1:A2:118:VAL:O	1:A2:128:ASN:ND2	2.50	0.43
19:B2:816:CLA:CMB	19:B2:821:CLA:HMA3	2.47	0.43
1:A:506:VAL:HG23	19:A:837:CLA:HED3	2.00	0.43
1:A:590:ASP:OD1	1:A:725:ARG:NH1	2.51	0.43
2:B:59:LEU:HD23	2:B:143:LEU:HD23	2.00	0.43
1:A1:349:TRP:HE3	19:A1:806:CLA:HMD2	1.83	0.43
2:B1:481:LEU:HD21	12:X1:38:TYR:CD1	2.53	0.43
1:A:584:CYS:O	2:B:676:GLY:N	2.51	0.43
23:F:305:BCR:H382	23:F:305:BCR:H371	2.00	0.43
2:B1:468:GLN:OE1	19:B1:832:CLA:HMB1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:PHE:O	1:A:451:HIS:ND1	2.45	0.43
19:B:829:CLA:CAB	19:B:830:CLA:HMB2	2.48	0.43
1:AA:341:LEU:HD13	19:AA:826:CLA:HMD3	1.99	0.43
19:AA:822:CLA:HMA2	9:KK:64:ALA:HB2	1.99	0.43
2:BB:258:LEU:HD23	2:BB:269:TRP:CE2	2.53	0.43
2:BB:516:PHE:CE1	19:BB:823:CLA:HBC2	2.54	0.43
23:FF:303:BCR:H333	19:FF:305:CLA:H142	2.00	0.43
2:B1:531:ALA:HB2	19:B1:833:CLA:CBB	2.48	0.43
2:B:653:TRP:O	2:B:657:PHE:N	2.46	0.43
11:M:14:VAL:CG2	23:M:101:BCR:H391	2.48	0.43
1:A1:359:PHE:CG	19:A1:826:CLA:HMB2	2.54	0.43
19:B1:820:CLA:HBC2	19:B1:820:CLA:HHD	2.01	0.43
1:A2:436:ALA:O	1:A2:440:HIS:ND1	2.52	0.43
23:J2:104:BCR:H23C	23:J2:104:BCR:H392	2.01	0.43
24:L2:203:AJP:OBZ	24:L2:203:AJP:OBC	2.36	0.43
1:A:694:TRP:CE2	21:A:843:PQN:H2M3	2.52	0.43
1:A1:282:LEU:HD23	1:A1:289:LEU:HD23	2.00	0.43
19:A:830:CLA:HMB1	19:A:830:CLA:HBB1	2.01	0.43
2:B:531:ALA:HB2	19:B:834:CLA:CBB	2.49	0.43
28:B:856:DGD:HO2D	28:B:856:DGD:C1A	2.30	0.43
19:AA:842:CLA:H41	19:AA:842:CLA:H71	2.01	0.43
2:BB:531:ALA:HB2	19:BB:833:CLA:CBB	2.48	0.43
24:L1:204:AJP:OBZ	24:L1:204:AJP:OBC	2.36	0.43
19:B2:821:CLA:HMB1	19:B2:821:CLA:HBB1	1.99	0.43
3:C:11:CYS:SG	3:C:12:ILE:N	2.92	0.43
19:AA:806:CLA:HMA2	19:AA:813:CLA:HMD2	2.01	0.43
2:B2:30:ASP:O	2:B2:34:HIS:ND1	2.52	0.43
2:B2:257:PHE:CD2	2:B2:499:VAL:HG23	2.53	0.43
19:B2:831:CLA:HMD2	19:B2:832:CLA:CHC	2.49	0.43
19:B2:834:CLA:H43	19:X2:101:CLA:C4D	2.49	0.43
13:F2:88:ILE:HG12	19:J2:103:CLA:HMB3	2.01	0.43
1:A:39:LEU:HD11	1:A:55:LEU:HD12	2.01	0.43
1:A:313:ARG:O	19:A:822:CLA:HED2	2.18	0.43
2:B:43:TYR:CZ	2:B:334:LEU:HD21	2.54	0.43
1:AA:477:ILE:O	1:AA:477:ILE:HG22	2.19	0.43
2:BB:123:TRP:CH2	19:BB:810:CLA:H191	2.54	0.43
1:A1:196:SER:O	1:A1:200:HIS:ND1	2.45	0.43
19:A1:805:CLA:HBC2	19:A1:831:CLA:H43	2.00	0.43
19:A1:841:CLA:H93	21:A1:843:PQN:H293	2.00	0.43
2:B1:273:MET:SD	19:B1:815:CLA:HED1	2.59	0.43
23:B1:838:BCR:HC8	23:B1:838:BCR:H311	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:24:ASP:OD2	4:D1:96:HIS:ND1	2.51	0.43
4:D1:101:VAL:HG11	4:D1:107:ASN:HB2	2.00	0.43
19:A2:805:CLA:CGA	19:A2:842:CLA:H43	2.49	0.43
19:A2:840:CLA:CBB	19:A2:841:CLA:HBC3	2.49	0.43
19:B2:809:CLA:CMC	23:B2:840:BCR:H343	2.49	0.43
1:A:694:TRP:CZ2	21:A:843:PQN:H2M3	2.54	0.43
1:A1:114:SER:OG	1:A1:131:VAL:HG21	2.19	0.43
19:A1:815:CLA:HHB	23:A1:847:BCR:H331	2.00	0.43
19:A1:829:CLA:HMB1	19:A1:829:CLA:HBB1	2.00	0.43
19:A1:839:CLA:CBB	19:A1:840:CLA:HBC3	2.49	0.43
19:B:820:CLA:O1A	23:B:842:BCR:H352	2.19	0.43
1:AA:245:LEU:CD2	19:AA:818:CLA:HBC1	2.48	0.43
2:BB:105:THR:HG22	2:BB:111:GLY:C	2.39	0.43
2:B1:118:SER:O	2:B1:375:LEU:HD21	2.19	0.42
2:B1:257:PHE:CD2	2:B1:499:VAL:HG23	2.53	0.42
2:B1:428:TRP:HZ3	19:B1:834:CLA:HBC2	1.84	0.42
2:B1:433:LEU:HD11	19:B1:833:CLA:HMC3	2.01	0.42
19:B1:809:CLA:CMC	23:B1:839:BCR:H343	2.49	0.42
1:A2:13:ALA:HB3	1:A2:315:ASN:OD1	2.18	0.42
1:A2:342:TYR:O	1:A2:346:THR:OG1	2.23	0.42
16:L2:147:LEU:HD21	19:LL:201:CLA:O1A	2.18	0.42
1:A:424:ASN:OD1	1:A:429:ARG:NH1	2.52	0.42
19:A:833:CLA:HMA1	19:A:834:CLA:O1D	2.18	0.42
19:AA:826:CLA:HAB	19:AA:833:CLA:HMD2	2.00	0.42
1:A1:57:HIS:O	19:A1:806:CLA:HMC3	2.19	0.42
1:A1:521:VAL:HG11	1:A1:618:VAL:O	2.19	0.42
19:B1:827:CLA:HED3	12:X1:11:ASN:CB	2.49	0.42
1:A2:336:GLU:N	1:A2:336:GLU:OE1	2.52	0.42
2:B2:643:ASN:OD1	2:B2:646:GLY:N	2.48	0.42
2:B:74:PHE:CZ	2:B:78:ILE:HD11	2.54	0.42
2:B:478:LEU:HB3	2:B:480:THR:HG23	2.01	0.42
23:B:843:BCR:H24C	23:B:843:BCR:H371	1.92	0.42
2:BB:415:VAL:HG11	23:BB:841:BCR:H401	2.01	0.42
23:FF:306:BCR:H382	23:FF:306:BCR:H371	2.01	0.42
22:L1:211:LHG:C9	19:L:202:CLA:HMD2	2.49	0.42
2:B2:466:PHE:CD1	2:B2:480:THR:HG21	2.54	0.42
19:A:820:CLA:H92	19:A:837:CLA:O1A	2.19	0.42
2:B1:125:TYR:O	2:B1:130:ARG:NH1	2.52	0.42
2:B1:167:TRP:CZ2	19:B1:808:CLA:HMA1	2.55	0.42
19:A2:815:CLA:HBA2	19:A2:815:CLA:H3A	1.89	0.42
19:A2:835:CLA:H93	19:B2:837:CLA:H142	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:694:TRP:CE2	21:AA:844:PQN:H2M3	2.54	0.42
20:AA:803:CL0:H22	2:BB:632:TRP:HD1	1.84	0.42
18:LL:52:ALA:HB2	19:LL:202:CLA:HMD1	2.00	0.42
19:A1:824:CLA:HMC1	19:A1:828:CLA:H202	2.01	0.42
19:B1:830:CLA:HMD2	19:B1:831:CLA:CHC	2.50	0.42
1:A2:553:GLY:O	1:A2:557:ALA:HB2	2.19	0.42
19:A2:805:CLA:H41	19:A2:805:CLA:H71	2.01	0.42
19:B2:806:CLA:H41	19:B2:806:CLA:H72	2.01	0.42
23:B2:839:BCR:HC8	23:B2:839:BCR:H311	2.01	0.42
19:B:834:CLA:C9	19:B:835:CLA:HBC1	2.40	0.42
2:BB:223:GLN:NE2	2:BB:227:THR:OG1	2.53	0.42
9:KK:76:LEU:O	9:KK:80:LEU:HD23	2.20	0.42
1:A1:370:HIS:ND1	19:A1:819:CLA:OBD	2.53	0.42
19:B1:831:CLA:CHD	19:B1:845:CLA:HMD2	2.50	0.42
3:C1:7:ILE:HD13	3:C1:40:ALA:C	2.39	0.42
1:A2:395:ILE:HG22	1:A2:603:LEU:HD12	2.01	0.42
2:B2:459:ILE:HG22	13:F2:74:LEU:HB2	2.00	0.42
2:B:46:ILE:O	2:B:49:THR:OG1	2.35	0.42
2:B:343:ALA:HB2	23:B:843:BCR:H372	2.01	0.42
11:M:3:SER:OG	11:M:4:ILE:N	2.53	0.42
1:AA:334:THR:HG21	22:AA:847:LHG:HC12	2.01	0.42
1:AA:532:ASP:O	1:AA:536:HIS:ND1	2.46	0.42
2:BB:594:VAL:HG22	2:BB:598:THR:HG23	2.01	0.42
23:BB:841:BCR:C8	23:BB:841:BCR:H331	2.50	0.42
19:A1:814:CLA:HBB1	19:A1:814:CLA:HMB1	2.02	0.42
2:B1:105:THR:HG23	2:B1:105:THR:O	2.19	0.42
1:A2:21:PRO:HG3	1:A2:185:ALA:HB2	2.01	0.42
1:A2:343:GLU:OE2	1:A2:343:GLU:N	2.53	0.42
20:A2:803:CL0:H48	19:B2:850:CLA:HMA3	2.01	0.42
1:A:318:ILE:HG12	19:A:824:CLA:HMD1	2.01	0.42
2:BB:491:THR:O	2:BB:491:THR:HG23	2.20	0.42
19:BB:821:CLA:HMB1	19:BB:821:CLA:HBB1	2.02	0.42
1:A1:297:HIS:CE1	19:A1:820:CLA:HMB3	2.54	0.42
23:J1:104:BCR:H392	23:J1:104:BCR:H23C	2.02	0.42
1:A2:196:SER:O	1:A2:200:HIS:ND1	2.43	0.42
1:A2:364:THR:HG22	1:A2:394:HIS:HB3	2.00	0.42
1:A2:448:LEU:O	1:A2:452:SER:N	2.53	0.42
19:B2:832:CLA:CHD	19:B2:846:CLA:HMD2	2.50	0.42
23:B2:842:BCR:H24C	23:B2:842:BCR:H371	1.90	0.42
1:A:357:LEU:HD21	19:A:832:CLA:CBB	2.50	0.42
23:FF:306:BCR:H381	19:JJ:103:CLA:HBC3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:593:THR:O	2:B1:597:VAL:HG23	2.19	0.42
1:A2:426:VAL:O	1:A2:430:VAL:HG23	2.20	0.42
2:B2:182:LEU:HD21	19:B2:810:CLA:C2	2.50	0.42
2:B:374:ALA:HB1	19:B:824:CLA:HMA1	2.01	0.42
2:B:514:SER:O	2:B:514:SER:OG	2.34	0.42
2:B:707:LEU:N	21:B:838:PQN:O4	2.48	0.42
19:L:202:CLA:H91	19:L:202:CLA:H143	2.01	0.42
2:BB:174:ARG:HB2	19:BB:810:CLA:HBC2	2.01	0.42
8:JJ:23:THR:HG21	23:JJ:104:BCR:H403	2.02	0.42
9:KK:68:PHE:CE2	9:KK:72:LEU:HD11	2.55	0.42
18:LL:101:LEU:HD21	18:LL:105:PHE:CZ	2.55	0.42
1:A1:600:TYR:CE2	20:A1:802:CL0:H36	2.54	0.42
2:B1:440:LEU:HD11	23:F1:306:BCR:H311	2.01	0.42
6:F1:34:ASN:ND2	6:F1:67:GLY:O	2.50	0.42
20:A2:803:CL0:H16	2:B2:631:LEU:HD22	2.02	0.42
19:A2:804:CLA:H193	19:A2:852:CLA:H192	2.00	0.42
19:B2:834:CLA:HBB2	19:B2:835:CLA:O2D	2.20	0.42
19:B2:849:CLA:HMB3	19:B2:850:CLA:CAD	2.50	0.42
1:A:698:ILE:O	1:A:702:VAL:HG23	2.20	0.42
2:B:534:LEU:HD12	19:B:835:CLA:CED	2.50	0.42
3:C:12:ILE:HD11	3:C:59:PRO:HG2	2.02	0.42
2:BB:71:GLN:NE2	19:BB:804:CLA:O1D	2.49	0.42
18:LL:126:VAL:O	18:LL:126:VAL:HG13	2.20	0.42
19:A:805:CLA:H41	19:A:805:CLA:H71	2.02	0.41
23:F:305:BCR:H15C	23:F:305:BCR:H351	1.78	0.41
23:J:104:BCR:H392	23:J:104:BCR:H23C	2.02	0.41
19:AA:810:CLA:H43	19:AA:830:CLA:HMD2	2.01	0.41
23:LL:204:BCR:H15C	23:LL:204:BCR:H351	1.95	0.41
1:A1:707:LYS:HA	6:F1:159:ILE:HD11	2.01	0.41
10:L1:11:LEU:O	10:L1:17:ASN:ND2	2.53	0.41
1:A2:558:ARG:NH2	4:D2:42:GLU:OE2	2.52	0.41
20:A2:803:CL0:H4	19:A2:852:CLA:OBD	2.20	0.41
2:B2:592:ASN:OD1	19:B2:849:CLA:H42	2.20	0.41
19:A:805:CLA:CGA	19:A:842:CLA:H43	2.49	0.41
19:A:815:CLA:HBA2	19:A:815:CLA:H3A	1.90	0.41
1:AA:81:LEU:O	1:AA:85:THR:HG23	2.19	0.41
1:AA:112:ARG:HB2	1:AA:131:VAL:HG22	2.02	0.41
2:BB:724:TYR:CD1	19:BB:852:CLA:HED1	2.56	0.41
19:BB:832:CLA:O1D	19:BB:833:CLA:HMB1	2.20	0.41
19:B2:811:CLA:HMB1	19:B2:811:CLA:HBB1	2.01	0.41
1:A:558:ARG:NH2	4:D:42:GLU:OE2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:THR:HG21	2:B:589:TRP:CZ2	2.55	0.41
2:B:630:TYR:O	2:B:634:ASN:ND2	2.53	0.41
19:B:833:CLA:C3D	19:B:833:CLA:HED3	2.51	0.41
1:AA:575:CYS:SG	1:AA:577:GLY:N	2.87	0.41
19:AA:830:CLA:HMC1	19:AA:830:CLA:HBC2	2.02	0.41
2:BB:45:LYS:NZ	19:BB:801:CLA:HED1	2.36	0.41
2:BB:293:THR:O	2:BB:295:PHE:N	2.53	0.41
19:FF:301:CLA:H42	8:JJ:22:ALA:HA	2.02	0.41
1:A1:199:ASN:OD1	1:A1:314:THR:HG21	2.20	0.41
2:B1:491:THR:O	2:B1:491:THR:HG23	2.21	0.41
19:B2:826:CLA:H41	19:B2:826:CLA:H72	2.02	0.41
14:I2:33:PHE:CE1	23:I2:103:BCR:H342	2.56	0.41
16:L2:62:ARG:NH1	16:L2:131:ASP:OD1	2.53	0.41
1:AA:341:LEU:CD1	19:AA:826:CLA:HMD3	2.50	0.41
10:L1:152:GLY:O	10:L1:156:VAL:HG23	2.20	0.41
2:B2:653:TRP:O	2:B2:657:PHE:N	2.50	0.41
2:B2:731:PHE:O	2:B2:735:SER:OG	2.29	0.41
1:A:81:LEU:O	1:A:85:THR:HG23	2.21	0.41
1:A:121:ILE:HG23	1:A:122:VAL:N	2.35	0.41
2:B:422:ILE:HG23	19:B:835:CLA:HBB2	2.01	0.41
1:AA:115:ALA:HB3	1:AA:140:ILE:CD1	2.51	0.41
6:FF:46:ASN:OD1	6:FF:46:ASN:N	2.53	0.41
1:A1:413:MET:CE	1:A1:431:ILE:HD11	2.51	0.41
2:B2:196:HIS:O	2:B2:207:VAL:HG11	2.21	0.41
19:A:826:CLA:HAB	19:A:833:CLA:HMD2	2.03	0.41
19:B:818:CLA:HBB1	19:B:818:CLA:HHC	2.02	0.41
1:AA:320:HIS:HB3	1:AA:325:ILE:HD11	2.02	0.41
2:BB:536:THR:HG21	2:BB:589:TRP:CZ2	2.56	0.41
19:A1:833:CLA:HED1	10:L1:32:ASN:OD1	2.21	0.41
10:L1:61:ARG:NH2	19:L1:205:CLA:HED1	2.35	0.41
1:A2:494:ALA:HB3	1:A2:495:PRO:HD3	2.02	0.41
2:B2:167:TRP:CZ2	19:B2:808:CLA:HMA1	2.55	0.41
1:A:36:ASP:OD1	1:A:37:ARG:N	2.54	0.41
2:B:294:ASN:OD1	19:B:809:CLA:HMA2	2.20	0.41
2:BB:255:LEU:HD21	2:BB:278:LEU:HD23	2.03	0.41
2:BB:652:VAL:HG11	19:BB:805:CLA:CBC	2.51	0.41
1:A2:297:HIS:CE1	19:A2:821:CLA:HMB3	2.55	0.41
18:L:131:ASP:OD1	18:L:131:ASP:N	2.54	0.41
19:AA:825:CLA:HMA1	19:AA:845:CLA:HBC3	2.01	0.41
2:BB:724:TYR:CE1	19:BB:852:CLA:HED1	2.55	0.41
1:A1:397:ILE:HD13	19:A1:829:CLA:HBC3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:685:MET:O	1:A1:689:SER:OG	2.32	0.41
19:A1:852:CLA:HMB3	19:B1:848:CLA:C19	2.50	0.41
2:B1:15:ASP:O	2:B1:20:ARG:NH1	2.53	0.41
2:B1:429:VAL:HG11	2:B1:535:HIS:CD2	2.56	0.41
2:B2:536:THR:HG21	2:B2:589:TRP:CZ2	2.56	0.41
3:C2:42:SER:O	4:D2:114:ARG:NH1	2.54	0.41
23:F2:305:BCR:H381	19:J2:103:CLA:HBC3	2.03	0.41
1:A:93:PHE:HE1	19:A:809:CLA:HMD3	1.86	0.41
1:A:126:ILE:HG21	2:B:450:PHE:HA	2.03	0.41
1:A:199:ASN:HD21	1:A:312:TYR:H	1.69	0.41
19:A:831:CLA:HMD2	19:A:831:CLA:H92	2.03	0.41
23:B:842:BCR:C8	23:B:842:BCR:H331	2.50	0.41
1:AA:584:CYS:O	2:BB:676:GLY:N	2.53	0.41
2:BB:272:ASP:O	2:BB:276:HIS:N	2.53	0.41
1:A1:180:HIS:HE1	19:A1:811:CLA:HMA3	1.86	0.41
19:A1:834:CLA:HMA1	23:I1:101:BCR:H282	2.02	0.41
19:B1:811:CLA:HBB1	19:B1:811:CLA:HMB1	2.03	0.41
19:A2:826:CLA:HAB	19:A2:833:CLA:HMD2	2.02	0.41
2:B2:602:HIS:CD2	2:B2:732:LEU:HD12	2.56	0.41
19:B2:827:CLA:HED3	12:X2:11:ASN:CB	2.51	0.41
23:A:854:BCR:H362	9:K:71:ILE:HD11	2.03	0.41
2:B:444:ASN:OD1	2:B:457:ILE:N	2.47	0.41
2:BB:91:ILE:HD11	2:BB:114:ASN:OD1	2.21	0.41
2:BB:587:LEU:HD12	2:BB:717:LEU:HD21	2.03	0.41
19:BB:806:CLA:H41	19:BB:806:CLA:H72	2.01	0.41
3:CC:13:GLY:O	3:CC:38:GLN:NE2	2.54	0.41
19:A1:814:CLA:HBA2	19:A1:814:CLA:H3A	1.89	0.40
2:B1:584:TYR:OH	2:B1:671:LEU:HD22	2.21	0.40
10:L1:57:LEU:HD13	10:L1:61:ARG:HD3	2.03	0.40
1:A2:234:VAL:HA	1:A2:237:ILE:HD12	2.03	0.40
2:B:319:PHE:CD2	19:B:820:CLA:HMA1	2.56	0.40
19:AA:831:CLA:HMD2	19:AA:831:CLA:H92	2.02	0.40
2:BB:58:PHE:CD1	2:BB:142:LEU:HD22	2.54	0.40
2:BB:270:LEU:HD23	2:BB:273:MET:SD	2.61	0.40
2:BB:699:ARG:NH2	4:DD:25:GLU:OE2	2.54	0.40
1:A1:304:VAL:HG12	19:A1:822:CLA:HMC1	2.02	0.40
19:A1:819:CLA:H92	19:A1:836:CLA:O1A	2.21	0.40
10:L1:72:TYR:OH	19:L1:207:CLA:OBD	2.29	0.40
1:A2:53:HIS:HD2	19:A2:806:CLA:HBC1	1.86	0.40
19:A:832:CLA:HMB1	19:A:832:CLA:HBB1	2.02	0.40
19:A:840:CLA:CBB	19:A:841:CLA:HBC3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:LEU:HD12	19:B:835:CLA:HED3	2.03	0.40
2:BB:319:PHE:HD2	19:BB:820:CLA:HMA1	1.86	0.40
10:L1:61:ARG:NH2	10:L1:65:GLU:OE1	2.54	0.40
1:A2:444:VAL:HG12	1:A2:448:LEU:HD12	2.04	0.40
1:A:329:HIS:O	22:A:846:LHG:O2	2.34	0.40
2:B:394:GLY:HA2	23:B:843:BCR:H393	2.03	0.40
2:B:638:LEU:HD21	2:B:657:PHE:CG	2.57	0.40
19:B:854:CLA:H62	19:B:854:CLA:H41	1.96	0.40
1:AA:122:VAL:CG2	19:BB:829:CLA:HMD1	2.50	0.40
2:BB:194:LEU:HA	2:BB:198:ALA:HB3	2.03	0.40
3:CC:17:CYS:SG	3:CC:18:VAL:N	2.95	0.40
19:FF:301:CLA:H43	19:FF:302:CLA:CBC	2.52	0.40
3:C1:35:LYS:HA	5:E1:32:ILE:HG22	2.02	0.40
19:B2:852:CLA:HHD	19:B2:852:CLA:HBC2	2.02	0.40
13:F2:95:TYR:OH	13:F2:137:PHE:O	2.17	0.40
1:A:662:TYR:OH	2:B:445:ASP:OD2	2.39	0.40
2:B:399:VAL:CG2	2:B:548:ALA:HB1	2.51	0.40
19:BB:822:CLA:H143	19:BB:831:CLA:HBB2	2.04	0.40
1:A1:388:LEU:HD23	1:A1:610:PHE:CD1	2.57	0.40
2:B1:422:ILE:HG23	19:B1:834:CLA:CBB	2.52	0.40
2:B1:534:LEU:HD12	19:B1:834:CLA:CED	2.42	0.40
19:B2:851:CLA:HMC3	19:F2:301:CLA:C4D	2.52	0.40
1:A:697:LEU:HB2	2:B:543:LYS:HZ2	1.87	0.40
19:AA:828:CLA:HAB	23:AA:851:BCR:H311	2.03	0.40
2:BB:409:GLY:N	2:BB:413:GLU:OE1	2.50	0.40
19:BB:832:CLA:HED3	19:BB:832:CLA:C3D	2.52	0.40
6:FF:114:ASP:OD1	6:FF:120:LYS:NZ	2.34	0.40

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	A	738/740 (100%)	713 (97%)	24 (3%)	1 (0%)	51	83
1	A1	738/740 (100%)	710 (96%)	27 (4%)	1 (0%)	51	83
1	A2	738/740 (100%)	714 (97%)	23 (3%)	1 (0%)	51	83
1	AA	738/740 (100%)	709 (96%)	28 (4%)	1 (0%)	51	83
2	B	737/739 (100%)	712 (97%)	25 (3%)	0	100	100
2	B1	737/739 (100%)	715 (97%)	22 (3%)	0	100	100
2	B2	737/739 (100%)	713 (97%)	24 (3%)	0	100	100
2	BB	737/739 (100%)	710 (96%)	27 (4%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	C1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	CC	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
4	D1	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
4	D2	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
4	DD	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
5	E1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
5	E2	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
6	F	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
6	F1	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	FF	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
7	I	29/31 (94%)	29 (100%)	0	0	100	100
7	I1	29/31 (94%)	29 (100%)	0	0	100	100
7	II	29/31 (94%)	29 (100%)	0	0	100	100
8	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
8	J1	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
8	J2	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
8	JJ	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
9	K	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
9	K1	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	KK	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
10	L1	164/166 (99%)	160 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	MM	29/31 (94%)	29 (100%)	0	0	100	100
12	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X1	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X2	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	XX	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
13	F2	135/137 (98%)	125 (93%)	7 (5%)	3 (2%)	6	35
14	I2	31/33 (94%)	31 (100%)	0	0	100	100
15	K2	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
16	L2	165/167 (99%)	160 (97%)	5 (3%)	0	100	100
17	E	61/63 (97%)	61 (100%)	0	0	100	100
17	EE	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	L	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	22	61
18	LL	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
All	All	8958/9106 (98%)	8634 (96%)	316 (4%)	8 (0%)	54	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	122	VAL
13	F2	159	ILE
1	A1	122	VAL
1	A	122	VAL
1	AA	477	ILE
13	F2	158	GLU
13	F2	160	THR
18	L	118	PRO

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	A	594/594 (100%)	594 (100%)	0	100	100
1	A1	594/594 (100%)	594 (100%)	0	100	100
1	A2	594/594 (100%)	594 (100%)	0	100	100
1	AA	594/594 (100%)	594 (100%)	0	100	100
2	B	601/601 (100%)	601 (100%)	0	100	100
2	B1	601/601 (100%)	601 (100%)	0	100	100
2	B2	601/601 (100%)	601 (100%)	0	100	100
2	BB	601/601 (100%)	600 (100%)	1 (0%)	93	98
3	C	68/68 (100%)	68 (100%)	0	100	100
3	C1	68/68 (100%)	67 (98%)	1 (2%)	65	85
3	C2	68/68 (100%)	67 (98%)	1 (2%)	65	85
3	CC	68/68 (100%)	68 (100%)	0	100	100
4	D	107/107 (100%)	107 (100%)	0	100	100
4	D1	107/107 (100%)	107 (100%)	0	100	100
4	D2	107/107 (100%)	107 (100%)	0	100	100
4	DD	107/107 (100%)	107 (100%)	0	100	100
5	E1	53/53 (100%)	53 (100%)	0	100	100
5	E2	53/53 (100%)	53 (100%)	0	100	100
6	F	108/108 (100%)	108 (100%)	0	100	100
6	F1	108/108 (100%)	108 (100%)	0	100	100
6	FF	108/108 (100%)	108 (100%)	0	100	100
7	I	28/28 (100%)	28 (100%)	0	100	100
7	I1	28/28 (100%)	28 (100%)	0	100	100
7	II	28/28 (100%)	28 (100%)	0	100	100
8	J	38/41 (93%)	38 (100%)	0	100	100
8	J1	38/41 (93%)	38 (100%)	0	100	100
8	J2	38/41 (93%)	38 (100%)	0	100	100
8	JJ	38/41 (93%)	38 (100%)	0	100	100
9	K	46/54 (85%)	46 (100%)	0	100	100
9	K1	54/54 (100%)	54 (100%)	0	100	100
9	KK	46/54 (85%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	L1	127/127 (100%)	126 (99%)	1 (1%)	81 93
11	M	26/26 (100%)	26 (100%)	0	100 100
11	M1	26/26 (100%)	26 (100%)	0	100 100
11	M2	26/26 (100%)	26 (100%)	0	100 100
11	MM	26/26 (100%)	26 (100%)	0	100 100
12	X	31/31 (100%)	31 (100%)	0	100 100
12	X1	31/31 (100%)	31 (100%)	0	100 100
12	X2	31/31 (100%)	31 (100%)	0	100 100
12	XX	31/31 (100%)	31 (100%)	0	100 100
13	F2	106/106 (100%)	106 (100%)	0	100 100
14	I2	30/30 (100%)	30 (100%)	0	100 100
15	K2	54/54 (100%)	54 (100%)	0	100 100
16	L2	128/128 (100%)	127 (99%)	1 (1%)	81 93
17	E	55/55 (100%)	55 (100%)	0	100 100
17	EE	55/55 (100%)	55 (100%)	0	100 100
18	L	117/117 (100%)	116 (99%)	1 (1%)	78 91
18	LL	117/117 (100%)	117 (100%)	0	100 100
All	All	7309/7337 (100%)	7303 (100%)	6 (0%)	93 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C1	44	ARG
10	L1	61	ARG
3	C2	44	ARG
16	L2	61	ARG
18	L	61	ARG
2	BB	34	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	158	GLN
1	A1	180	HIS
1	A1	199	ASN

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Mol	Chain	Res	Type
1	A1	715	GLN
2	B1	29	ASN
2	B1	468	GLN
2	B1	610	GLN
5	E1	19	GLN
5	E1	51	ASN
10	L1	114	ASN
1	A2	53	HIS
1	A2	715	GLN
2	B2	114	ASN
2	B2	341	HIS
2	B2	468	GLN
2	B2	610	GLN
5	E2	19	GLN
16	L2	114	ASN
1	A	216	HIS
2	B	41	ASN
2	B	289	HIS
2	B	306	ASN
2	B	380	GLN
4	D	125	ASN
4	D	128	GLN
17	E	51	ASN
1	AA	158	GLN
2	BB	223	GLN
2	BB	498	ASN
17	EE	51	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 (i)

Of 594 ligands modelled in this entry, 22 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 572 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	$\#\|Z\| > 2$
19	CLA	B1	824	-	55,63,73	1.62	8 (14%)	64,101,113	1.39	8 (12%)
19	CLA	B	821	2	65,73,73	1.42	6 (9%)	76,113,113	1.40	7 (9%)
23	BCR	B1	842	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
19	CLA	B1	826	-	65,73,73	1.54	8 (12%)	76,113,113	1.49	9 (11%)
19	CLA	A1	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.33	9 (11%)
19	CLA	BB	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
19	CLA	A1	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.56	8 (13%)
19	CLA	B	832	-	45,53,73	1.81	8 (17%)	52,89,113	1.42	4 (7%)
19	CLA	AA	808	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	7 (9%)
23	BCR	A	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
23	BCR	A2	849	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	8 (14%)
19	CLA	A	808	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	10 (13%)
23	BCR	II	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.22	8 (14%)
19	CLA	BB	813	-	42,50,73	1.80	6 (14%)	48,85,113	1.56	7 (14%)
19	CLA	B1	828	-	65,73,73	1.49	6 (9%)	76,113,113	1.28	7 (9%)
19	CLA	A	806	-	56,64,73	1.61	9 (16%)	65,102,113	1.57	11 (16%)
23	BCR	K2	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
23	BCR	M	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.33	10 (17%)
19	CLA	B2	808	-	60,68,73	1.54	6 (10%)	70,107,113	1.34	7 (10%)
22	LHG	BB	851	-	48,48,48	0.77	2 (4%)	51,54,54	0.98	4 (7%)
25	LMG	B	851	-	55,55,55	0.68	0	63,63,63	1.28	7 (11%)
19	CLA	BB	809	-	45,53,73	1.75	7 (15%)	52,89,113	1.59	8 (15%)
23	BCR	F2	304	-	41,41,41	1.20	2 (4%)	56,56,56	1.25	9 (16%)
19	CLA	A2	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.54	8 (13%)
19	CLA	B2	806	2	65,73,73	1.46	8 (12%)	76,113,113	1.43	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	B2	842	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	7 (12%)
22	LHG	X1	102	-	39,39,48	0.82	2 (5%)	42,45,54	0.93	2 (4%)
19	CLA	B	860	-	65,73,73	1.46	7 (10%)	76,113,113	1.56	10 (13%)
19	CLA	B1	802	-	65,73,73	1.45	7 (10%)	76,113,113	1.34	9 (11%)
19	CLA	B2	822	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	A	801	-	65,73,73	1.45	8 (12%)	76,113,113	1.36	8 (10%)
19	CLA	A2	840	-	56,64,73	1.56	7 (12%)	65,102,113	1.42	7 (10%)
19	CLA	B2	817	-	42,50,73	1.81	6 (14%)	48,85,113	1.57	6 (12%)
19	CLA	B	835	-	45,53,73	1.72	6 (13%)	52,89,113	1.58	9 (17%)
19	CLA	B	837	-	60,68,73	1.55	7 (11%)	70,107,113	1.37	7 (10%)
23	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	4 (7%)
19	CLA	A2	828	-	56,64,73	1.57	6 (10%)	65,102,113	1.47	7 (10%)
19	CLA	AA	842	-	65,73,73	1.48	8 (12%)	76,113,113	1.43	11 (14%)
19	CLA	AA	840	-	56,64,73	1.57	7 (12%)	65,102,113	1.36	6 (9%)
19	CLA	BB	834	-	45,53,73	1.74	7 (15%)	52,89,113	1.58	7 (13%)
19	CLA	AA	838	-	44,52,73	1.78	7 (15%)	49,87,113	1.65	8 (16%)
23	BCR	J1	104	-	41,41,41	1.13	2 (4%)	56,56,56	1.34	6 (10%)
23	BCR	LL	204	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	5 (8%)
19	CLA	A	842	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	12 (15%)
19	CLA	B1	833	-	65,73,73	1.49	8 (12%)	76,113,113	1.65	16 (21%)
19	CLA	BB	812	-	41,49,73	1.81	6 (14%)	47,84,113	1.61	6 (12%)
19	CLA	A	838	-	44,52,73	1.78	7 (15%)	49,87,113	1.63	8 (16%)
23	BCR	JJ	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	8 (14%)
22	LHG	A	845	-	48,48,48	0.80	2 (4%)	51,54,54	0.98	3 (5%)
19	CLA	A2	807	-	65,73,73	1.45	8 (12%)	76,113,113	1.33	8 (10%)
23	BCR	L1	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	AA	818	-	45,53,73	1.77	6 (13%)	52,89,113	1.54	6 (11%)
19	CLA	A2	802	-	46,54,73	1.74	6 (13%)	53,90,113	1.55	7 (13%)
19	CLA	B1	809	-	45,53,73	1.78	6 (13%)	52,89,113	1.56	8 (15%)
22	LHG	B1	847	-	32,32,48	0.87	1 (3%)	35,38,54	1.03	3 (8%)
19	CLA	A2	806	-	56,64,73	1.62	9 (16%)	65,102,113	1.56	10 (15%)
19	CLA	B1	813	-	42,50,73	1.81	6 (14%)	48,85,113	1.51	7 (14%)
19	CLA	A2	837	-	45,53,73	1.79	7 (15%)	52,89,113	1.57	7 (13%)
19	CLA	A2	822	-	51,59,73	1.67	6 (11%)	59,96,113	1.49	9 (15%)
19	CLA	B2	823	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	PQN	A1	843	-	34,34,34	0.63	0	42,45,45	1.10	3 (7%)
19	CLA	A1	829	-	62,70,73	1.48	6 (9%)	72,109,113	1.37	8 (11%)
19	CLA	B	830	-	56,64,73	1.53	7 (12%)	65,102,113	1.46	9 (13%)
23	BCR	AA	848	-	40,40,41	1.09	2 (5%)	54,54,56	1.28	10 (18%)
23	BCR	AA	854	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	12 (21%)
19	CLA	B1	845	-	40,47,73	1.84	6 (15%)	45,80,113	1.60	7 (15%)
19	CLA	BB	824	-	55,63,73	1.60	7 (12%)	64,101,113	1.41	7 (10%)
23	BCR	J	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.38	10 (17%)
23	BCR	J1	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	BB	826	-	65,73,73	1.57	9 (13%)	76,113,113	1.53	12 (15%)
19	CLA	A1	824	-	42,50,73	1.82	7 (16%)	48,85,113	1.54	7 (14%)
27	SF4	C2	102	-	0,12,12	-	-	-		
19	CLA	A1	833	-	41,49,73	1.81	7 (17%)	47,84,113	1.57	8 (17%)
19	CLA	BB	820	-	45,53,73	1.76	8 (17%)	52,89,113	1.83	13 (25%)
19	CLA	A	813	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	8 (10%)
19	CLA	B1	815	-	65,73,73	1.45	6 (9%)	76,113,113	1.54	11 (14%)
19	CLA	LL	202	-	65,73,73	1.48	9 (13%)	76,113,113	1.45	9 (11%)
27	SF4	C	101	-	0,12,12	-	-	-		
22	LHG	XX	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	A2	818	-	45,53,73	1.79	6 (13%)	52,89,113	1.54	7 (13%)
19	CLA	B2	809	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	8 (15%)
19	CLA	A1	809	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	11 (14%)
19	CLA	LL	203	-	42,50,73	1.84	6 (14%)	48,85,113	1.84	9 (18%)
19	CLA	B2	815	-	65,73,73	1.46	6 (9%)	76,113,113	1.47	10 (13%)
22	LHG	BB	850	-	32,32,48	0.89	1 (3%)	35,38,54	1.03	3 (8%)
19	CLA	BB	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.46	7 (9%)
27	SF4	BB	857	-	0,12,12	-	-	-		
19	CLA	F	301	-	60,68,73	1.54	7 (11%)	70,107,113	1.52	10 (14%)
19	CLA	A1	828	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	8 (10%)
23	BCR	B	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	6 (10%)
19	CLA	A	811	1	51,59,73	1.66	9 (17%)	59,96,113	1.57	9 (15%)
19	CLA	AA	834	-	41,49,73	1.81	7 (17%)	47,84,113	1.54	6 (12%)
27	SF4	B1	851	-	0,12,12	-	-	-		
19	CLA	B	820	-	45,53,73	1.77	7 (15%)	52,89,113	1.80	11 (21%)
19	CLA	BB	819	-	41,49,73	1.80	6 (14%)	47,84,113	1.59	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B1	836	-	60,68,73	1.53	6 (10%)	70,107,113	1.46	9 (12%)
19	CLA	A2	801	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	7 (9%)
19	CLA	B2	811	-	61,69,73	1.52	6 (9%)	71,108,113	1.29	5 (7%)
19	CLA	A	824	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	8 (15%)
19	CLA	B1	807	-	65,73,73	1.49	6 (9%)	76,113,113	1.55	13 (17%)
19	CLA	A1	813	-	42,50,73	1.81	6 (14%)	48,85,113	1.52	7 (14%)
23	BCR	F	303	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
27	SF4	C	102	3	0,12,12	-	-	-		
25	LMG	B1	844	-	55,55,55	0.68	0	63,63,63	1.28	4 (6%)
19	CLA	B1	806	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	10 (13%)
19	CLA	A2	838	-	44,52,73	1.76	6 (13%)	49,87,113	1.64	7 (14%)
19	CLA	AA	813	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	8 (10%)
19	CLA	B2	827	-	45,53,73	1.80	9 (20%)	52,89,113	1.51	7 (13%)
23	BCR	F1	306	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	8 (14%)
19	CLA	A1	827	-	56,64,73	1.58	6 (10%)	65,102,113	1.46	7 (10%)
19	CLA	AA	827	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	5 (6%)
19	CLA	A2	831	-	65,73,73	1.46	8 (12%)	76,113,113	1.32	8 (10%)
19	CLA	A1	819	-	58,66,73	1.58	10 (17%)	67,104,113	1.46	10 (14%)
19	CLA	K1	105	9	39,48,73	1.88	6 (15%)	45,82,113	1.68	9 (20%)
19	CLA	A2	816	-	50,58,73	1.66	6 (12%)	58,95,113	1.47	8 (13%)
19	CLA	A	814	-	42,50,73	1.83	6 (14%)	48,85,113	1.49	7 (14%)
19	CLA	AA	845	-	41,49,73	1.81	6 (14%)	47,84,113	1.62	7 (14%)
19	CLA	AA	826	-	45,53,73	1.76	7 (15%)	52,89,113	1.57	8 (15%)
23	BCR	KK	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	10 (17%)
19	CLA	AA	820	-	58,66,73	1.57	9 (15%)	67,104,113	1.48	9 (13%)
19	CLA	B1	801	-	65,73,73	1.46	6 (9%)	76,113,113	1.52	10 (13%)
19	CLA	A2	835	-	65,73,73	1.50	9 (13%)	76,113,113	1.35	9 (11%)
19	CLA	B	834	-	65,73,73	1.45	8 (12%)	76,113,113	1.63	16 (21%)
28	DGD	B	856	-	43,43,67	1.06	0	57,57,81	1.40	6 (10%)
20	CL0	AA	803	-	65,73,73	2.01	15 (23%)	76,113,113	2.54	25 (32%)
23	BCR	L2	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	8 (14%)
19	CLA	BB	802	-	65,73,73	1.47	8 (12%)	76,113,113	1.34	9 (11%)
19	CLA	B	813	-	42,50,73	1.80	7 (16%)	48,85,113	1.50	7 (14%)
19	CLA	B1	848	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	4 (5%)
19	CLA	A	821	-	65,73,73	1.43	7 (10%)	76,113,113	1.43	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	PQN	B2	838	-	34,34,34	0.62	0	42,45,45	0.87	0
23	BCR	B2	839	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
19	CLA	B1	835	-	65,73,73	1.47	8 (12%)	76,113,113	1.28	6 (7%)
27	SF4	B2	853	-	0,12,12	-	-	-		
19	CLA	AA	812	-	46,54,73	1.73	6 (13%)	53,90,113	1.56	7 (13%)
19	CLA	A1	806	-	65,73,73	1.46	8 (12%)	76,113,113	1.32	8 (10%)
19	CLA	A	837	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
19	CLA	A	841	-	46,54,73	1.68	6 (13%)	53,90,113	1.55	6 (11%)
19	CLA	A2	815	-	55,63,73	1.57	6 (10%)	64,101,113	1.41	7 (10%)
19	CLA	B1	831	-	45,53,73	1.82	8 (17%)	52,89,113	1.46	5 (9%)
19	CLA	B1	816	-	57,65,73	1.60	7 (12%)	66,103,113	1.39	8 (12%)
19	CLA	AA	829	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	A	825	-	52,60,73	1.64	6 (11%)	60,97,113	1.46	7 (11%)
19	CLA	BB	836	-	60,68,73	1.52	7 (11%)	70,107,113	1.73	12 (17%)
19	CLA	A	833	-	50,58,73	1.68	8 (16%)	58,95,113	1.42	5 (8%)
19	CLA	A	829	-	65,73,73	1.45	8 (12%)	76,113,113	1.39	8 (10%)
19	CLA	K2	102	-	45,53,73	1.77	6 (13%)	52,89,113	1.59	9 (17%)
19	CLA	J1	103	-	41,49,73	1.87	6 (14%)	47,84,113	1.54	6 (12%)
19	CLA	L1	207	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	6 (7%)
19	CLA	K	102	-	46,54,73	1.73	6 (13%)	53,90,113	1.51	7 (13%)
19	CLA	B	859	-	60,68,73	1.53	8 (13%)	70,107,113	1.72	16 (22%)
19	CLA	BB	830	-	56,64,73	1.56	6 (10%)	65,102,113	1.39	7 (10%)
19	CLA	J	101	8	41,49,73	1.84	6 (14%)	47,84,113	1.58	7 (14%)
19	CLA	A1	814	-	55,63,73	1.57	6 (10%)	64,101,113	1.43	7 (10%)
19	CLA	B2	819	-	41,49,73	1.81	7 (17%)	47,84,113	1.63	6 (12%)
19	CLA	A	828	-	56,64,73	1.55	6 (10%)	65,102,113	1.45	8 (12%)
19	CLA	A2	841	-	46,54,73	1.69	6 (13%)	53,90,113	1.56	6 (11%)
19	CLA	A	835	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	8 (10%)
28	DGD	BB	854	-	43,43,67	1.05	0	57,57,81	1.41	7 (12%)
19	CLA	K1	103	-	46,54,73	1.74	6 (13%)	53,90,113	1.55	7 (13%)
19	CLA	A2	825	-	42,50,73	1.83	8 (19%)	48,85,113	1.60	7 (14%)
19	CLA	A1	823	-	45,53,73	1.75	7 (15%)	52,89,113	1.62	8 (15%)
19	CLA	A1	831	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
19	CLA	A2	810	1	65,73,73	1.47	7 (10%)	76,113,113	1.45	11 (14%)
19	CLA	BB	852	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A1	818	-	60,68,73	1.53	6 (10%)	70,107,113	1.40	8 (11%)
19	CLA	F	302	-	42,50,73	1.83	7 (16%)	48,85,113	1.63	7 (14%)
23	BCR	B2	843	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	6 (10%)
19	CLA	A1	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
23	BCR	F2	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
19	CLA	B2	821	-	65,73,73	1.43	6 (9%)	76,113,113	1.41	9 (11%)
19	CLA	BB	832	-	65,73,73	1.54	8 (12%)	76,113,113	1.48	10 (13%)
19	CLA	B	814	-	59,67,73	1.55	7 (11%)	68,105,113	1.50	8 (11%)
23	BCR	B1	843	-	41,41,41	1.21	3 (7%)	56,56,56	1.19	6 (10%)
19	CLA	X2	101	-	45,53,73	1.79	6 (13%)	52,89,113	1.54	6 (11%)
19	CLA	AA	807	-	65,73,73	1.46	7 (10%)	76,113,113	1.27	6 (7%)
19	CLA	AA	843	-	65,73,73	1.45	7 (10%)	76,113,113	1.53	9 (11%)
23	BCR	B1	841	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	6 (10%)
19	CLA	A	804	-	65,73,73	1.47	8 (12%)	76,113,113	1.33	8 (10%)
19	CLA	AA	805	-	60,68,73	1.50	7 (11%)	70,107,113	1.46	9 (12%)
19	CLA	BB	818	-	41,49,73	1.82	6 (14%)	47,84,113	1.50	7 (14%)
25	LMG	B1	852	-	30,30,55	1.00	0	38,38,63	1.23	4 (10%)
23	BCR	A1	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
19	CLA	AA	819	-	60,68,73	1.54	6 (10%)	70,107,113	1.39	8 (11%)
19	CLA	BB	814	-	59,67,73	1.54	10 (16%)	68,105,113	1.48	10 (14%)
23	BCR	I2	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	A	819	-	60,68,73	1.53	7 (11%)	70,107,113	1.40	8 (11%)
25	LMG	B2	854	-	30,30,55	0.99	0	38,38,63	1.23	4 (10%)
27	SF4	C1	101	-	0,12,12	-	-	-		
20	CL0	A2	803	-	65,73,73	1.97	15 (23%)	76,113,113	2.55	25 (32%)
19	CLA	L2	206	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	6 (7%)
19	CLA	B	810	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	AA	836	-	65,73,73	1.47	8 (12%)	76,113,113	1.33	6 (7%)
19	CLA	AA	853	-	65,73,73	1.47	9 (13%)	76,113,113	1.28	9 (11%)
19	CLA	BB	823	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	6 (7%)
19	CLA	A	836	-	65,73,73	1.47	8 (12%)	76,113,113	1.35	7 (9%)
19	CLA	B2	803	-	65,73,73	1.45	8 (12%)	76,113,113	1.44	7 (9%)
19	CLA	B	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	7 (9%)
19	CLA	BB	835	-	65,73,73	1.48	9 (13%)	76,113,113	1.33	8 (10%)
27	SF4	C2	101	-	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	BB	821	-	65,73,73	1.44	6 (9%)	76,113,113	1.29	7 (9%)
19	CLA	A2	852	-	65,73,73	1.49	8 (12%)	76,113,113	1.37	8 (10%)
19	CLA	AA	830	-	62,70,73	1.46	7 (11%)	72,109,113	1.37	8 (11%)
19	CLA	B2	835	-	45,53,73	1.74	6 (13%)	52,89,113	1.54	8 (15%)
19	CLA	B1	849	-	65,73,73	1.49	9 (13%)	76,113,113	1.28	7 (9%)
19	CLA	A1	835	-	65,73,73	1.48	8 (12%)	76,113,113	1.32	5 (6%)
23	BCR	I2	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.27	9 (16%)
23	BCR	J2	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.35	8 (14%)
19	CLA	A2	804	-	65,73,73	1.45	7 (10%)	76,113,113	1.31	7 (9%)
19	CLA	A2	844	-	41,49,73	1.81	7 (17%)	47,84,113	1.59	6 (12%)
23	BCR	A2	847	-	40,40,41	1.09	2 (5%)	54,54,56	1.26	7 (12%)
23	BCR	A	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	9 (16%)
23	BCR	A2	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	8 (14%)
19	CLA	B1	820	-	45,53,73	1.79	6 (13%)	52,89,113	1.50	7 (13%)
25	LMG	B2	845	-	55,55,55	0.69	0	63,63,63	1.27	5 (7%)
27	SF4	CC	102	-	0,12,12	-	-	-		
23	BCR	II	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	8 (14%)
19	CLA	B	828	-	45,53,73	1.75	7 (15%)	52,89,113	1.51	7 (13%)
23	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	8 (14%)
19	CLA	B2	801	-	65,73,73	1.45	6 (9%)	76,113,113	1.54	11 (14%)
19	CLA	B2	846	-	40,47,73	1.84	7 (17%)	45,80,113	1.60	7 (15%)
19	CLA	B1	834	-	45,53,73	1.73	6 (13%)	52,89,113	1.55	8 (15%)
19	CLA	B1	810	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	9 (11%)
23	BCR	FF	306	-	41,41,41	1.15	3 (7%)	56,56,56	1.48	10 (17%)
19	CLA	B	816	-	57,65,73	1.59	8 (14%)	66,103,113	1.45	8 (12%)
19	CLA	B1	804	-	62,70,73	1.52	8 (12%)	72,109,113	1.42	9 (12%)
19	CLA	B	829	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	7 (9%)
23	BCR	MM	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.36	10 (17%)
19	CLA	A1	815	-	50,58,73	1.66	6 (12%)	58,95,113	1.48	8 (13%)
19	CLA	AA	839	-	52,60,73	1.62	6 (11%)	60,97,113	1.50	8 (13%)
19	CLA	A2	808	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
19	CLA	AA	814	-	42,50,73	1.81	6 (14%)	48,85,113	1.52	7 (14%)
23	BCR	AA	852	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	7 (12%)
19	CLA	B2	813	-	42,50,73	1.80	6 (14%)	48,85,113	1.50	8 (16%)
19	CLA	A2	834	-	41,49,73	1.81	7 (17%)	47,84,113	1.58	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	JJ	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	10 (17%)
23	BCR	A2	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	XX	101	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	6 (11%)
22	LHG	LL	205	-	33,33,48	0.94	3 (9%)	36,39,54	1.05	4 (11%)
22	LHG	X	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	AA	823	-	60,68,73	1.54	7 (11%)	70,107,113	1.50	10 (14%)
22	LHG	L2	208	-	34,34,48	0.87	1 (2%)	37,40,54	1.05	3 (8%)
19	CLA	BB	815	-	65,73,73	1.45	6 (9%)	76,113,113	1.48	10 (13%)
19	CLA	A	834	-	41,49,73	1.81	7 (17%)	47,84,113	1.56	8 (17%)
19	CLA	A1	810	-	51,59,73	1.67	9 (17%)	59,96,113	1.56	9 (15%)
19	CLA	A2	817	-	44,52,73	1.79	7 (15%)	49,87,113	1.53	6 (12%)
19	CLA	AA	821	-	65,73,73	1.43	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	A1	852	-	65,73,73	1.48	8 (12%)	76,113,113	1.27	5 (6%)
19	CLA	A1	841	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	10 (13%)
19	CLA	B	836	-	65,73,73	1.48	7 (10%)	76,113,113	1.36	8 (10%)
19	CLA	A1	844	-	41,49,73	1.81	6 (14%)	47,84,113	1.59	7 (14%)
19	CLA	B	808	-	60,68,73	1.51	6 (10%)	70,107,113	1.29	6 (8%)
26	ECH	B	841	-	42,42,42	0.90	1 (2%)	55,58,58	2.48	22 (40%)
23	BCR	A1	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.37	9 (16%)
22	LHG	X2	103	-	48,48,48	0.77	1 (2%)	51,54,54	0.96	4 (7%)
23	BCR	AA	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	5 (8%)
19	CLA	AA	832	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	9 (11%)
23	BCR	A1	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	8 (14%)
19	CLA	B1	850	-	60,68,73	1.54	7 (11%)	70,107,113	1.67	16 (22%)
19	CLA	B1	808	-	60,68,73	1.53	6 (10%)	70,107,113	1.33	7 (10%)
19	CLA	B2	849	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	4 (5%)
19	CLA	A	832	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	9 (11%)
19	CLA	B	811	-	61,69,73	1.50	7 (11%)	71,108,113	1.30	5 (7%)
23	BCR	B2	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.19	6 (10%)
19	CLA	A1	826	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	5 (6%)
22	LHG	B	852	-	32,32,48	0.89	1 (3%)	35,38,54	1.02	3 (8%)
19	CLA	B1	822	-	65,73,73	1.48	7 (10%)	76,113,113	1.33	7 (9%)
19	CLA	A1	820	-	65,73,73	1.42	7 (10%)	76,113,113	1.43	10 (13%)
23	BCR	A2	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	K	101	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	L2	204	16	61,69,73	1.51	6 (9%)	71,108,113	1.44	10 (14%)
23	BCR	A1	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	6 (10%)
25	LMG	B2	847	-	32,32,55	0.94	1 (3%)	40,40,63	1.22	2 (5%)
23	BCR	AA	850	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	9 (16%)
19	CLA	J2	103	-	41,49,73	1.87	6 (14%)	47,84,113	1.52	7 (14%)
23	BCR	FF	303	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
19	CLA	L	204	-	65,73,73	1.44	7 (10%)	76,113,113	1.48	9 (11%)
19	CLA	B2	834	-	65,73,73	1.52	8 (12%)	76,113,113	1.61	15 (19%)
21	PQN	AA	844	-	34,34,34	0.66	0	42,45,45	1.06	4 (9%)
19	CLA	A1	834	-	65,73,73	1.49	8 (12%)	76,113,113	1.33	9 (11%)
19	CLA	B2	812	-	41,49,73	1.81	6 (14%)	47,84,113	1.64	7 (14%)
23	BCR	F	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	A	812	-	46,54,73	1.73	6 (13%)	53,90,113	1.58	7 (13%)
19	CLA	BB	829	-	56,64,73	1.55	8 (14%)	65,102,113	1.41	10 (15%)
23	BCR	B	844	-	41,41,41	1.24	4 (9%)	56,56,56	1.22	7 (12%)
19	CLA	B2	828	-	45,53,73	1.76	6 (13%)	52,89,113	1.52	7 (13%)
19	CLA	AA	815	-	55,63,73	1.57	6 (10%)	64,101,113	1.44	7 (10%)
19	CLA	B	818	-	41,49,73	1.88	5 (12%)	47,84,113	1.53	6 (12%)
25	LMG	B	845	-	55,55,55	0.69	0	63,63,63	1.27	4 (6%)
19	CLA	J2	101	8	41,49,73	1.85	6 (14%)	47,84,113	1.54	7 (14%)
19	CLA	AA	809	-	50,58,73	1.65	6 (12%)	58,95,113	1.54	9 (15%)
23	BCR	L1	209	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	9 (16%)
25	LMG	I1	102	-	35,35,55	1.04	1 (2%)	43,43,63	1.27	3 (6%)
19	CLA	A	826	-	45,53,73	1.75	7 (15%)	52,89,113	1.55	8 (15%)
19	CLA	A	820	-	58,66,73	1.57	9 (15%)	67,104,113	1.47	10 (14%)
25	LMG	B1	846	-	32,32,55	0.93	0	40,40,63	1.21	4 (10%)
23	BCR	F2	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	9 (16%)
19	CLA	A	840	-	56,64,73	1.57	7 (12%)	65,102,113	1.42	7 (10%)
19	CLA	L	203	-	65,73,73	1.50	8 (12%)	76,113,113	1.41	9 (11%)
19	CLA	A2	812	-	46,54,73	1.73	8 (17%)	53,90,113	1.53	9 (16%)
19	CLA	B2	826	-	65,73,73	1.54	7 (10%)	76,113,113	1.47	9 (11%)
23	BCR	AA	855	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	8 (14%)
19	CLA	F2	301	-	60,68,73	1.56	7 (11%)	70,107,113	1.46	10 (14%)
19	CLA	A	818	-	45,53,73	1.78	6 (13%)	52,89,113	1.53	6 (11%)
23	BCR	A	854	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	804	-	62,70,73	1.52	7 (11%)	72,109,113	1.39	10 (13%)
19	CLA	L2	205	-	59,67,73	1.54	8 (13%)	68,105,113	1.53	8 (11%)
19	CLA	B	833	-	65,73,73	1.50	8 (12%)	76,113,113	1.50	11 (14%)
27	SF4	B	861	-	0,12,12	-	-	-		
19	CLA	B2	818	-	41,49,73	1.85	6 (14%)	47,84,113	1.53	6 (12%)
22	LHG	AA	846	-	48,48,48	0.79	2 (4%)	51,54,54	0.97	3 (5%)
19	CLA	B2	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.56	13 (17%)
19	CLA	B1	823	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	6 (7%)
19	CLA	B	809	-	45,53,73	1.76	7 (15%)	52,89,113	1.58	8 (15%)
19	CLA	B2	850	-	65,73,73	1.49	9 (13%)	76,113,113	1.33	7 (9%)
22	LHG	A	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
21	PQN	A	843	-	34,34,34	0.60	0	42,45,45	1.09	3 (7%)
19	CLA	B1	812	-	41,49,73	1.82	6 (14%)	47,84,113	1.64	7 (14%)
19	CLA	B1	818	-	41,49,73	1.85	6 (14%)	47,84,113	1.53	6 (12%)
19	CLA	K2	104	-	42,49,73	1.82	7 (16%)	48,83,113	1.60	6 (12%)
21	PQN	B1	837	-	34,34,34	0.70	0	42,45,45	0.88	0
19	CLA	AA	824	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	8 (15%)
19	CLA	A2	820	-	58,66,73	1.58	10 (17%)	67,104,113	1.48	9 (13%)
19	CLA	B2	824	-	55,63,73	1.59	6 (10%)	64,101,113	1.43	7 (10%)
27	SF4	C1	102	-	0,12,12	-	-	-		
23	BCR	BB	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
19	CLA	B	846	-	40,47,73	1.84	7 (17%)	45,80,113	1.64	7 (15%)
19	CLA	A1	801	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	9 (11%)
19	CLA	FF	305	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	7 (9%)
23	BCR	F1	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	9 (16%)
19	CLA	BB	810	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	7 (9%)
23	BCR	K2	105	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	X1	101	-	45,53,73	1.78	6 (13%)	52,89,113	1.55	6 (11%)
19	CLA	B	815	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	11 (14%)
19	CLA	B2	814	-	59,67,73	1.57	7 (11%)	68,105,113	1.39	8 (11%)
19	CLA	B	827	-	45,53,73	1.77	9 (20%)	52,89,113	1.51	7 (13%)
19	CLA	A2	829	-	65,73,73	1.48	10 (15%)	76,113,113	1.31	9 (11%)
19	CLA	A1	838	-	52,60,73	1.63	6 (11%)	60,97,113	1.51	7 (11%)
19	CLA	A1	825	-	45,53,73	1.74	7 (15%)	52,89,113	1.59	8 (15%)
19	CLA	A	831	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	LMG	I2	105	-	35,35,55	0.92	1 (2%)	43,43,63	1.22	4 (9%)
19	CLA	A1	812	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
19	CLA	BB	806	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	10 (13%)
19	CLA	A1	816	-	44,52,73	1.79	7 (15%)	49,87,113	1.52	6 (12%)
23	BCR	BB	838	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	7 (12%)
23	BCR	F	305	-	41,41,41	1.15	3 (7%)	56,56,56	1.49	10 (17%)
19	CLA	A1	803	-	65,73,73	1.44	6 (9%)	76,113,113	1.33	7 (9%)
23	BCR	B	843	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	6 (10%)
19	CLA	AA	828	-	56,64,73	1.57	6 (10%)	65,102,113	1.47	8 (12%)
19	CLA	BB	822	-	65,73,73	1.49	8 (12%)	76,113,113	1.35	5 (6%)
19	CLA	B2	802	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	8 (10%)
19	CLA	AA	835	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
19	CLA	B2	837	-	60,68,73	1.53	6 (10%)	70,107,113	1.44	9 (12%)
19	CLA	BB	828	-	45,53,73	1.75	7 (15%)	52,89,113	1.55	7 (13%)
19	CLA	BB	801	-	65,73,73	1.44	6 (9%)	76,113,113	1.62	9 (11%)
19	CLA	B	825	-	65,73,73	1.44	6 (9%)	76,113,113	1.39	10 (13%)
19	CLA	B2	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	9 (11%)
19	CLA	B2	833	-	65,73,73	1.51	6 (9%)	76,113,113	1.51	10 (13%)
22	LHG	A2	845	-	48,48,48	0.76	1 (2%)	51,54,54	0.96	3 (5%)
23	BCR	I	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	6 (10%)
19	CLA	BB	816	-	57,65,73	1.59	8 (14%)	66,103,113	1.43	8 (12%)
19	CLA	B	806	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	10 (13%)
19	CLA	BB	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.39	9 (11%)
23	BCR	B	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
19	CLA	JJ	103	-	41,49,73	1.85	6 (14%)	47,84,113	1.54	7 (14%)
19	CLA	A2	805	-	60,68,73	1.51	6 (10%)	70,107,113	1.43	8 (11%)
22	LHG	B	853	-	48,48,48	0.75	1 (2%)	51,54,54	0.98	4 (7%)
20	CL0	A1	802	-	65,73,73	2.04	15 (23%)	76,113,113	2.44	28 (36%)
19	CLA	BB	831	-	45,53,73	1.80	8 (17%)	52,89,113	1.47	6 (11%)
23	BCR	J2	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	10 (17%)
19	CLA	FF	301	-	60,68,73	1.53	6 (10%)	70,107,113	1.38	9 (12%)
19	CLA	B2	831	-	56,64,73	1.57	6 (10%)	65,102,113	1.41	7 (10%)
23	BCR	II	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	5 (8%)
23	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
19	CLA	A	817	-	44,52,73	1.78	6 (13%)	49,87,113	1.54	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B1	829	-	56,64,73	1.58	9 (16%)	65,102,113	1.44	9 (13%)
19	CLA	A1	817	-	45,53,73	1.78	6 (13%)	52,89,113	1.54	7 (13%)
19	CLA	B1	805	-	64,72,73	1.47	9 (14%)	74,111,113	1.42	9 (12%)
19	CLA	A2	819	-	60,68,73	1.53	7 (11%)	70,107,113	1.39	9 (12%)
21	PQN	BB	837	-	34,34,34	0.66	0	42,45,45	0.85	0
19	CLA	AA	806	-	56,64,73	1.62	9 (16%)	65,102,113	1.57	10 (15%)
19	CLA	B	823	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	7 (9%)
19	CLA	B	801	-	65,73,73	1.43	6 (9%)	76,113,113	1.64	12 (15%)
19	CLA	A	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.53	10 (17%)
19	CLA	B	831	-	56,64,73	1.55	6 (10%)	65,102,113	1.40	8 (12%)
19	CLA	AA	822	-	51,59,73	1.68	6 (11%)	59,96,113	1.46	6 (10%)
23	BCR	J	104	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	8 (14%)
19	CLA	B2	804	-	62,70,73	1.52	8 (12%)	72,109,113	1.43	9 (12%)
23	BCR	L	205	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	9 (16%)
23	BCR	K	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	7 (12%)
25	LMG	II	105	-	42,42,55	0.82	1 (2%)	50,50,63	1.24	6 (12%)
19	CLA	B1	803	-	65,73,73	1.46	9 (13%)	76,113,113	1.41	8 (10%)
19	CLA	B	819	-	41,49,73	1.81	7 (17%)	47,84,113	1.58	7 (14%)
19	CLA	B1	819	-	41,49,73	1.82	6 (14%)	47,84,113	1.58	7 (14%)
19	CLA	AA	801	-	65,73,73	1.45	9 (13%)	76,113,113	1.33	7 (9%)
23	BCR	I	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
19	CLA	A1	842	-	65,73,73	1.45	9 (13%)	76,113,113	1.58	12 (15%)
19	CLA	BB	855	-	65,73,73	1.49	9 (13%)	76,113,113	1.36	6 (7%)
19	CLA	A	823	-	60,68,73	1.54	7 (11%)	70,107,113	1.51	10 (14%)
19	CLA	B	812	-	41,49,73	1.78	6 (14%)	47,84,113	1.70	8 (17%)
20	CL0	A	803	-	65,73,73	2.03	14 (21%)	76,113,113	2.52	26 (34%)
22	LHG	A1	845	-	48,48,48	0.78	2 (4%)	51,54,54	0.96	3 (5%)
23	BCR	BB	842	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	5 (8%)
19	CLA	BB	811	-	61,69,73	1.51	7 (11%)	71,108,113	1.31	5 (7%)
19	CLA	AA	816	-	50,58,73	1.68	8 (16%)	58,95,113	1.49	9 (15%)
23	BCR	M1	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	A1	836	-	45,53,73	1.79	7 (15%)	52,89,113	1.56	7 (13%)
26	ECH	BB	840	-	42,42,42	0.89	0	55,58,58	2.44	18 (32%)
22	LHG	X1	103	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	3 (5%)
19	CLA	A	816	-	50,58,73	1.67	6 (12%)	58,95,113	1.47	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B2	851	-	60,68,73	1.54	7 (11%)	70,107,113	1.68	16 (22%)
19	CLA	A	805	-	60,68,73	1.50	6 (10%)	70,107,113	1.45	8 (11%)
19	CLA	A1	805	-	56,64,73	1.65	9 (16%)	65,102,113	1.44	8 (12%)
19	CLA	A	810	1	65,73,73	1.48	7 (10%)	76,113,113	1.47	11 (14%)
19	CLA	J1	101	-	41,49,73	1.84	6 (14%)	47,84,113	1.55	7 (14%)
19	CLA	A2	827	-	65,73,73	1.49	8 (12%)	76,113,113	1.40	7 (9%)
19	CLA	A	852	-	65,73,73	1.48	9 (13%)	76,113,113	1.35	7 (9%)
19	CLA	BB	817	-	42,50,73	1.79	6 (14%)	48,85,113	1.60	6 (12%)
19	CLA	BB	833	-	65,73,73	1.45	8 (12%)	76,113,113	1.64	16 (21%)
19	CLA	AA	831	-	65,73,73	1.46	7 (10%)	76,113,113	1.33	7 (9%)
19	CLA	F2	302	-	42,50,73	1.83	7 (16%)	48,85,113	1.66	7 (14%)
19	CLA	B2	810	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	8 (10%)
19	CLA	B	822	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	6 (7%)
23	BCR	A	847	-	40,40,41	1.09	2 (5%)	54,54,56	1.28	11 (20%)
19	CLA	A2	839	-	52,60,73	1.62	6 (11%)	60,97,113	1.50	7 (11%)
23	BCR	M2	102	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	9 (16%)
19	CLA	F1	305	-	45,53,73	1.76	6 (13%)	52,89,113	1.50	7 (13%)
19	CLA	B2	852	-	65,73,73	1.46	7 (10%)	76,113,113	1.54	10 (13%)
23	BCR	B1	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	3 (5%)
19	CLA	A2	814	-	42,50,73	1.81	6 (14%)	48,85,113	1.52	7 (14%)
19	CLA	KK	102	-	46,54,73	1.73	6 (13%)	53,90,113	1.53	7 (13%)
23	BCR	A1	847	-	40,40,41	1.10	2 (5%)	54,54,56	1.26	7 (12%)
19	CLA	L	202	18	61,69,73	1.50	7 (11%)	71,108,113	1.61	11 (15%)
23	BCR	BB	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	6 (10%)
19	CLA	B2	832	-	45,53,73	1.80	8 (17%)	52,89,113	1.45	5 (9%)
19	CLA	A2	823	-	60,68,73	1.53	7 (11%)	70,107,113	1.56	9 (12%)
19	CLA	B	817	-	42,50,73	1.80	6 (14%)	48,85,113	1.63	7 (14%)
19	CLA	B1	827	-	45,53,73	1.79	9 (20%)	52,89,113	1.50	7 (13%)
19	CLA	A2	821	-	65,73,73	1.43	7 (10%)	76,113,113	1.38	8 (10%)
22	LHG	B2	848	-	32,32,48	0.90	2 (6%)	35,38,54	0.98	2 (5%)
25	LMG	BB	844	-	55,55,55	0.69	1 (1%)	63,63,63	1.27	4 (6%)
19	CLA	A	844	-	41,49,73	1.81	7 (17%)	47,84,113	1.60	6 (12%)
19	CLA	B	858	-	65,73,73	1.49	8 (12%)	76,113,113	1.35	8 (10%)
19	CLA	A2	836	-	65,73,73	1.47	9 (13%)	76,113,113	1.42	7 (9%)
23	BCR	L	206	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A2	832	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
23	BCR	K1	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
19	CLA	B1	814	-	59,67,73	1.56	6 (10%)	68,105,113	1.39	7 (10%)
19	CLA	B2	816	-	57,65,73	1.59	7 (12%)	66,103,113	1.40	7 (10%)
19	CLA	B2	805	-	64,72,73	1.47	8 (12%)	74,111,113	1.44	9 (12%)
19	CLA	A	815	-	55,63,73	1.57	6 (10%)	64,101,113	1.44	7 (10%)
19	CLA	F1	301	-	60,68,73	1.56	7 (11%)	70,107,113	1.50	10 (14%)
27	SF4	CC	101	-	0,12,12	-	-	-		
19	CLA	A	827	-	65,73,73	1.50	9 (13%)	76,113,113	1.27	4 (5%)
19	CLA	B	824	-	55,63,73	1.59	6 (10%)	64,101,113	1.39	7 (10%)
19	CLA	AA	811	1	51,59,73	1.67	9 (17%)	59,96,113	1.60	10 (16%)
22	LHG	A1	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
19	CLA	K1	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.66	9 (17%)
19	CLA	B	826	-	65,73,73	1.54	9 (13%)	76,113,113	1.47	12 (15%)
21	PQN	B	838	-	34,34,34	0.63	0	42,45,45	0.87	1 (2%)
19	CLA	A	839	-	52,60,73	1.62	6 (11%)	60,97,113	1.51	9 (15%)
19	CLA	A2	830	-	62,70,73	1.45	6 (9%)	72,109,113	1.38	8 (11%)
23	BCR	F1	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	BB	845	-	40,47,73	1.84	7 (17%)	45,80,113	1.65	7 (15%)
19	CLA	AA	817	-	44,52,73	1.78	6 (13%)	49,87,113	1.53	6 (12%)
19	CLA	B1	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	9 (11%)
19	CLA	A1	804	-	60,68,73	1.51	6 (10%)	70,107,113	1.33	7 (10%)
19	CLA	B1	832	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	9 (11%)
19	CLA	B	805	-	64,72,73	1.47	8 (12%)	74,111,113	1.44	9 (12%)
23	BCR	I1	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.27	8 (14%)
19	CLA	B1	821	2	65,73,73	1.43	7 (10%)	76,113,113	1.37	9 (11%)
19	CLA	A1	822	-	60,68,73	1.52	8 (13%)	70,107,113	1.47	10 (14%)
19	CLA	LL	201	18	61,69,73	1.50	7 (11%)	71,108,113	1.65	11 (15%)
25	LMG	M	102	-	46,46,55	0.82	0	54,54,63	1.28	7 (12%)
26	ECH	B1	840	-	42,42,42	0.82	1 (2%)	55,58,58	2.43	19 (34%)
19	CLA	A	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.28	8 (10%)
19	CLA	BB	805	-	64,72,73	1.48	8 (12%)	74,111,113	1.43	9 (12%)
19	CLA	B	803	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
19	CLA	B	854	-	65,73,73	1.45	8 (12%)	76,113,113	1.35	4 (5%)
25	LMG	L1	210	-	55,55,55	0.68	0	63,63,63	1.28	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	X	101	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	6 (11%)
19	CLA	B1	830	-	56,64,73	1.58	5 (8%)	65,102,113	1.41	6 (9%)
23	BCR	A2	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	10 (17%)
23	BCR	K1	106	-	41,41,41	1.14	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	B2	820	-	45,53,73	1.78	7 (15%)	52,89,113	1.71	10 (19%)
19	CLA	BB	804	-	62,70,73	1.53	8 (12%)	72,109,113	1.40	10 (13%)
19	CLA	A1	821	-	51,59,73	1.67	6 (11%)	59,96,113	1.48	9 (15%)
19	CLA	A2	811	-	51,59,73	1.66	9 (17%)	59,96,113	1.55	9 (15%)
23	BCR	BB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	7 (12%)
19	CLA	BB	827	-	45,53,73	1.77	9 (20%)	52,89,113	1.49	7 (13%)
23	BCR	A	853	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	J	103	-	41,49,73	1.86	7 (17%)	47,84,113	1.52	5 (10%)
19	CLA	L1	205	10	61,69,73	1.51	6 (9%)	71,108,113	1.46	11 (15%)
19	CLA	AA	810	-	65,73,73	1.48	7 (10%)	76,113,113	1.46	12 (15%)
23	BCR	AA	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
19	CLA	A	830	-	62,70,73	1.46	7 (11%)	72,109,113	1.38	8 (11%)
22	LHG	L	207	-	33,33,48	0.94	3 (9%)	36,39,54	1.05	4 (11%)
19	CLA	AA	841	-	46,54,73	1.68	6 (13%)	53,90,113	1.55	7 (13%)
23	BCR	BB	843	-	41,41,41	1.21	4 (9%)	56,56,56	1.19	6 (10%)
19	CLA	A2	826	-	45,53,73	1.76	8 (17%)	52,89,113	1.61	8 (15%)
19	CLA	A1	839	-	56,64,73	1.56	7 (12%)	65,102,113	1.39	7 (10%)
19	CLA	A2	842	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	10 (13%)
23	BCR	L1	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	A2	813	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
19	CLA	B2	829	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
19	CLA	AA	833	-	50,58,73	1.68	8 (16%)	58,95,113	1.37	5 (8%)
19	CLA	B2	830	-	56,64,73	1.57	9 (16%)	65,102,113	1.45	9 (13%)
23	BCR	B2	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
19	CLA	B1	811	-	61,69,73	1.52	6 (9%)	71,108,113	1.28	5 (7%)
19	CLA	KK	101	-	45,53,73	1.78	6 (13%)	52,89,113	1.66	9 (17%)
23	BCR	I2	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	BB	808	-	60,68,73	1.52	7 (11%)	70,107,113	1.37	7 (10%)
22	LHG	AA	847	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
19	CLA	B	802	-	65,73,73	1.46	8 (12%)	76,113,113	1.34	8 (10%)
23	BCR	B1	838	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	B	839	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
19	CLA	B1	817	-	42,50,73	1.81	6 (14%)	48,85,113	1.58	6 (12%)
22	LHG	L1	211	-	32,32,48	0.96	3 (9%)	35,38,54	1.02	3 (8%)
19	CLA	A1	840	-	46,54,73	1.69	6 (13%)	53,90,113	1.56	6 (11%)
26	ECH	B2	841	-	42,42,42	0.80	1 (2%)	55,58,58	2.41	18 (32%)
19	CLA	BB	856	-	60,68,73	1.52	8 (13%)	70,107,113	1.70	16 (22%)
19	CLA	FF	302	-	42,50,73	1.83	6 (14%)	48,85,113	1.63	7 (14%)
19	CLA	A2	824	-	45,53,73	1.75	6 (13%)	52,89,113	1.60	8 (15%)
21	PQN	A2	843	-	34,34,34	0.63	0	42,45,45	1.09	3 (7%)
19	CLA	A1	837	1	44,52,73	1.77	6 (13%)	49,87,113	1.65	8 (16%)
22	LHG	X2	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.93	2 (4%)
19	CLA	B2	836	-	65,73,73	1.48	9 (13%)	76,113,113	1.29	6 (7%)
19	CLA	AA	837	-	45,53,73	1.79	7 (15%)	52,89,113	1.55	7 (13%)
23	BCR	A1	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
23	BCR	FF	304	-	41,41,41	1.22	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	AA	825	-	52,60,73	1.64	6 (11%)	60,97,113	1.44	7 (11%)
19	CLA	A1	832	-	50,58,73	1.68	8 (16%)	58,95,113	1.45	7 (12%)
19	CLA	A1	811	-	46,54,73	1.73	7 (15%)	53,90,113	1.54	8 (15%)
19	CLA	F1	302	-	42,50,73	1.82	7 (16%)	48,85,113	1.65	8 (16%)
19	CLA	A2	833	-	50,58,73	1.69	8 (16%)	58,95,113	1.39	8 (13%)
19	CLA	JJ	101	8	41,49,73	1.84	6 (14%)	47,84,113	1.58	7 (14%)
19	CLA	A	822	-	51,59,73	1.68	5 (9%)	59,96,113	1.48	7 (11%)
19	CLA	L1	206	-	65,73,73	1.47	8 (12%)	76,113,113	1.42	9 (11%)
19	CLA	AA	804	-	65,73,73	1.46	6 (9%)	76,113,113	1.34	7 (9%)
22	LHG	A2	846	-	37,37,48	0.82	1 (2%)	40,43,54	1.02	3 (7%)

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
19	CLA	B1	824	-	1/1/18/20	13/25/103/115	-
19	CLA	B	821	2	1/1/20/20	14/37/115/115	-
23	BCR	B1	842	-	-	16/29/63/63	0/2/2/2
19	CLA	B1	826	-	1/1/20/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A1	830	-	1/1/20/20	14/37/115/115	-
19	CLA	BB	803	-	1/1/20/20	14/37/115/115	-
19	CLA	A1	808	-	1/1/17/20	1/19/97/115	-
19	CLA	B	832	-	1/1/15/20	4/13/91/115	-
19	CLA	AA	808	-	1/1/20/20	14/37/115/115	-
23	BCR	A	851	-	-	19/29/63/63	0/2/2/2
23	BCR	A2	849	-	-	13/29/63/63	0/2/2/2
19	CLA	A	808	-	1/1/20/20	13/37/115/115	-
23	BCR	II	101	-	-	17/29/63/63	0/2/2/2
19	CLA	BB	813	-	1/1/14/20	6/10/88/115	-
19	CLA	B1	828	-	1/1/20/20	11/37/115/115	-
19	CLA	A	806	-	1/1/18/20	8/27/105/115	-
23	BCR	K2	103	-	-	12/29/63/63	0/2/2/2
23	BCR	M	101	-	-	22/29/63/63	0/2/2/2
19	CLA	B2	808	-	1/1/19/20	11/31/109/115	-
22	LHG	BB	851	-	-	20/53/53/53	-
25	LMG	B	851	-	-	17/50/70/70	0/1/1/1
19	CLA	BB	809	-	1/1/15/20	6/13/91/115	-
23	BCR	F2	304	-	-	15/29/63/63	0/2/2/2
19	CLA	A2	809	-	1/1/17/20	2/19/97/115	-
19	CLA	B2	806	2	1/1/20/20	15/37/115/115	-
23	BCR	B2	842	-	-	21/29/63/63	0/2/2/2
22	LHG	X1	102	-	-	17/44/44/53	-
19	CLA	B1	802	-	1/1/20/20	13/37/115/115	-
19	CLA	A	801	-	1/1/20/20	11/37/115/115	-
19	CLA	B2	822	-	1/1/20/20	7/37/115/115	-
19	CLA	B	860	-	1/1/20/20	15/37/115/115	-
19	CLA	A2	840	-	1/1/18/20	4/27/105/115	-
19	CLA	B2	817	-	1/1/14/20	2/10/88/115	-
19	CLA	B	835	-	1/1/15/20	1/13/91/115	-
19	CLA	B	837	-	1/1/19/20	10/31/109/115	-
23	BCR	A	850	-	-	15/29/63/63	0/2/2/2
19	CLA	A2	828	-	1/1/18/20	11/27/105/115	-
19	CLA	AA	842	-	1/1/20/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	840	-	1/1/18/20	7/27/105/115	-
19	CLA	BB	834	-	1/1/15/20	1/13/91/115	-
19	CLA	AA	838	-	1/1/14/20	4/11/90/115	-
23	BCR	J1	104	-	-	18/29/63/63	0/2/2/2
23	BCR	LL	204	-	-	18/29/63/63	0/2/2/2
19	CLA	A	842	-	1/1/20/20	11/37/115/115	-
19	CLA	B1	833	-	1/1/19/20	18/37/115/115	-
19	CLA	BB	812	-	1/1/14/20	6/8/86/115	-
19	CLA	A	838	-	1/1/14/20	5/11/90/115	-
23	BCR	JJ	104	-	-	16/29/63/63	0/2/2/2
22	LHG	A	845	-	-	19/53/53/53	-
19	CLA	A2	807	-	1/1/20/20	16/37/115/115	-
23	BCR	L1	208	-	-	17/29/63/63	0/2/2/2
19	CLA	AA	818	-	1/1/15/20	3/13/91/115	-
19	CLA	A2	802	-	1/1/15/20	9/15/93/115	-
19	CLA	B1	809	-	1/1/15/20	6/13/91/115	-
22	LHG	B1	847	-	-	14/37/37/53	-
19	CLA	A2	806	-	1/1/18/20	9/27/105/115	-
19	CLA	B1	813	-	1/1/14/20	6/10/88/115	-
19	CLA	A2	837	-	1/1/15/20	6/13/91/115	-
19	CLA	A2	822	-	1/1/17/20	5/21/99/115	-
19	CLA	B2	823	-	1/1/20/20	17/37/115/115	-
21	PQN	A1	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A1	829	-	1/1/19/20	16/34/112/115	-
19	CLA	B	830	-	1/1/18/20	4/27/105/115	-
23	BCR	AA	848	-	-	13/27/61/63	0/2/2/2
23	BCR	AA	854	-	-	18/29/63/63	0/2/2/2
19	CLA	B1	845	-	1/1/12/20	0/5/79/115	-
19	CLA	BB	824	-	1/1/18/20	12/25/103/115	-
23	BCR	J	102	-	-	19/29/63/63	0/2/2/2
23	BCR	J1	102	-	-	19/29/63/63	0/2/2/2
19	CLA	BB	826	-	1/1/20/20	17/37/115/115	-
19	CLA	A1	824	-	1/1/14/20	2/10/88/115	-
27	SF4	C2	102	-	-	-	0/6/5/5
19	CLA	A1	833	-	1/1/14/20	4/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	BB	820	-	1/1/15/20	10/13/91/115	-
19	CLA	A	813	-	1/1/20/20	9/37/115/115	-
19	CLA	B1	815	-	1/1/20/20	16/37/115/115	-
19	CLA	LL	202	-	1/1/20/20	6/37/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
22	LHG	XX	102	-	-	18/44/44/53	-
19	CLA	A2	818	-	1/1/15/20	3/13/91/115	-
19	CLA	B2	809	-	1/1/15/20	6/13/91/115	-
19	CLA	A1	809	-	1/1/20/20	11/37/115/115	-
19	CLA	LL	203	-	1/1/14/20	8/10/88/115	-
19	CLA	B2	815	-	1/1/20/20	15/37/115/115	-
22	LHG	BB	850	-	-	13/37/37/53	-
19	CLA	BB	807	-	1/1/20/20	11/37/115/115	-
27	SF4	BB	857	-	-	-	0/6/5/5
19	CLA	F	301	-	1/1/19/20	12/31/109/115	-
19	CLA	A1	828	-	1/1/20/20	20/37/115/115	-
23	BCR	B	842	-	-	18/29/63/63	0/2/2/2
19	CLA	A	811	1	1/1/17/20	6/21/99/115	-
19	CLA	AA	834	-	1/1/14/20	4/8/86/115	-
27	SF4	B1	851	-	-	-	0/6/5/5
19	CLA	B	820	-	1/1/15/20	9/13/91/115	-
19	CLA	BB	819	-	1/1/14/20	2/8/86/115	-
19	CLA	B1	836	-	1/1/19/20	10/31/109/115	-
19	CLA	A2	801	-	1/1/20/20	13/37/115/115	-
19	CLA	B2	811	-	1/1/19/20	15/33/111/115	-
19	CLA	A	824	-	1/1/15/20	9/13/91/115	-
19	CLA	B1	807	-	1/1/20/20	11/37/115/115	-
19	CLA	A1	813	-	1/1/14/20	4/10/88/115	-
23	BCR	F	303	-	-	18/29/63/63	0/2/2/2
27	SF4	C	102	3	-	-	0/6/5/5
25	LMG	B1	844	-	-	20/50/70/70	0/1/1/1
19	CLA	B1	806	-	1/1/20/20	15/37/115/115	-
19	CLA	A2	838	-	1/1/14/20	4/11/90/115	-
19	CLA	AA	813	-	1/1/20/20	9/37/115/115	-
19	CLA	B2	827	-	1/1/15/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	F1	306	-	-	25/29/63/63	0/2/2/2
19	CLA	A1	827	-	1/1/18/20	11/27/105/115	-
19	CLA	AA	827	-	1/1/20/20	16/37/115/115	-
19	CLA	A2	831	-	1/1/20/20	13/37/115/115	-
19	CLA	A2	816	-	1/1/17/20	6/19/97/115	-
19	CLA	K1	105	9	1/1/13/20	6/8/82/115	-
19	CLA	A	814	-	1/1/14/20	3/10/88/115	-
19	CLA	A1	819	-	-	9/29/107/115	-
19	CLA	AA	845	-	1/1/14/20	3/8/86/115	-
19	CLA	AA	826	-	1/1/15/20	9/13/91/115	-
23	BCR	KK	103	-	-	19/29/63/63	0/2/2/2
19	CLA	AA	820	-	1/1/18/20	11/29/107/115	-
19	CLA	B1	801	-	1/1/20/20	20/37/115/115	-
19	CLA	A2	835	-	1/1/20/20	7/37/115/115	-
19	CLA	B	834	-	1/1/19/20	18/37/115/115	-
28	DGD	B	856	-	-	22/31/71/95	0/2/2/2
20	CL0	AA	803	-	4/4/25/25	15/37/135/135	-
23	BCR	L2	207	-	-	19/29/63/63	0/2/2/2
19	CLA	BB	802	-	1/1/20/20	16/37/115/115	-
19	CLA	B	813	-	1/1/14/20	6/10/88/115	-
19	CLA	B1	848	-	1/1/20/20	16/37/115/115	-
19	CLA	A	821	-	1/1/20/20	13/37/115/115	-
21	PQN	B2	838	-	-	7/23/43/43	0/2/2/2
23	BCR	B2	839	-	-	19/29/63/63	0/2/2/2
19	CLA	B1	835	-	1/1/20/20	10/37/115/115	-
27	SF4	B2	853	-	-	-	0/6/5/5
19	CLA	AA	812	-	1/1/15/20	7/15/93/115	-
19	CLA	A1	806	-	1/1/20/20	16/37/115/115	-
19	CLA	A	837	-	1/1/15/20	4/13/91/115	-
19	CLA	A	841	-	1/1/15/20	5/15/93/115	-
19	CLA	A2	815	-	1/1/18/20	9/25/103/115	-
19	CLA	B1	831	-	1/1/15/20	6/13/91/115	-
19	CLA	B1	816	-	1/1/18/20	9/28/106/115	-
19	CLA	AA	829	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	825	-	1/1/17/20	3/22/100/115	-
19	CLA	BB	836	-	1/1/19/20	10/31/109/115	-
19	CLA	A	833	-	1/1/17/20	5/19/97/115	-
19	CLA	A	829	-	1/1/20/20	14/37/115/115	-
19	CLA	K2	102	-	1/1/15/20	1/13/91/115	-
19	CLA	J1	103	-	1/1/14/20	0/8/86/115	-
19	CLA	L1	207	-	1/1/20/20	12/37/115/115	-
19	CLA	K	102	-	1/1/15/20	11/15/93/115	-
19	CLA	B	859	-	1/1/19/20	13/31/109/115	-
19	CLA	BB	830	-	1/1/18/20	8/27/105/115	-
19	CLA	J	101	8	1/1/14/20	3/8/86/115	-
19	CLA	A1	814	-	1/1/18/20	9/25/103/115	-
19	CLA	B2	819	-	1/1/14/20	3/8/86/115	-
19	CLA	A	828	-	1/1/18/20	11/27/105/115	-
19	CLA	A2	841	-	1/1/15/20	6/15/93/115	-
19	CLA	A	835	-	1/1/20/20	8/37/115/115	-
28	DGD	BB	854	-	-	21/31/71/95	0/2/2/2
19	CLA	K1	103	-	1/1/15/20	8/15/93/115	-
19	CLA	A2	825	-	1/1/14/20	3/10/88/115	-
19	CLA	A1	823	-	1/1/15/20	6/13/91/115	-
19	CLA	A1	831	-	1/1/20/20	8/37/115/115	-
19	CLA	A2	810	1	1/1/20/20	10/37/115/115	-
19	CLA	BB	852	-	1/1/20/20	13/37/115/115	-
19	CLA	A1	818	-	1/1/19/20	13/31/109/115	-
19	CLA	F	302	-	1/1/14/20	4/10/88/115	-
23	BCR	B2	843	-	-	18/29/63/63	0/2/2/2
19	CLA	A1	807	-	1/1/20/20	14/37/115/115	-
23	BCR	F2	303	-	-	21/29/63/63	0/2/2/2
19	CLA	B2	821	-	1/1/20/20	14/37/115/115	-
19	CLA	BB	832	-	-	12/37/115/115	-
19	CLA	B	814	-	1/1/18/20	10/30/108/115	-
23	BCR	B1	843	-	-	13/29/63/63	0/2/2/2
19	CLA	X2	101	-	1/1/15/20	4/13/91/115	-
19	CLA	AA	807	-	1/1/20/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	843	-	1/1/20/20	15/37/115/115	-
23	BCR	B1	841	-	-	20/29/63/63	0/2/2/2
19	CLA	A	804	-	1/1/20/20	17/37/115/115	-
19	CLA	AA	805	-	1/1/19/20	8/31/109/115	-
19	CLA	BB	818	-	1/1/14/20	2/8/86/115	-
25	LMG	B1	852	-	-	5/25/45/70	0/1/1/1
23	BCR	A1	851	-	-	19/29/63/63	0/2/2/2
19	CLA	AA	819	-	1/1/19/20	13/31/109/115	-
19	CLA	BB	814	-	1/1/18/20	11/30/108/115	-
23	BCR	I2	103	-	-	18/29/63/63	0/2/2/2
19	CLA	A	819	-	1/1/19/20	11/31/109/115	-
25	LMG	B2	854	-	-	5/25/45/70	0/1/1/1
27	SF4	C1	101	-	-	-	0/6/5/5
20	CL0	A2	803	-	4/4/25/25	16/37/135/135	-
19	CLA	L2	206	-	1/1/20/20	14/37/115/115	-
19	CLA	B	810	-	1/1/20/20	15/37/115/115	-
19	CLA	AA	836	-	1/1/20/20	16/37/115/115	-
19	CLA	AA	853	-	1/1/20/20	18/37/115/115	-
19	CLA	BB	823	-	1/1/20/20	14/37/115/115	-
19	CLA	A	836	-	1/1/20/20	13/37/115/115	-
19	CLA	B2	803	-	1/1/20/20	13/37/115/115	-
19	CLA	B	807	-	1/1/20/20	11/37/115/115	-
19	CLA	BB	835	-	1/1/20/20	9/37/115/115	-
27	SF4	C2	101	-	-	-	0/6/5/5
19	CLA	BB	821	-	1/1/20/20	17/37/115/115	-
19	CLA	A2	852	-	1/1/20/20	13/37/115/115	-
19	CLA	AA	830	-	1/1/19/20	14/34/112/115	-
19	CLA	B2	835	-	1/1/15/20	2/13/91/115	-
19	CLA	B1	849	-	1/1/20/20	4/37/115/115	-
19	CLA	A1	835	-	1/1/20/20	11/37/115/115	-
23	BCR	I2	101	-	-	17/29/63/63	0/2/2/2
23	BCR	J2	102	-	-	18/29/63/63	0/2/2/2
19	CLA	A2	804	-	1/1/20/20	19/37/115/115	-
19	CLA	A2	844	-	1/1/14/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A2	847	-	-	12/27/61/63	0/2/2/2
23	BCR	A	849	-	-	18/29/63/63	0/2/2/2
23	BCR	A2	853	-	-	17/29/63/63	0/2/2/2
19	CLA	B1	820	-	1/1/15/20	9/13/91/115	-
25	LMG	B2	845	-	-	21/50/70/70	0/1/1/1
27	SF4	CC	102	-	-	-	0/6/5/5
23	BCR	II	104	-	-	18/29/63/63	0/2/2/2
19	CLA	B	828	-	1/1/15/20	4/13/91/115	-
23	BCR	A	848	-	-	18/29/63/63	0/2/2/2
19	CLA	B2	801	-	1/1/20/20	18/37/115/115	-
19	CLA	B2	846	-	1/1/12/20	0/5/79/115	-
19	CLA	B1	834	-	1/1/15/20	1/13/91/115	-
19	CLA	B1	810	-	1/1/20/20	16/37/115/115	-
23	BCR	FF	306	-	-	22/29/63/63	0/2/2/2
19	CLA	B	816	-	1/1/18/20	9/28/106/115	-
19	CLA	B1	804	-	1/1/19/20	10/34/112/115	-
19	CLA	B	829	-	1/1/20/20	14/37/115/115	-
23	BCR	MM	101	-	-	23/29/63/63	0/2/2/2
19	CLA	A1	815	-	1/1/17/20	9/19/97/115	-
19	CLA	AA	839	-	1/1/17/20	8/22/100/115	-
19	CLA	A2	808	-	1/1/20/20	15/37/115/115	-
19	CLA	AA	814	-	1/1/14/20	3/10/88/115	-
23	BCR	AA	852	-	-	19/29/63/63	0/2/2/2
19	CLA	B2	813	-	1/1/14/20	6/10/88/115	-
19	CLA	A2	834	-	1/1/14/20	4/8/86/115	-
23	BCR	JJ	102	-	-	20/29/63/63	0/2/2/2
23	BCR	A2	848	-	-	15/29/63/63	0/2/2/2
19	CLA	XX	101	-	1/1/15/20	7/13/91/115	-
22	LHG	LL	205	-	-	13/38/38/53	-
22	LHG	X	102	-	-	19/44/44/53	-
19	CLA	AA	823	-	1/1/19/20	13/31/109/115	-
22	LHG	L2	208	-	-	17/39/39/53	-
19	CLA	BB	815	-	1/1/20/20	17/37/115/115	-
19	CLA	A	834	-	1/1/14/20	4/8/86/115	-
19	CLA	A1	810	-	1/1/17/20	7/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A2	817	-	1/1/14/20	1/11/90/115	-
19	CLA	AA	821	-	1/1/20/20	15/37/115/115	-
19	CLA	A1	852	-	1/1/20/20	18/37/115/115	-
19	CLA	A1	841	-	1/1/20/20	9/37/115/115	-
19	CLA	B	836	-	1/1/20/20	9/37/115/115	-
19	CLA	A1	844	-	1/1/14/20	3/8/86/115	-
19	CLA	B	808	-	1/1/19/20	10/31/109/115	-
26	ECH	B	841	-	-	16/29/66/66	0/2/2/2
23	BCR	A1	853	-	-	16/29/63/63	0/2/2/2
22	LHG	X2	103	-	-	22/53/53/53	-
23	BCR	AA	851	-	-	15/29/63/63	0/2/2/2
19	CLA	AA	832	-	1/1/20/20	6/37/115/115	-
23	BCR	A1	849	-	-	13/29/63/63	0/2/2/2
19	CLA	B1	850	-	1/1/19/20	11/31/109/115	-
19	CLA	B1	808	-	1/1/19/20	11/31/109/115	-
19	CLA	B2	849	-	1/1/20/20	14/37/115/115	-
19	CLA	A	832	-	1/1/20/20	9/37/115/115	-
19	CLA	B	811	-	1/1/19/20	16/33/111/115	-
23	BCR	B2	844	-	-	13/29/63/63	0/2/2/2
19	CLA	A1	826	-	1/1/20/20	14/37/115/115	-
22	LHG	B	852	-	-	14/37/37/53	-
19	CLA	B1	822	-	1/1/20/20	2/37/115/115	-
19	CLA	A1	820	-	1/1/20/20	18/37/115/115	-
23	BCR	A2	850	-	-	13/29/63/63	0/2/2/2
19	CLA	K	101	-	1/1/15/20	1/13/91/115	-
19	CLA	L2	204	16	1/1/19/20	16/33/111/115	-
23	BCR	A1	850	-	-	14/29/63/63	0/2/2/2
25	LMG	B2	847	-	-	9/27/47/70	0/1/1/1
23	BCR	AA	850	-	-	16/29/63/63	0/2/2/2
19	CLA	J2	103	-	1/1/14/20	0/8/86/115	-
23	BCR	FF	303	-	-	19/29/63/63	0/2/2/2
19	CLA	L	204	-	1/1/20/20	17/37/115/115	-
19	CLA	B2	834	-	1/1/19/20	20/37/115/115	-
21	PQN	AA	844	-	-	4/23/43/43	0/2/2/2
19	CLA	A1	834	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	812	-	1/1/14/20	4/8/86/115	-
23	BCR	F	304	-	-	15/29/63/63	0/2/2/2
19	CLA	A	812	-	1/1/15/20	7/15/93/115	-
19	CLA	BB	829	-	1/1/18/20	7/27/105/115	-
23	BCR	B	844	-	-	15/29/63/63	0/2/2/2
19	CLA	B2	828	-	1/1/15/20	1/13/91/115	-
19	CLA	AA	815	-	1/1/18/20	9/25/103/115	-
19	CLA	B	818	-	1/1/14/20	4/8/86/115	-
25	LMG	B	845	-	-	21/50/70/70	0/1/1/1
19	CLA	J2	101	8	1/1/14/20	3/8/86/115	-
19	CLA	AA	809	-	1/1/17/20	2/19/97/115	-
23	BCR	L1	209	-	-	18/29/63/63	0/2/2/2
25	LMG	I1	102	-	-	18/30/50/70	0/1/1/1
19	CLA	A	826	-	1/1/15/20	9/13/91/115	-
19	CLA	A	820	-	-	11/29/107/115	-
25	LMG	B1	846	-	-	10/27/47/70	0/1/1/1
23	BCR	F2	305	-	-	26/29/63/63	0/2/2/2
19	CLA	A	840	-	1/1/18/20	5/27/105/115	-
19	CLA	L	203	-	1/1/20/20	6/37/115/115	-
19	CLA	A2	812	-	1/1/15/20	5/15/93/115	-
19	CLA	B2	826	-	1/1/20/20	16/37/115/115	-
23	BCR	AA	855	-	-	18/29/63/63	0/2/2/2
19	CLA	F2	301	-	1/1/19/20	10/31/109/115	-
19	CLA	A	818	-	1/1/15/20	3/13/91/115	-
23	BCR	A	854	-	-	18/29/63/63	0/2/2/2
19	CLA	B	804	-	1/1/19/20	8/34/112/115	-
19	CLA	L2	205	-	1/1/18/20	6/30/108/115	-
19	CLA	B	833	-	-	12/37/115/115	-
27	SF4	B	861	-	-	-	0/6/5/5
19	CLA	B2	818	-	1/1/14/20	2/8/86/115	-
22	LHG	AA	846	-	-	19/53/53/53	-
19	CLA	B2	807	-	1/1/20/20	14/37/115/115	-
19	CLA	B1	823	-	1/1/20/20	16/37/115/115	-
19	CLA	B	809	-	1/1/15/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	850	-	1/1/20/20	4/37/115/115	-
22	LHG	A	846	-	-	12/42/42/53	-
21	PQN	A	843	-	-	8/23/43/43	0/2/2/2
19	CLA	B1	812	-	1/1/14/20	6/8/86/115	-
19	CLA	B1	818	-	1/1/14/20	2/8/86/115	-
19	CLA	K2	104	-	1/1/13/20	4/7/81/115	-
21	PQN	B1	837	-	-	7/23/43/43	0/2/2/2
19	CLA	AA	824	-	1/1/15/20	9/13/91/115	-
19	CLA	A2	820	-	1/1/18/20	11/29/107/115	-
19	CLA	B2	824	-	1/1/18/20	13/25/103/115	-
27	SF4	C1	102	-	-	-	0/6/5/5
23	BCR	BB	839	-	-	9/29/63/63	0/2/2/2
19	CLA	B	846	-	1/1/12/20	1/5/79/115	-
19	CLA	A1	801	-	1/1/20/20	13/37/115/115	-
19	CLA	FF	305	-	1/1/20/20	11/37/115/115	-
23	BCR	F1	304	-	-	15/29/63/63	0/2/2/2
19	CLA	BB	810	-	1/1/20/20	16/37/115/115	-
23	BCR	K2	105	-	-	17/29/63/63	0/2/2/2
19	CLA	X1	101	-	1/1/15/20	4/13/91/115	-
19	CLA	B	815	-	1/1/20/20	18/37/115/115	-
19	CLA	B2	814	-	1/1/18/20	12/30/108/115	-
19	CLA	B	827	-	1/1/15/20	8/13/91/115	-
19	CLA	A2	829	-	1/1/20/20	17/37/115/115	-
19	CLA	A1	838	-	1/1/17/20	8/22/100/115	-
19	CLA	A1	825	-	1/1/15/20	9/13/91/115	-
19	CLA	A	831	-	1/1/20/20	13/37/115/115	-
25	LMG	I2	105	-	-	10/29/49/70	0/1/1/1
19	CLA	A1	812	-	1/1/20/20	9/37/115/115	-
19	CLA	BB	806	-	1/1/20/20	15/37/115/115	-
19	CLA	A1	816	-	1/1/14/20	2/11/90/115	-
23	BCR	BB	838	-	-	15/29/63/63	0/2/2/2
23	BCR	F	305	-	-	23/29/63/63	0/2/2/2
19	CLA	A1	803	-	1/1/20/20	17/37/115/115	-
23	BCR	B	843	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	828	-	1/1/18/20	11/27/105/115	-
19	CLA	BB	822	-	1/1/20/20	8/37/115/115	-
19	CLA	B2	802	-	1/1/20/20	9/37/115/115	-
19	CLA	AA	835	-	1/1/20/20	8/37/115/115	-
19	CLA	B2	837	-	1/1/19/20	10/31/109/115	-
19	CLA	BB	828	-	1/1/15/20	1/13/91/115	-
19	CLA	BB	801	-	1/1/20/20	21/37/115/115	-
19	CLA	B	825	-	1/1/20/20	20/37/115/115	-
19	CLA	B2	825	-	1/1/20/20	20/37/115/115	-
19	CLA	B2	833	-	-	11/37/115/115	-
22	LHG	A2	845	-	-	16/53/53/53	-
23	BCR	I	102	-	-	10/29/63/63	0/2/2/2
19	CLA	BB	816	-	1/1/18/20	8/28/106/115	-
19	CLA	B	806	-	1/1/20/20	15/37/115/115	-
19	CLA	BB	825	-	1/1/20/20	20/37/115/115	-
23	BCR	B	848	-	-	16/29/63/63	0/2/2/2
19	CLA	JJ	103	-	1/1/14/20	0/8/86/115	-
19	CLA	A2	805	-	1/1/19/20	8/31/109/115	-
22	LHG	B	853	-	-	23/53/53/53	-
20	CL0	A1	802	-	4/4/25/25	13/37/135/135	-
19	CLA	BB	831	-	1/1/15/20	4/13/91/115	-
23	BCR	J2	104	-	-	16/29/63/63	0/2/2/2
19	CLA	FF	301	-	1/1/19/20	13/31/109/115	-
19	CLA	B2	831	-	1/1/18/20	9/27/105/115	-
23	BCR	II	102	-	-	9/29/63/63	0/2/2/2
23	BCR	B	840	-	-	9/29/63/63	0/2/2/2
19	CLA	A	817	-	1/1/14/20	3/11/90/115	-
19	CLA	B1	829	-	1/1/18/20	5/27/105/115	-
19	CLA	A1	817	-	1/1/15/20	3/13/91/115	-
19	CLA	B1	805	-	1/1/19/20	9/36/114/115	-
19	CLA	A2	819	-	1/1/19/20	9/31/109/115	-
21	PQN	BB	837	-	-	7/23/43/43	0/2/2/2
19	CLA	AA	806	-	1/1/18/20	8/27/105/115	-
19	CLA	B	823	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	801	-	1/1/20/20	17/37/115/115	-
19	CLA	A	809	-	1/1/17/20	2/19/97/115	-
19	CLA	B	831	-	1/1/18/20	5/27/105/115	-
19	CLA	AA	822	-	-	8/21/99/115	-
23	BCR	J	104	-	-	16/29/63/63	0/2/2/2
19	CLA	B2	804	-	1/1/19/20	10/34/112/115	-
23	BCR	L	205	-	-	17/29/63/63	0/2/2/2
23	BCR	K	103	-	-	19/29/63/63	0/2/2/2
25	LMG	II	105	-	-	20/37/57/70	0/1/1/1
19	CLA	B1	803	-	1/1/20/20	13/37/115/115	-
19	CLA	B	819	-	1/1/14/20	2/8/86/115	-
19	CLA	B1	819	-	1/1/14/20	3/8/86/115	-
19	CLA	AA	801	-	1/1/20/20	13/37/115/115	-
23	BCR	I	101	-	-	20/29/63/63	0/2/2/2
19	CLA	A1	842	-	1/1/20/20	15/37/115/115	-
19	CLA	BB	855	-	1/1/20/20	6/37/115/115	-
19	CLA	A	823	-	1/1/19/20	14/31/109/115	-
19	CLA	B	812	-	1/1/14/20	4/8/86/115	-
20	CL0	A	803	-	4/4/25/25	18/37/135/135	-
22	LHG	A1	845	-	-	20/53/53/53	-
23	BCR	BB	842	-	-	16/29/63/63	0/2/2/2
19	CLA	BB	811	-	1/1/19/20	18/33/111/115	-
19	CLA	AA	816	-	1/1/17/20	9/19/97/115	-
23	BCR	M1	101	-	-	17/29/63/63	0/2/2/2
19	CLA	A1	836	-	1/1/15/20	6/13/91/115	-
26	ECH	BB	840	-	-	16/29/66/66	0/2/2/2
22	LHG	X1	103	-	-	20/53/53/53	-
19	CLA	A	816	-	1/1/17/20	7/19/97/115	-
19	CLA	B2	851	-	1/1/19/20	11/31/109/115	-
19	CLA	A	805	-	1/1/19/20	8/31/109/115	-
19	CLA	A	810	1	1/1/20/20	11/37/115/115	-
19	CLA	A1	805	-	-	6/27/105/115	-
19	CLA	J1	101	-	1/1/13/20	3/8/86/115	-
19	CLA	A2	827	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	852	-	1/1/20/20	16/37/115/115	-
19	CLA	BB	817	-	1/1/14/20	1/10/88/115	-
19	CLA	BB	833	-	1/1/19/20	16/37/115/115	-
19	CLA	AA	831	-	1/1/20/20	14/37/115/115	-
19	CLA	F2	302	-	1/1/14/20	4/10/88/115	-
19	CLA	B2	810	-	1/1/20/20	17/37/115/115	-
19	CLA	B	822	-	1/1/20/20	4/37/115/115	-
23	BCR	A	847	-	-	14/27/61/63	0/2/2/2
19	CLA	A2	839	-	1/1/17/20	8/22/100/115	-
23	BCR	M2	102	-	-	19/29/63/63	0/2/2/2
19	CLA	F1	305	-	1/1/15/20	4/13/91/115	-
19	CLA	B2	852	-	1/1/20/20	15/37/115/115	-
23	BCR	B1	839	-	-	9/29/63/63	0/2/2/2
19	CLA	A2	814	-	1/1/14/20	4/10/88/115	-
19	CLA	KK	102	-	1/1/15/20	10/15/93/115	-
23	BCR	A1	847	-	-	12/27/61/63	0/2/2/2
19	CLA	L	202	18	1/1/19/20	14/33/111/115	-
23	BCR	BB	841	-	-	20/29/63/63	0/2/2/2
19	CLA	B2	832	-	1/1/15/20	6/13/91/115	-
19	CLA	A2	823	-	1/1/19/20	12/31/109/115	-
19	CLA	B	817	-	1/1/14/20	4/10/88/115	-
19	CLA	B1	827	-	1/1/15/20	6/13/91/115	-
19	CLA	A2	821	-	1/1/20/20	13/37/115/115	-
22	LHG	B2	848	-	-	8/37/37/53	-
25	LMG	BB	844	-	-	18/50/70/70	0/1/1/1
19	CLA	A	844	-	1/1/14/20	4/8/86/115	-
19	CLA	B	858	-	1/1/20/20	5/37/115/115	-
19	CLA	A2	836	-	-	14/37/115/115	-
23	BCR	L	206	-	-	18/29/63/63	0/2/2/2
19	CLA	A2	832	-	1/1/20/20	6/37/115/115	-
23	BCR	K1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	B1	814	-	1/1/18/20	12/30/108/115	-
19	CLA	B2	816	-	1/1/18/20	8/28/106/115	-
19	CLA	B2	805	-	1/1/19/20	9/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	815	-	1/1/18/20	9/25/103/115	-
19	CLA	F1	301	-	1/1/19/20	10/31/109/115	-
27	SF4	CC	101	-	-	-	0/6/5/5
19	CLA	A	827	-	1/1/20/20	16/37/115/115	-
19	CLA	B	824	-	1/1/18/20	12/25/103/115	-
19	CLA	AA	811	1	1/1/17/20	6/21/99/115	-
22	LHG	A1	846	-	-	12/42/42/53	-
19	CLA	K1	102	-	1/1/15/20	1/13/91/115	-
19	CLA	B	826	-	1/1/20/20	14/37/115/115	-
21	PQN	B	838	-	-	7/23/43/43	0/2/2/2
19	CLA	A	839	-	1/1/17/20	8/22/100/115	-
19	CLA	A2	830	-	1/1/19/20	18/34/112/115	-
23	BCR	F1	303	-	-	17/29/63/63	0/2/2/2
19	CLA	BB	845	-	1/1/12/20	1/5/79/115	-
19	CLA	AA	817	-	1/1/14/20	2/11/90/115	-
19	CLA	B1	825	-	1/1/20/20	18/37/115/115	-
19	CLA	A1	804	-	1/1/19/20	9/31/109/115	-
19	CLA	B1	832	-	1/1/20/20	12/37/115/115	-
19	CLA	B	805	-	1/1/19/20	9/36/114/115	-
23	BCR	I1	101	-	-	17/29/63/63	0/2/2/2
19	CLA	B1	821	2	1/1/20/20	14/37/115/115	-
19	CLA	A1	822	-	1/1/19/20	15/31/109/115	-
19	CLA	LL	201	18	1/1/19/20	13/33/111/115	-
25	LMG	M	102	-	-	15/41/61/70	0/1/1/1
26	ECH	B1	840	-	-	16/29/66/66	0/2/2/2
19	CLA	A	807	-	1/1/20/20	17/37/115/115	-
19	CLA	BB	805	-	1/1/19/20	9/36/114/115	-
19	CLA	B	803	-	1/1/20/20	13/37/115/115	-
19	CLA	B	854	-	1/1/20/20	13/37/115/115	-
25	LMG	L1	210	-	-	16/50/70/70	0/1/1/1
19	CLA	X	101	-	1/1/15/20	3/13/91/115	-
19	CLA	B1	830	-	1/1/18/20	8/27/105/115	-
23	BCR	A2	851	-	-	17/29/63/63	0/2/2/2
23	BCR	K1	106	-	-	18/29/63/63	0/2/2/2
19	CLA	B2	820	-	1/1/15/20	10/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	BB	804	-	1/1/19/20	9/34/112/115	-
19	CLA	A1	821	-	1/1/17/20	4/21/99/115	-
19	CLA	A2	811	-	1/1/17/20	6/21/99/115	-
23	BCR	BB	847	-	-	17/29/63/63	0/2/2/2
19	CLA	BB	827	-	1/1/15/20	2/13/91/115	-
23	BCR	A	853	-	-	18/29/63/63	0/2/2/2
19	CLA	J	103	-	-	6/8/86/115	-
19	CLA	L1	205	10	1/1/19/20	11/33/111/115	-
19	CLA	AA	810	-	1/1/20/20	10/37/115/115	-
23	BCR	AA	849	-	-	18/29/63/63	0/2/2/2
19	CLA	A	830	-	1/1/19/20	15/34/112/115	-
22	LHG	L	207	-	-	13/38/38/53	-
19	CLA	AA	841	-	1/1/15/20	5/15/93/115	-
23	BCR	BB	843	-	-	13/29/63/63	0/2/2/2
19	CLA	A2	826	-	1/1/15/20	9/13/91/115	-
19	CLA	A1	839	-	1/1/18/20	7/27/105/115	-
19	CLA	A2	842	-	1/1/20/20	10/37/115/115	-
23	BCR	L1	201	-	-	12/29/63/63	0/2/2/2
19	CLA	A2	813	-	1/1/20/20	11/37/115/115	-
19	CLA	B2	829	-	1/1/20/20	13/37/115/115	-
19	CLA	AA	833	-	1/1/17/20	4/19/97/115	-
19	CLA	B2	830	-	1/1/18/20	4/27/105/115	-
23	BCR	B2	840	-	-	8/29/63/63	0/2/2/2
19	CLA	B1	811	-	1/1/19/20	15/33/111/115	-
19	CLA	KK	101	-	1/1/15/20	1/13/91/115	-
23	BCR	I2	102	-	-	11/29/63/63	0/2/2/2
19	CLA	BB	808	-	1/1/19/20	13/31/109/115	-
22	LHG	AA	847	-	-	12/42/42/53	-
19	CLA	B	802	-	1/1/20/20	11/37/115/115	-
23	BCR	B1	838	-	-	19/29/63/63	0/2/2/2
23	BCR	B	839	-	-	16/29/63/63	0/2/2/2
19	CLA	B1	817	-	1/1/14/20	2/10/88/115	-
22	LHG	L1	211	-	-	14/37/37/53	-
19	CLA	A1	840	-	1/1/15/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	ECH	B2	841	-	-	16/29/66/66	0/2/2/2
19	CLA	BB	856	-	1/1/19/20	13/31/109/115	-
19	CLA	FF	302	-	1/1/14/20	4/10/88/115	-
19	CLA	A2	824	-	1/1/15/20	4/13/91/115	-
21	PQN	A2	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A1	837	1	1/1/14/20	4/11/90/115	-
22	LHG	X2	102	-	-	15/44/44/53	-
19	CLA	B2	836	-	1/1/20/20	11/37/115/115	-
19	CLA	AA	837	-	1/1/15/20	0/13/91/115	-
23	BCR	A1	848	-	-	14/29/63/63	0/2/2/2
23	BCR	FF	304	-	-	14/29/63/63	0/2/2/2
19	CLA	AA	825	-	1/1/17/20	2/22/100/115	-
19	CLA	A1	832	-	1/1/17/20	9/19/97/115	-
19	CLA	A1	811	-	1/1/15/20	5/15/93/115	-
19	CLA	F1	302	-	1/1/14/20	4/10/88/115	-
19	CLA	A2	833	-	1/1/17/20	5/19/97/115	-
19	CLA	JJ	101	8	1/1/14/20	3/8/86/115	-
19	CLA	A	822	-	1/1/17/20	7/21/99/115	-
19	CLA	L1	206	-	1/1/20/20	3/37/115/115	-
19	CLA	AA	804	-	1/1/20/20	16/37/115/115	-
22	LHG	A2	846	-	-	12/42/42/53	-

All (2929) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	818	CLA	C4B-NB	8.40	1.42	1.35
19	BB	826	CLA	C4B-NB	8.11	1.42	1.35
19	B2	826	CLA	C4B-NB	8.00	1.42	1.35
19	B1	826	CLA	C4B-NB	7.89	1.42	1.35
19	BB	822	CLA	C4B-NB	7.71	1.42	1.35
19	B	826	CLA	C4B-NB	7.69	1.42	1.35
19	A1	805	CLA	C4B-NB	7.61	1.42	1.35
19	F2	301	CLA	C4B-NB	7.61	1.42	1.35
19	F1	301	CLA	C4B-NB	7.60	1.42	1.35
19	J2	103	CLA	C4B-NB	7.59	1.42	1.35
19	B1	818	CLA	C4B-NB	7.59	1.42	1.35
19	J1	103	CLA	C4B-NB	7.58	1.42	1.35
19	X2	101	CLA	C4B-NB	7.57	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	818	CLA	C4B-NB	7.55	1.41	1.35
19	F2	302	CLA	C4B-NB	7.54	1.41	1.35
19	B	829	CLA	C4B-NB	7.53	1.41	1.35
19	FF	302	CLA	C4B-NB	7.52	1.41	1.35
19	B2	829	CLA	C4B-NB	7.51	1.41	1.35
19	B1	828	CLA	C4B-NB	7.51	1.41	1.35
19	F	302	CLA	C4B-NB	7.50	1.41	1.35
19	J	103	CLA	C4B-NB	7.49	1.41	1.35
19	AA	822	CLA	C4B-NB	7.49	1.41	1.35
19	L2	206	CLA	C4B-NB	7.48	1.41	1.35
19	B2	823	CLA	C4B-NB	7.48	1.41	1.35
19	A2	806	CLA	C4B-NB	7.48	1.41	1.35
19	A2	814	CLA	C4B-NB	7.48	1.41	1.35
19	A	814	CLA	C4B-NB	7.48	1.41	1.35
19	F	301	CLA	C4B-NB	7.48	1.41	1.35
19	BB	832	CLA	C4B-NB	7.47	1.41	1.35
19	A1	813	CLA	C4B-NB	7.47	1.41	1.35
19	FF	305	CLA	C4B-NB	7.45	1.41	1.35
19	BB	804	CLA	C4B-NB	7.45	1.41	1.35
19	B	837	CLA	C4B-NB	7.44	1.41	1.35
19	F1	302	CLA	C4B-NB	7.43	1.41	1.35
19	A1	836	CLA	C4B-NB	7.43	1.41	1.35
19	X1	101	CLA	C4B-NB	7.43	1.41	1.35
19	AA	806	CLA	C4B-NB	7.43	1.41	1.35
19	JJ	103	CLA	C4B-NB	7.42	1.41	1.35
19	A	827	CLA	C4B-NB	7.42	1.41	1.35
19	AA	817	CLA	C4B-NB	7.41	1.41	1.35
19	A	817	CLA	C4B-NB	7.39	1.41	1.35
19	A	837	CLA	C4B-NB	7.39	1.41	1.35
19	AA	837	CLA	C4B-NB	7.39	1.41	1.35
19	JJ	101	CLA	C4B-NB	7.39	1.41	1.35
19	A	806	CLA	C4B-NB	7.39	1.41	1.35
19	A	810	CLA	C4B-NB	7.39	1.41	1.35
19	AA	810	CLA	C4B-NB	7.38	1.41	1.35
19	B2	816	CLA	C4B-NB	7.38	1.41	1.35
19	B1	823	CLA	C4B-NB	7.38	1.41	1.35
19	B	804	CLA	C4B-NB	7.38	1.41	1.35
19	B1	816	CLA	C4B-NB	7.37	1.41	1.35
19	A1	816	CLA	C4B-NB	7.37	1.41	1.35
19	A2	817	CLA	C4B-NB	7.37	1.41	1.35
19	B2	833	CLA	C4B-NB	7.36	1.41	1.35
19	J1	101	CLA	C4B-NB	7.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J2	101	CLA	C4B-NB	7.36	1.41	1.35
19	A	822	CLA	C4B-NB	7.36	1.41	1.35
19	X	101	CLA	C4B-NB	7.35	1.41	1.35
19	AA	814	CLA	C4B-NB	7.35	1.41	1.35
19	B1	820	CLA	C4B-NB	7.35	1.41	1.35
19	A2	818	CLA	C4B-NB	7.35	1.41	1.35
19	B1	809	CLA	C4B-NB	7.35	1.41	1.35
19	A2	837	CLA	C4B-NB	7.35	1.41	1.35
19	A	824	CLA	C4B-NB	7.35	1.41	1.35
19	B1	831	CLA	C4B-NB	7.34	1.41	1.35
19	B2	817	CLA	C4B-NB	7.34	1.41	1.35
19	J	101	CLA	C4B-NB	7.34	1.41	1.35
19	B1	822	CLA	C4B-NB	7.34	1.41	1.35
19	B1	807	CLA	C4B-NB	7.33	1.41	1.35
19	B2	809	CLA	C4B-NB	7.33	1.41	1.35
19	B2	811	CLA	C4B-NB	7.33	1.41	1.35
19	AA	825	CLA	C4B-NB	7.33	1.41	1.35
19	B1	817	CLA	C4B-NB	7.32	1.41	1.35
19	A	825	CLA	C4B-NB	7.32	1.41	1.35
19	AA	827	CLA	C4B-NB	7.31	1.41	1.35
19	AA	838	CLA	C4B-NB	7.31	1.41	1.35
19	B2	804	CLA	C4B-NB	7.31	1.41	1.35
19	B	807	CLA	C4B-NB	7.31	1.41	1.35
19	K1	105	CLA	C4B-NB	7.31	1.41	1.35
19	B2	827	CLA	C4B-NB	7.31	1.41	1.35
19	AA	824	CLA	C4B-NB	7.31	1.41	1.35
19	B2	846	CLA	C4B-NB	7.30	1.41	1.35
19	A2	825	CLA	C4B-NB	7.30	1.41	1.35
19	A	818	CLA	C4B-NB	7.30	1.41	1.35
19	A1	817	CLA	C4B-NB	7.30	1.41	1.35
19	BB	823	CLA	C4B-NB	7.30	1.41	1.35
19	A1	837	CLA	C4B-NB	7.30	1.41	1.35
19	A2	822	CLA	C4B-NB	7.29	1.41	1.35
19	XX	101	CLA	C4B-NB	7.29	1.41	1.35
19	A1	812	CLA	C4B-NB	7.29	1.41	1.35
19	B1	845	CLA	C4B-NB	7.29	1.41	1.35
19	B1	827	CLA	C4B-NB	7.29	1.41	1.35
19	B1	804	CLA	C4B-NB	7.29	1.41	1.35
19	AA	818	CLA	C4B-NB	7.29	1.41	1.35
19	AA	842	CLA	C4B-NB	7.29	1.41	1.35
19	L1	207	CLA	C4B-NB	7.29	1.41	1.35
19	A	838	CLA	C4B-NB	7.28	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	101	CLA	C4B-NB	7.28	1.41	1.35
19	LL	203	CLA	C4B-NB	7.28	1.41	1.35
19	A2	838	CLA	C4B-NB	7.28	1.41	1.35
19	A1	834	CLA	C4B-NB	7.28	1.41	1.35
19	KK	101	CLA	C4B-NB	7.28	1.41	1.35
19	A2	802	CLA	C4B-NB	7.28	1.41	1.35
19	BB	807	CLA	C4B-NB	7.28	1.41	1.35
19	B1	819	CLA	C4B-NB	7.28	1.41	1.35
19	B	823	CLA	C4B-NB	7.28	1.41	1.35
19	BB	813	CLA	C4B-NB	7.27	1.41	1.35
19	B1	811	CLA	C4B-NB	7.27	1.41	1.35
19	K1	103	CLA	C4B-NB	7.27	1.41	1.35
19	AA	819	CLA	C4B-NB	7.27	1.41	1.35
19	B2	814	CLA	C4B-NB	7.27	1.41	1.35
19	A1	821	CLA	C4B-NB	7.27	1.41	1.35
19	A1	809	CLA	C4B-NB	7.27	1.41	1.35
19	F1	305	CLA	C4B-NB	7.27	1.41	1.35
19	B2	813	CLA	C4B-NB	7.26	1.41	1.35
19	AA	833	CLA	C4B-NB	7.26	1.41	1.35
19	A2	835	CLA	C4B-NB	7.26	1.41	1.35
19	A1	835	CLA	C4B-NB	7.26	1.41	1.35
19	BB	811	CLA	C4B-NB	7.26	1.41	1.35
19	A1	832	CLA	C4B-NB	7.26	1.41	1.35
19	A2	833	CLA	C4B-NB	7.26	1.41	1.35
19	FF	301	CLA	C4B-NB	7.26	1.41	1.35
19	A1	818	CLA	C4B-NB	7.26	1.41	1.35
19	K2	104	CLA	C4B-NB	7.26	1.41	1.35
19	K	102	CLA	C4B-NB	7.26	1.41	1.35
19	A1	831	CLA	C4B-NB	7.25	1.41	1.35
19	A2	819	CLA	C4B-NB	7.25	1.41	1.35
19	B2	801	CLA	C4B-NB	7.25	1.41	1.35
19	AA	808	CLA	C4B-NB	7.25	1.41	1.35
19	A1	824	CLA	C4B-NB	7.24	1.41	1.35
19	B2	807	CLA	C4B-NB	7.24	1.41	1.35
19	BB	845	CLA	C4B-NB	7.24	1.41	1.35
19	A2	813	CLA	C4B-NB	7.24	1.41	1.35
19	B2	832	CLA	C4B-NB	7.24	1.41	1.35
19	A	833	CLA	C4B-NB	7.24	1.41	1.35
19	BB	827	CLA	C4B-NB	7.24	1.41	1.35
19	B1	814	CLA	C4B-NB	7.24	1.41	1.35
19	B2	837	CLA	C4B-NB	7.24	1.41	1.35
19	B	817	CLA	C4B-NB	7.24	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	836	CLA	C4B-NB	7.24	1.41	1.35
19	B	811	CLA	C4B-NB	7.24	1.41	1.35
19	B	846	CLA	C4B-NB	7.24	1.41	1.35
19	AA	835	CLA	C4B-NB	7.23	1.41	1.35
19	A	819	CLA	C4B-NB	7.23	1.41	1.35
19	B	816	CLA	C4B-NB	7.23	1.41	1.35
19	BB	805	CLA	C4B-NB	7.23	1.41	1.35
19	A	832	CLA	C4B-NB	7.22	1.41	1.35
19	B2	808	CLA	C4B-NB	7.22	1.41	1.35
19	B1	813	CLA	C4B-NB	7.22	1.41	1.35
19	B2	851	CLA	C4B-NB	7.22	1.41	1.35
19	B1	812	CLA	C4B-NB	7.22	1.41	1.35
19	B1	850	CLA	C4B-NB	7.22	1.41	1.35
19	BB	816	CLA	C4B-NB	7.22	1.41	1.35
19	B1	832	CLA	C4B-NB	7.21	1.41	1.35
19	AA	832	CLA	C4B-NB	7.21	1.41	1.35
19	BB	855	CLA	C4B-NB	7.21	1.41	1.35
19	A1	826	CLA	C4B-NB	7.21	1.41	1.35
19	B	832	CLA	C4B-NB	7.21	1.41	1.35
19	B1	824	CLA	C4B-NB	7.21	1.41	1.35
19	A2	810	CLA	C4B-NB	7.21	1.41	1.35
19	KK	102	CLA	C4B-NB	7.21	1.41	1.35
19	B2	822	CLA	C4B-NB	7.20	1.41	1.35
19	B1	801	CLA	C4B-NB	7.20	1.41	1.35
19	AA	823	CLA	C4B-NB	7.20	1.41	1.35
19	B1	830	CLA	C4B-NB	7.20	1.41	1.35
19	B2	828	CLA	C4B-NB	7.19	1.41	1.35
19	A1	841	CLA	C4B-NB	7.19	1.41	1.35
19	B2	831	CLA	C4B-NB	7.19	1.41	1.35
19	A	823	CLA	C4B-NB	7.19	1.41	1.35
19	B1	808	CLA	C4B-NB	7.19	1.41	1.35
19	A2	823	CLA	C4B-NB	7.19	1.41	1.35
19	A2	832	CLA	C4B-NB	7.19	1.41	1.35
19	K2	102	CLA	C4B-NB	7.18	1.41	1.35
19	BB	817	CLA	C4B-NB	7.18	1.41	1.35
19	B2	812	CLA	C4B-NB	7.18	1.41	1.35
19	A	808	CLA	C4B-NB	7.17	1.41	1.35
19	B	822	CLA	C4B-NB	7.17	1.41	1.35
19	L	203	CLA	C4B-NB	7.17	1.41	1.35
19	B	813	CLA	C4B-NB	7.17	1.41	1.35
19	A2	824	CLA	C4B-NB	7.16	1.41	1.35
19	A2	827	CLA	C4B-NB	7.16	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	849	CLA	C4B-NB	7.16	1.41	1.35
19	B2	805	CLA	C4B-NB	7.16	1.41	1.35
19	B	827	CLA	C4B-NB	7.16	1.41	1.35
19	B2	819	CLA	C4B-NB	7.16	1.41	1.35
19	B2	834	CLA	C4B-NB	7.16	1.41	1.35
19	B	833	CLA	C4B-NB	7.16	1.41	1.35
19	B	819	CLA	C4B-NB	7.15	1.41	1.35
19	A1	823	CLA	C4B-NB	7.15	1.41	1.35
19	B2	849	CLA	C4B-NB	7.15	1.41	1.35
19	A	812	CLA	C4B-NB	7.15	1.41	1.35
19	AA	813	CLA	C4B-NB	7.15	1.41	1.35
19	A1	811	CLA	C4B-NB	7.14	1.41	1.35
19	BB	818	CLA	C4B-NB	7.14	1.41	1.35
19	B	805	CLA	C4B-NB	7.14	1.41	1.35
19	BB	852	CLA	C4B-NB	7.14	1.41	1.35
19	BB	828	CLA	C4B-NB	7.14	1.41	1.35
19	BB	835	CLA	C4B-NB	7.14	1.41	1.35
19	B1	815	CLA	C4B-NB	7.14	1.41	1.35
19	B2	806	CLA	C4B-NB	7.14	1.41	1.35
19	L2	205	CLA	C4B-NB	7.13	1.41	1.35
19	B1	835	CLA	C4B-NB	7.13	1.41	1.35
19	AA	828	CLA	C4B-NB	7.13	1.41	1.35
19	BB	812	CLA	C4B-NB	7.13	1.41	1.35
19	A	835	CLA	C4B-NB	7.12	1.41	1.35
19	B	809	CLA	C4B-NB	7.12	1.41	1.35
19	B	836	CLA	C4B-NB	7.12	1.41	1.35
19	K1	102	CLA	C4B-NB	7.12	1.41	1.35
19	B1	805	CLA	C4B-NB	7.12	1.41	1.35
19	B	814	CLA	C4B-NB	7.12	1.41	1.35
19	AA	826	CLA	C4B-NB	7.12	1.41	1.35
19	AA	812	CLA	C4B-NB	7.12	1.41	1.35
19	A1	807	CLA	C4B-NB	7.12	1.41	1.35
19	A1	844	CLA	C4B-NB	7.12	1.41	1.35
19	BB	801	CLA	C4B-NB	7.12	1.41	1.35
19	L1	205	CLA	C4B-NB	7.11	1.41	1.35
19	A1	808	CLA	C4B-NB	7.11	1.41	1.35
19	A2	812	CLA	C4B-NB	7.11	1.41	1.35
19	B2	815	CLA	C4B-NB	7.11	1.41	1.35
19	B	828	CLA	C4B-NB	7.11	1.41	1.35
19	A	816	CLA	C4B-NB	7.11	1.41	1.35
19	A2	844	CLA	C4B-NB	7.11	1.41	1.35
19	B1	810	CLA	C4B-NB	7.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	836	CLA	C4B-NB	7.10	1.41	1.35
19	A2	808	CLA	C4B-NB	7.10	1.41	1.35
19	A	836	CLA	C4B-NB	7.10	1.41	1.35
19	B2	836	CLA	C4B-NB	7.09	1.41	1.35
19	A1	827	CLA	C4B-NB	7.09	1.41	1.35
19	A2	809	CLA	C4B-NB	7.09	1.41	1.35
19	A	842	CLA	C4B-NB	7.09	1.41	1.35
19	AA	845	CLA	C4B-NB	7.09	1.41	1.35
19	A1	833	CLA	C4B-NB	7.08	1.41	1.35
19	BB	809	CLA	C4B-NB	7.08	1.41	1.35
19	A	813	CLA	C4B-NB	7.08	1.41	1.35
19	A	844	CLA	C4B-NB	7.08	1.41	1.35
19	A2	816	CLA	C4B-NB	7.08	1.41	1.35
19	L1	206	CLA	C4B-NB	7.08	1.41	1.35
19	A	826	CLA	C4B-NB	7.08	1.41	1.35
19	L2	204	CLA	C4B-NB	7.08	1.41	1.35
19	BB	821	CLA	C4B-NB	7.08	1.41	1.35
19	A2	805	CLA	C4B-NB	7.07	1.41	1.35
19	A2	826	CLA	C4B-NB	7.07	1.41	1.35
19	B	858	CLA	C4B-NB	7.07	1.41	1.35
19	B	801	CLA	C4B-NB	7.07	1.41	1.35
19	A	809	CLA	C4B-NB	7.06	1.41	1.35
19	L	202	CLA	C4B-NB	7.06	1.41	1.35
19	BB	824	CLA	C4B-NB	7.06	1.41	1.35
19	A	834	CLA	C4B-NB	7.05	1.41	1.35
19	A2	834	CLA	C4B-NB	7.05	1.41	1.35
19	A2	842	CLA	C4B-NB	7.05	1.41	1.35
19	B2	820	CLA	C4B-NB	7.05	1.41	1.35
19	BB	831	CLA	C4B-NB	7.04	1.41	1.35
19	A	831	CLA	C4B-NB	7.04	1.41	1.35
19	B	824	CLA	C4B-NB	7.04	1.41	1.35
19	LL	201	CLA	C4B-NB	7.04	1.41	1.35
19	BB	819	CLA	C4B-NB	7.03	1.41	1.35
19	A1	825	CLA	C4B-NB	7.03	1.41	1.35
19	A2	828	CLA	C4B-NB	7.03	1.41	1.35
19	B	859	CLA	C4B-NB	7.03	1.41	1.35
19	A	840	CLA	C4B-NB	7.03	1.41	1.35
19	AA	805	CLA	C4B-NB	7.03	1.41	1.35
19	B1	825	CLA	C4B-NB	7.02	1.41	1.35
19	A1	815	CLA	C4B-NB	7.02	1.41	1.35
19	AA	840	CLA	C4B-NB	7.02	1.41	1.35
19	A	804	CLA	C4B-NB	7.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	839	CLA	C4B-NB	7.01	1.41	1.35
19	B1	848	CLA	C4B-NB	7.01	1.41	1.35
19	AA	809	CLA	C4B-NB	7.01	1.41	1.35
19	BB	830	CLA	C4B-NB	7.01	1.41	1.35
19	A1	822	CLA	C4B-NB	7.01	1.41	1.35
19	A2	839	CLA	C4B-NB	7.01	1.41	1.35
19	B2	850	CLA	C4B-NB	7.01	1.41	1.35
19	B	854	CLA	C4B-NB	7.01	1.41	1.35
19	AA	804	CLA	C4B-NB	7.00	1.41	1.35
19	AA	816	CLA	C4B-NB	7.00	1.41	1.35
19	A	839	CLA	C4B-NB	7.00	1.41	1.35
19	B2	824	CLA	C4B-NB	7.00	1.41	1.35
19	AA	834	CLA	C4B-NB	7.00	1.41	1.35
19	A1	838	CLA	C4B-NB	7.00	1.41	1.35
19	B1	829	CLA	C4B-NB	7.00	1.41	1.35
19	A2	829	CLA	C4B-NB	7.00	1.41	1.35
19	A2	836	CLA	C4B-NB	7.00	1.41	1.35
19	A	805	CLA	C4B-NB	7.00	1.41	1.35
19	A1	814	CLA	C4B-NB	7.00	1.41	1.35
19	AA	830	CLA	C4B-NB	7.00	1.41	1.35
19	A1	839	CLA	C4B-NB	6.99	1.41	1.35
19	A1	804	CLA	C4B-NB	6.99	1.41	1.35
19	A2	804	CLA	C4B-NB	6.99	1.41	1.35
19	B2	825	CLA	C4B-NB	6.99	1.41	1.35
19	BB	814	CLA	C4B-NB	6.99	1.41	1.35
19	B	812	CLA	C4B-NB	6.98	1.41	1.35
19	A1	829	CLA	C4B-NB	6.98	1.41	1.35
19	B	815	CLA	C4B-NB	6.98	1.41	1.35
19	BB	856	CLA	C4B-NB	6.98	1.41	1.35
19	B	803	CLA	C4B-NB	6.97	1.41	1.35
19	A2	840	CLA	C4B-NB	6.97	1.41	1.35
19	B2	802	CLA	C4B-NB	6.96	1.41	1.35
19	B2	821	CLA	C4B-NB	6.96	1.41	1.35
19	BB	815	CLA	C4B-NB	6.96	1.41	1.35
19	AA	821	CLA	C4B-NB	6.96	1.41	1.35
19	AA	831	CLA	C4B-NB	6.96	1.41	1.35
19	A1	830	CLA	C4B-NB	6.96	1.41	1.35
19	BB	825	CLA	C4B-NB	6.95	1.41	1.35
19	B2	810	CLA	C4B-NB	6.95	1.41	1.35
19	A2	815	CLA	C4B-NB	6.94	1.41	1.35
19	A2	821	CLA	C4B-NB	6.94	1.41	1.35
19	BB	834	CLA	C4B-NB	6.94	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	807	CLA	C4B-NB	6.93	1.41	1.35
19	B	810	CLA	C4B-NB	6.93	1.41	1.35
19	L	204	CLA	C4B-NB	6.93	1.41	1.35
19	A1	852	CLA	C4B-NB	6.92	1.41	1.35
19	B1	806	CLA	C4B-NB	6.92	1.41	1.35
19	B1	834	CLA	C4B-NB	6.92	1.41	1.35
19	A2	811	CLA	C4B-NB	6.92	1.41	1.35
19	LL	202	CLA	C4B-NB	6.92	1.41	1.35
19	A1	810	CLA	C4B-NB	6.91	1.41	1.35
19	A2	852	CLA	C4B-NB	6.91	1.41	1.35
19	A	830	CLA	C4B-NB	6.91	1.41	1.35
19	A1	803	CLA	C4B-NB	6.91	1.41	1.35
19	B2	830	CLA	C4B-NB	6.91	1.41	1.35
19	A	821	CLA	C4B-NB	6.91	1.41	1.35
19	AA	807	CLA	C4B-NB	6.90	1.41	1.35
19	BB	810	CLA	C4B-NB	6.90	1.41	1.35
19	A	828	CLA	C4B-NB	6.90	1.41	1.35
19	AA	815	CLA	C4B-NB	6.90	1.41	1.35
19	B1	833	CLA	C4B-NB	6.89	1.41	1.35
19	B	820	CLA	C4B-NB	6.89	1.41	1.35
19	B1	803	CLA	C4B-NB	6.88	1.41	1.35
19	BB	806	CLA	C4B-NB	6.88	1.41	1.35
19	B	821	CLA	C4B-NB	6.87	1.41	1.35
19	A	815	CLA	C4B-NB	6.87	1.41	1.35
19	AA	820	CLA	C4B-NB	6.87	1.41	1.35
19	B	825	CLA	C4B-NB	6.87	1.41	1.35
19	A1	806	CLA	C4B-NB	6.86	1.41	1.35
19	A2	831	CLA	C4B-NB	6.86	1.41	1.35
19	B1	802	CLA	C4B-NB	6.86	1.41	1.35
19	BB	836	CLA	C4B-NB	6.85	1.41	1.35
19	BB	802	CLA	C4B-NB	6.85	1.41	1.35
19	BB	808	CLA	C4B-NB	6.84	1.41	1.35
19	B	831	CLA	C4B-NB	6.84	1.41	1.35
19	B	802	CLA	C4B-NB	6.83	1.41	1.35
19	A	820	CLA	C4B-NB	6.83	1.41	1.35
19	B	806	CLA	C4B-NB	6.83	1.41	1.35
19	A1	828	CLA	C4B-NB	6.83	1.41	1.35
19	BB	803	CLA	C4B-NB	6.83	1.41	1.35
19	B1	821	CLA	C4B-NB	6.82	1.41	1.35
19	B2	852	CLA	C4B-NB	6.82	1.41	1.35
19	A1	820	CLA	C4B-NB	6.82	1.41	1.35
19	AA	811	CLA	C4B-NB	6.82	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	803	CLA	C4B-NB	6.81	1.41	1.35
19	A1	819	CLA	C4B-NB	6.81	1.41	1.35
19	A	852	CLA	C4B-NB	6.81	1.41	1.35
19	B	860	CLA	C4B-NB	6.80	1.41	1.35
19	B	830	CLA	C4B-NB	6.80	1.41	1.35
19	A2	801	CLA	C4B-NB	6.79	1.41	1.35
19	AA	841	CLA	C4B-NB	6.79	1.41	1.35
19	B	835	CLA	C4B-NB	6.79	1.41	1.35
19	AA	853	CLA	C4B-NB	6.78	1.41	1.35
19	B	808	CLA	C4B-NB	6.76	1.41	1.35
19	A2	820	CLA	C4B-NB	6.75	1.41	1.35
19	A	841	CLA	C4B-NB	6.75	1.41	1.35
19	AA	829	CLA	C4B-NB	6.75	1.41	1.35
19	A	801	CLA	C4B-NB	6.75	1.41	1.35
19	A	829	CLA	C4B-NB	6.74	1.41	1.35
19	A2	807	CLA	C4B-NB	6.74	1.41	1.35
19	AA	801	CLA	C4B-NB	6.74	1.41	1.35
19	A1	840	CLA	C4B-NB	6.74	1.41	1.35
19	A2	841	CLA	C4B-NB	6.73	1.41	1.35
19	A1	801	CLA	C4B-NB	6.71	1.41	1.35
19	BB	820	CLA	C4B-NB	6.71	1.41	1.35
19	B2	835	CLA	C4B-NB	6.70	1.41	1.35
19	A1	842	CLA	C4B-NB	6.69	1.41	1.35
19	A	811	CLA	C4B-NB	6.69	1.41	1.35
19	AA	843	CLA	C4B-NB	6.68	1.41	1.35
19	A2	830	CLA	C4B-NB	6.66	1.41	1.35
20	A	803	CL0	C1D-ND	6.54	1.45	1.37
20	A2	803	CL0	C1D-ND	6.47	1.45	1.37
20	A1	802	CL0	C1D-ND	6.40	1.45	1.37
19	BB	829	CLA	C4B-NB	6.40	1.40	1.35
19	B	834	CLA	C4B-NB	6.37	1.40	1.35
19	BB	833	CLA	C4B-NB	6.27	1.40	1.35
20	AA	803	CL0	C1D-ND	6.25	1.45	1.37
20	A	803	CL0	O2D-CGD	5.02	1.45	1.33
20	A1	802	CL0	CHC-C1C	4.96	1.47	1.35
20	AA	803	CL0	CHC-C1C	4.89	1.47	1.35
20	A	803	CL0	CHC-C1C	4.88	1.47	1.35
20	A	803	CL0	C3D-C4D	-4.84	1.33	1.44
20	A1	802	CL0	C3B-C2B	4.78	1.47	1.40
20	AA	803	CL0	C3B-C2B	4.77	1.47	1.40
20	A2	803	CL0	CHC-C1C	4.76	1.47	1.35
20	A1	802	CL0	O2D-CGD	4.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A1	802	CL0	C3D-C4D	-4.73	1.33	1.44
20	AA	803	CL0	O2D-CGD	4.73	1.44	1.33
20	AA	803	CL0	C3D-C4D	-4.64	1.33	1.44
20	A2	803	CL0	C3D-C4D	-4.58	1.33	1.44
20	A1	802	CL0	C3C-C2C	4.57	1.46	1.36
20	A	803	CL0	C3B-C2B	4.55	1.46	1.40
20	A2	803	CL0	O2D-CGD	4.54	1.44	1.33
20	AA	803	CL0	C3C-C2C	4.39	1.46	1.36
20	A	803	CL0	C3C-C2C	4.33	1.45	1.36
20	A2	803	CL0	C3B-C2B	4.29	1.46	1.40
20	A2	803	CL0	C3C-C2C	4.20	1.45	1.36
20	A1	802	CL0	O2A-CGA	4.12	1.45	1.33
23	AA	855	BCR	C1-C6	-4.06	1.48	1.53
19	LL	203	CLA	C1D-ND	4.06	1.42	1.37
19	B2	833	CLA	C1D-ND	4.05	1.42	1.37
23	A	854	BCR	C1-C6	-4.04	1.48	1.53
23	BB	839	BCR	C1-C6	-4.02	1.48	1.53
23	K2	105	BCR	C1-C6	-4.02	1.48	1.53
23	K1	106	BCR	C1-C6	-3.99	1.48	1.53
23	B	844	BCR	C30-C25	-3.97	1.48	1.53
23	B1	839	BCR	C1-C6	-3.96	1.48	1.53
23	B	840	BCR	C1-C6	-3.95	1.48	1.53
23	JJ	104	BCR	C1-C6	-3.95	1.48	1.53
23	B2	840	BCR	C1-C6	-3.94	1.48	1.53
19	B2	832	CLA	C1D-ND	3.89	1.42	1.37
19	B1	831	CLA	C1D-ND	3.88	1.42	1.37
23	B2	844	BCR	C30-C25	-3.88	1.48	1.53
23	M	101	BCR	C1-C6	-3.86	1.48	1.53
19	BB	832	CLA	C1D-ND	3.86	1.42	1.37
20	AA	803	CL0	O2A-CGA	3.85	1.44	1.33
23	B1	843	BCR	C30-C25	-3.85	1.48	1.53
23	J	102	BCR	C1-C6	-3.85	1.48	1.53
23	MM	101	BCR	C1-C6	-3.84	1.48	1.53
23	BB	847	BCR	C1-C6	-3.80	1.48	1.53
23	J2	104	BCR	C1-C6	-3.79	1.48	1.53
23	F1	304	BCR	C30-C25	-3.79	1.48	1.53
20	A	803	CL0	O2A-CGA	3.78	1.44	1.33
19	B1	830	CLA	C1D-ND	3.78	1.42	1.37
23	B	848	BCR	C1-C6	-3.78	1.48	1.53
19	J2	103	CLA	C1D-ND	3.78	1.42	1.37
19	B	818	CLA	C1D-ND	3.78	1.42	1.37
19	B	833	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	842	BCR	C1-C6	-3.77	1.48	1.53
19	J1	103	CLA	C1D-ND	3.77	1.42	1.37
19	F1	302	CLA	C1D-ND	3.77	1.42	1.37
23	J2	102	BCR	C1-C6	-3.76	1.48	1.53
23	JJ	102	BCR	C1-C6	-3.76	1.48	1.53
19	B2	831	CLA	C1D-ND	3.76	1.42	1.37
19	A	822	CLA	C1D-ND	3.76	1.42	1.37
19	B1	845	CLA	C1D-ND	3.76	1.42	1.37
19	B2	846	CLA	C1D-ND	3.76	1.42	1.37
19	BB	833	CLA	C1D-ND	3.76	1.42	1.37
19	F2	302	CLA	C1D-ND	3.76	1.42	1.37
19	J	103	CLA	C1D-ND	3.75	1.42	1.37
19	B1	812	CLA	C1D-ND	3.75	1.42	1.37
19	B2	812	CLA	C1D-ND	3.75	1.42	1.37
19	X2	101	CLA	C1D-ND	3.75	1.42	1.37
20	A	803	CL0	CHD-C1D	3.75	1.45	1.38
23	JJ	102	BCR	C30-C25	-3.74	1.48	1.53
23	B	843	BCR	C1-C6	-3.74	1.48	1.53
19	J2	101	CLA	C1D-ND	3.74	1.42	1.37
19	K2	104	CLA	C1D-ND	3.74	1.42	1.37
20	A2	803	CL0	O2A-CGA	3.73	1.44	1.33
19	AA	838	CLA	C1D-ND	3.73	1.42	1.37
19	A	838	CLA	C1D-ND	3.73	1.42	1.37
19	B1	833	CLA	C1D-ND	3.72	1.42	1.37
20	A2	803	CL0	CHD-C4C	3.72	1.47	1.39
23	BB	843	BCR	C30-C25	-3.72	1.48	1.53
19	B1	817	CLA	C1D-ND	3.72	1.42	1.37
19	F	302	CLA	C1D-ND	3.71	1.42	1.37
19	B2	822	CLA	C1D-ND	3.70	1.42	1.37
19	B	825	CLA	C1D-ND	3.70	1.42	1.37
23	I1	101	BCR	C30-C25	-3.70	1.48	1.53
19	B1	815	CLA	C1D-ND	3.70	1.42	1.37
23	B1	842	BCR	C1-C6	-3.70	1.48	1.53
23	FF	304	BCR	C30-C25	-3.70	1.48	1.53
23	J1	102	BCR	C1-C6	-3.70	1.48	1.53
23	BB	838	BCR	C1-C6	-3.70	1.48	1.53
19	B2	809	CLA	C1D-ND	3.70	1.42	1.37
19	B2	835	CLA	C4D-ND	-3.70	1.32	1.37
19	B1	809	CLA	C1D-ND	3.70	1.42	1.37
19	A	852	CLA	C1D-ND	3.70	1.42	1.37
19	K1	103	CLA	C1D-ND	3.69	1.42	1.37
19	A2	802	CLA	C1D-ND	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	839	CLA	C1D-ND	3.69	1.42	1.37
19	BB	830	CLA	C1D-ND	3.69	1.42	1.37
19	B2	817	CLA	C1D-ND	3.69	1.42	1.37
23	B2	843	BCR	C1-C6	-3.69	1.48	1.53
19	JJ	101	CLA	C1D-ND	3.69	1.42	1.37
20	AA	803	CL0	CHD-C4C	3.69	1.47	1.39
19	XX	101	CLA	C1D-ND	3.68	1.42	1.37
23	B	839	BCR	C1-C6	-3.68	1.48	1.53
19	A	817	CLA	C1D-ND	3.68	1.42	1.37
23	F2	304	BCR	C30-C25	-3.68	1.48	1.53
23	J1	102	BCR	C30-C25	-3.68	1.48	1.53
19	AA	817	CLA	C1D-ND	3.68	1.42	1.37
23	F	304	BCR	C1-C6	-3.68	1.48	1.53
19	B	823	CLA	C1D-ND	3.68	1.42	1.37
19	BB	801	CLA	C1D-ND	3.68	1.42	1.37
19	X	101	CLA	C1D-ND	3.67	1.42	1.37
19	AA	811	CLA	C1D-ND	3.67	1.42	1.37
19	FF	302	CLA	C1D-ND	3.67	1.42	1.37
19	X1	101	CLA	C1D-ND	3.67	1.42	1.37
19	L1	205	CLA	C1D-ND	3.67	1.42	1.37
19	BB	845	CLA	C1D-ND	3.67	1.42	1.37
19	KK	102	CLA	C1D-ND	3.67	1.42	1.37
19	J	101	CLA	C1D-ND	3.67	1.42	1.37
19	B1	825	CLA	C1D-ND	3.67	1.42	1.37
19	KK	101	CLA	C1D-ND	3.67	1.42	1.37
19	K1	102	CLA	C1D-ND	3.67	1.42	1.37
19	K	102	CLA	C1D-ND	3.67	1.42	1.37
19	J1	101	CLA	C1D-ND	3.67	1.42	1.37
19	K2	102	CLA	C1D-ND	3.67	1.42	1.37
19	A	833	CLA	C1D-ND	3.67	1.42	1.37
19	L2	204	CLA	C1D-ND	3.67	1.42	1.37
19	JJ	103	CLA	C1D-ND	3.67	1.42	1.37
19	F2	301	CLA	C1D-ND	3.66	1.42	1.37
19	A	832	CLA	C1D-ND	3.66	1.42	1.37
19	B1	832	CLA	C1D-ND	3.66	1.42	1.37
20	A	803	CL0	OBD-CAD	3.66	1.28	1.22
19	A1	829	CLA	C1D-ND	3.66	1.42	1.37
19	K1	105	CLA	C1D-ND	3.66	1.42	1.37
19	A1	831	CLA	C1D-ND	3.66	1.42	1.37
19	B	834	CLA	C1D-ND	3.66	1.42	1.37
19	B2	823	CLA	C1D-ND	3.66	1.42	1.37
19	AA	822	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	102	BCR	C30-C25	-3.66	1.48	1.53
19	K	101	CLA	C1D-ND	3.65	1.42	1.37
19	B	846	CLA	C1D-ND	3.65	1.42	1.37
19	AA	853	CLA	C1D-ND	3.65	1.42	1.37
19	B1	823	CLA	C1D-ND	3.65	1.42	1.37
19	A	824	CLA	C1D-ND	3.65	1.42	1.37
23	F	305	BCR	C1-C6	-3.65	1.48	1.53
19	A1	817	CLA	C1D-ND	3.65	1.42	1.37
19	B2	828	CLA	C1D-ND	3.65	1.42	1.37
19	AA	827	CLA	C1D-ND	3.65	1.42	1.37
19	A1	835	CLA	C1D-ND	3.64	1.42	1.37
19	AA	836	CLA	C1D-ND	3.64	1.42	1.37
19	A2	818	CLA	C1D-ND	3.64	1.42	1.37
19	B	809	CLA	C1D-ND	3.64	1.42	1.37
23	FF	306	BCR	C1-C6	-3.64	1.48	1.53
19	B1	813	CLA	C1D-ND	3.64	1.42	1.37
20	A1	802	CL0	CHD-C1D	3.64	1.45	1.38
19	B1	850	CLA	C1D-ND	3.64	1.42	1.37
19	BB	812	CLA	C1D-ND	3.64	1.42	1.37
23	I2	101	BCR	C30-C25	-3.64	1.48	1.53
20	AA	803	CL0	OBD-CAD	3.64	1.28	1.22
23	AA	852	BCR	C1-C6	-3.64	1.48	1.53
19	A	818	CLA	C1D-ND	3.64	1.42	1.37
19	AA	807	CLA	C1D-ND	3.64	1.42	1.37
23	F2	304	BCR	C1-C6	-3.64	1.48	1.53
19	A2	826	CLA	C1D-ND	3.64	1.42	1.37
19	AA	818	CLA	C1D-ND	3.63	1.42	1.37
19	B	831	CLA	C1D-ND	3.63	1.42	1.37
19	A	816	CLA	C1D-ND	3.63	1.42	1.37
19	B1	822	CLA	C1D-ND	3.63	1.42	1.37
19	F1	301	CLA	C1D-ND	3.63	1.42	1.37
19	BB	823	CLA	C1D-ND	3.63	1.42	1.37
19	BB	835	CLA	C1D-ND	3.63	1.42	1.37
23	KK	103	BCR	C1-C6	-3.63	1.48	1.53
19	A2	832	CLA	C1D-ND	3.63	1.42	1.37
19	B2	825	CLA	C1D-ND	3.63	1.42	1.37
19	BB	809	CLA	C1D-ND	3.63	1.42	1.37
23	BB	843	BCR	C1-C6	-3.63	1.48	1.53
19	BB	825	CLA	C1D-ND	3.63	1.42	1.37
23	F1	304	BCR	C1-C6	-3.63	1.48	1.53
23	B	844	BCR	C1-C6	-3.63	1.48	1.53
19	B2	811	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	813	CLA	C1D-ND	3.63	1.42	1.37
19	B2	834	CLA	C1D-ND	3.62	1.42	1.37
19	B	815	CLA	C1D-ND	3.62	1.42	1.37
19	B	826	CLA	C1D-ND	3.62	1.42	1.37
19	AA	816	CLA	C1D-ND	3.62	1.42	1.37
19	B2	814	CLA	C1D-ND	3.62	1.42	1.37
19	B	832	CLA	C1D-ND	3.62	1.42	1.37
19	AA	845	CLA	C1D-ND	3.62	1.42	1.37
23	FF	304	BCR	C1-C6	-3.62	1.48	1.53
19	A	807	CLA	C1D-ND	3.62	1.42	1.37
19	A	811	CLA	C1D-ND	3.62	1.42	1.37
23	K2	103	BCR	C1-C6	-3.62	1.48	1.53
19	AA	832	CLA	C1D-ND	3.61	1.42	1.37
19	A	823	CLA	C1D-ND	3.61	1.42	1.37
20	A2	803	CL0	OBD-CAD	3.61	1.28	1.22
19	B2	819	CLA	C1D-ND	3.61	1.42	1.37
19	B1	818	CLA	C1D-ND	3.61	1.42	1.37
19	B2	804	CLA	C1D-ND	3.61	1.42	1.37
23	K1	104	BCR	C1-C6	-3.61	1.48	1.53
19	B1	849	CLA	C1D-ND	3.61	1.42	1.37
19	B	817	CLA	C1D-ND	3.61	1.42	1.37
23	M1	101	BCR	C1-C6	-3.61	1.48	1.53
19	L2	206	CLA	C1D-ND	3.61	1.42	1.37
19	B2	836	CLA	C1D-ND	3.61	1.42	1.37
20	A1	802	CL0	OBD-CAD	3.61	1.28	1.22
19	B1	814	CLA	C1D-ND	3.61	1.42	1.37
19	B1	806	CLA	C1D-ND	3.60	1.42	1.37
19	AA	826	CLA	C1D-ND	3.60	1.42	1.37
19	BB	819	CLA	C1D-ND	3.60	1.42	1.37
19	AA	839	CLA	C1D-ND	3.60	1.42	1.37
19	A2	822	CLA	C1D-ND	3.60	1.42	1.37
19	A2	841	CLA	C1D-ND	3.60	1.42	1.37
19	B1	804	CLA	C1D-ND	3.60	1.42	1.37
19	A2	852	CLA	C1D-ND	3.60	1.42	1.37
19	BB	817	CLA	C1D-ND	3.60	1.42	1.37
19	BB	815	CLA	C1D-ND	3.60	1.42	1.37
23	K	103	BCR	C1-C6	-3.60	1.48	1.53
19	B2	835	CLA	C1D-ND	3.60	1.42	1.37
19	BB	831	CLA	C1D-ND	3.60	1.42	1.37
19	A	836	CLA	C1D-ND	3.60	1.42	1.37
19	A2	842	CLA	C1D-ND	3.59	1.42	1.37
19	B2	818	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	815	CLA	C1D-ND	3.59	1.42	1.37
19	B1	801	CLA	C1D-ND	3.59	1.42	1.37
19	A2	808	CLA	C1D-ND	3.59	1.42	1.37
19	A1	840	CLA	C1D-ND	3.59	1.42	1.37
19	B1	811	CLA	C1D-ND	3.59	1.42	1.37
19	B2	851	CLA	C1D-ND	3.59	1.42	1.37
23	L	206	BCR	C1-C6	-3.59	1.48	1.53
19	A1	805	CLA	C1D-ND	3.59	1.42	1.37
19	A	814	CLA	C1D-ND	3.59	1.42	1.37
19	AA	815	CLA	C1D-ND	3.59	1.42	1.37
19	F	301	CLA	C1D-ND	3.59	1.42	1.37
19	B1	836	CLA	C1D-ND	3.58	1.42	1.37
23	B1	838	BCR	C1-C6	-3.58	1.48	1.53
19	L1	207	CLA	C1D-ND	3.58	1.42	1.37
19	AA	823	CLA	C1D-ND	3.58	1.42	1.37
19	A2	807	CLA	C1D-ND	3.58	1.42	1.37
19	A	827	CLA	C1D-ND	3.58	1.42	1.37
19	A2	823	CLA	C1D-ND	3.58	1.42	1.37
23	B2	839	BCR	C1-C6	-3.58	1.48	1.53
19	LL	201	CLA	C1D-ND	3.58	1.42	1.37
20	AA	803	CL0	CHD-C1D	3.58	1.45	1.38
19	AA	808	CLA	C1D-ND	3.58	1.42	1.37
19	A1	808	CLA	C1D-ND	3.58	1.42	1.37
19	AA	833	CLA	C1D-ND	3.58	1.42	1.37
19	A2	813	CLA	C1D-ND	3.57	1.42	1.37
19	B1	820	CLA	C1D-ND	3.57	1.42	1.37
19	A2	815	CLA	C1D-ND	3.57	1.42	1.37
19	A	815	CLA	C1D-ND	3.57	1.42	1.37
19	L	203	CLA	C4D-ND	-3.57	1.32	1.37
19	A1	822	CLA	C1D-ND	3.57	1.42	1.37
19	A1	844	CLA	C1D-ND	3.57	1.42	1.37
19	F1	305	CLA	C1D-ND	3.57	1.42	1.37
19	A	809	CLA	C1D-ND	3.57	1.42	1.37
19	B2	808	CLA	C1D-ND	3.57	1.42	1.37
19	A1	806	CLA	C1D-ND	3.57	1.42	1.37
19	BB	828	CLA	C1D-ND	3.57	1.42	1.37
20	A	803	CL0	CHD-C4C	3.57	1.47	1.39
19	B1	819	CLA	C1D-ND	3.57	1.42	1.37
19	B2	815	CLA	C1D-ND	3.57	1.42	1.37
19	B	812	CLA	C1D-ND	3.57	1.42	1.37
19	B1	808	CLA	C1D-ND	3.57	1.42	1.37
19	BB	804	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	839	CLA	C1D-ND	3.57	1.42	1.37
19	A1	812	CLA	C1D-ND	3.56	1.42	1.37
19	A2	816	CLA	C1D-ND	3.56	1.42	1.37
19	B	836	CLA	C1D-ND	3.56	1.42	1.37
23	I2	101	BCR	C1-C6	-3.56	1.48	1.53
19	B	807	CLA	C1D-ND	3.56	1.42	1.37
19	A1	841	CLA	C1D-ND	3.56	1.42	1.37
19	A2	817	CLA	C1D-ND	3.56	1.42	1.37
19	BB	826	CLA	CMB-C2B	-3.56	1.44	1.51
20	A1	802	CL0	CHD-C4C	3.56	1.47	1.39
23	I1	101	BCR	C1-C6	-3.56	1.48	1.53
19	A2	844	CLA	C1D-ND	3.56	1.42	1.37
19	A	844	CLA	C1D-ND	3.56	1.42	1.37
19	A1	810	CLA	C1D-ND	3.56	1.42	1.37
19	A1	813	CLA	C1D-ND	3.56	1.42	1.37
19	B	803	CLA	C1D-ND	3.56	1.42	1.37
19	BB	807	CLA	C1D-ND	3.56	1.42	1.37
19	AA	841	CLA	C1D-ND	3.56	1.42	1.37
19	A2	812	CLA	C1D-ND	3.55	1.42	1.37
23	J2	102	BCR	C30-C25	-3.55	1.48	1.53
23	A1	850	BCR	C1-C6	-3.55	1.48	1.53
19	B1	835	CLA	C1D-ND	3.55	1.42	1.37
19	B2	802	CLA	C1D-ND	3.55	1.42	1.37
19	BB	808	CLA	C1D-ND	3.55	1.42	1.37
23	F	304	BCR	C30-C25	-3.55	1.48	1.53
19	AA	812	CLA	C1D-ND	3.55	1.42	1.37
20	A2	803	CL0	CHD-C1D	3.55	1.45	1.38
23	A2	848	BCR	C1-C6	-3.55	1.48	1.53
19	A	841	CLA	C1D-ND	3.55	1.42	1.37
19	A	837	CLA	C1D-ND	3.55	1.42	1.37
19	BB	811	CLA	C1D-ND	3.55	1.42	1.37
19	A	812	CLA	C1D-ND	3.55	1.42	1.37
19	B2	816	CLA	C1D-ND	3.54	1.42	1.37
19	A1	811	CLA	C1D-ND	3.54	1.42	1.37
19	A1	821	CLA	C1D-ND	3.54	1.42	1.37
19	A1	823	CLA	C1D-ND	3.54	1.42	1.37
19	B2	837	CLA	C1D-ND	3.54	1.42	1.37
19	B2	850	CLA	C1D-ND	3.54	1.42	1.37
19	A1	816	CLA	C1D-ND	3.54	1.42	1.37
23	A1	848	BCR	C1-C6	-3.54	1.48	1.53
19	B1	802	CLA	C1D-ND	3.54	1.42	1.37
19	B	858	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	814	CLA	C1D-ND	3.54	1.42	1.37
19	AA	837	CLA	C1D-ND	3.54	1.42	1.37
23	AA	854	BCR	C30-C25	-3.54	1.48	1.53
19	A1	824	CLA	C1D-ND	3.54	1.42	1.37
19	A2	833	CLA	C1D-ND	3.54	1.42	1.37
23	A2	850	BCR	C1-C6	-3.54	1.48	1.53
19	A1	827	CLA	C1D-ND	3.54	1.42	1.37
23	II	101	BCR	C1-C6	-3.53	1.48	1.53
19	AA	824	CLA	C1D-ND	3.53	1.42	1.37
19	B	804	CLA	C1D-ND	3.53	1.42	1.37
19	AA	840	CLA	C1D-ND	3.53	1.42	1.37
19	BB	813	CLA	C1D-ND	3.53	1.42	1.37
19	A2	814	CLA	C1D-ND	3.53	1.42	1.37
19	A2	838	CLA	C1D-ND	3.53	1.42	1.37
19	B	811	CLA	C1D-ND	3.53	1.42	1.37
19	B	828	CLA	C1D-ND	3.53	1.42	1.37
19	AA	814	CLA	C1D-ND	3.53	1.42	1.37
23	A1	847	BCR	C1-C6	-3.53	1.48	1.53
19	B2	807	CLA	C1D-ND	3.53	1.42	1.37
19	A2	809	CLA	C1D-ND	3.53	1.42	1.37
19	B	837	CLA	C1D-ND	3.53	1.42	1.37
19	AA	809	CLA	C1D-ND	3.53	1.42	1.37
23	A	853	BCR	C30-C25	-3.53	1.48	1.53
19	B1	807	CLA	C1D-ND	3.52	1.42	1.37
19	A2	810	CLA	C1D-ND	3.52	1.42	1.37
19	A2	828	CLA	C1D-ND	3.52	1.42	1.37
19	AA	821	CLA	C1D-ND	3.52	1.42	1.37
19	B1	816	CLA	C1D-ND	3.52	1.42	1.37
19	B2	801	CLA	C1D-ND	3.52	1.42	1.37
23	B1	843	BCR	C1-C6	-3.52	1.48	1.53
19	L	202	CLA	C1D-ND	3.52	1.42	1.37
23	M2	102	BCR	C1-C6	-3.52	1.48	1.53
19	BB	803	CLA	C1D-ND	3.52	1.42	1.37
19	A2	811	CLA	C1D-ND	3.51	1.42	1.37
19	AA	813	CLA	C1D-ND	3.51	1.42	1.37
19	AA	830	CLA	C1D-ND	3.51	1.42	1.37
19	A2	836	CLA	C1D-ND	3.51	1.42	1.37
23	A2	847	BCR	C1-C6	-3.51	1.48	1.53
23	II	104	BCR	C1-C6	-3.51	1.48	1.53
19	B	808	CLA	C1D-ND	3.51	1.42	1.37
19	B1	803	CLA	C1D-ND	3.51	1.42	1.37
19	A	813	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	825	CLA	C1D-ND	3.51	1.42	1.37
23	I	101	BCR	C1-C6	-3.51	1.48	1.53
19	B1	810	CLA	C1D-ND	3.51	1.42	1.37
19	A2	824	CLA	C1D-ND	3.51	1.42	1.37
19	A1	838	CLA	C1D-ND	3.51	1.42	1.37
19	BB	855	CLA	C1D-ND	3.51	1.42	1.37
19	AA	842	CLA	C1D-ND	3.51	1.42	1.37
19	B2	810	CLA	C1D-ND	3.50	1.42	1.37
19	B	801	CLA	C1D-ND	3.50	1.42	1.37
19	A1	839	CLA	C1D-ND	3.50	1.42	1.37
19	A	821	CLA	C1D-ND	3.50	1.42	1.37
23	B2	844	BCR	C1-C6	-3.50	1.49	1.53
19	A2	827	CLA	C1D-ND	3.50	1.42	1.37
19	BB	856	CLA	C1D-ND	3.50	1.42	1.37
19	A2	820	CLA	C1D-ND	3.50	1.42	1.37
19	A	819	CLA	C1D-ND	3.50	1.42	1.37
19	A2	840	CLA	C1D-ND	3.50	1.42	1.37
23	L1	209	BCR	C1-C6	-3.50	1.49	1.53
19	A1	832	CLA	C1D-ND	3.50	1.42	1.37
19	A1	818	CLA	C1D-ND	3.50	1.42	1.37
23	II	102	BCR	C1-C6	-3.49	1.49	1.53
19	B2	803	CLA	C1D-ND	3.49	1.42	1.37
19	A	840	CLA	C1D-ND	3.49	1.42	1.37
23	A1	853	BCR	C30-C25	-3.49	1.49	1.53
23	L2	207	BCR	C1-C6	-3.49	1.49	1.53
23	A2	853	BCR	C30-C25	-3.49	1.49	1.53
19	B	859	CLA	C1D-ND	3.49	1.42	1.37
19	A1	852	CLA	C1D-ND	3.49	1.42	1.37
19	A2	825	CLA	C1D-ND	3.49	1.42	1.37
19	B2	829	CLA	C1D-ND	3.49	1.42	1.37
19	AA	810	CLA	C1D-ND	3.49	1.42	1.37
23	AA	849	BCR	C1-C6	-3.49	1.49	1.53
19	A1	804	CLA	C1D-ND	3.49	1.42	1.37
19	A1	826	CLA	C1D-ND	3.49	1.42	1.37
19	A	835	CLA	C1D-ND	3.49	1.42	1.37
19	A1	837	CLA	C1D-ND	3.49	1.42	1.37
19	B1	826	CLA	C1D-ND	3.49	1.42	1.37
19	A	830	CLA	C1D-ND	3.49	1.42	1.37
19	A	842	CLA	C1D-ND	3.49	1.42	1.37
19	A1	825	CLA	C1D-ND	3.48	1.42	1.37
23	I2	103	BCR	C1-C6	-3.48	1.49	1.53
19	A	828	CLA	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	847	BCR	C1-C6	-3.48	1.49	1.53
19	LL	202	CLA	C4D-ND	-3.48	1.32	1.37
19	A1	801	CLA	C1D-ND	3.48	1.42	1.37
19	AA	819	CLA	C1D-ND	3.48	1.42	1.37
19	A1	833	CLA	C1D-ND	3.48	1.42	1.37
19	A2	819	CLA	C1D-ND	3.48	1.42	1.37
23	A	848	BCR	C1-C6	-3.48	1.49	1.53
19	B	814	CLA	C1D-ND	3.48	1.42	1.37
19	A2	837	CLA	C1D-ND	3.48	1.42	1.37
23	L	205	BCR	C1-C6	-3.48	1.49	1.53
19	A	808	CLA	C1D-ND	3.47	1.42	1.37
19	B	813	CLA	C1D-ND	3.47	1.42	1.37
23	L	206	BCR	C30-C25	-3.47	1.49	1.53
19	A1	836	CLA	C1D-ND	3.47	1.42	1.37
19	A	826	CLA	C1D-ND	3.47	1.42	1.37
23	J1	104	BCR	C1-C6	-3.47	1.49	1.53
19	A	806	CLA	C1D-ND	3.47	1.42	1.37
19	A2	806	CLA	C1D-ND	3.47	1.42	1.37
23	AA	848	BCR	C1-C6	-3.47	1.49	1.53
19	A1	807	CLA	C1D-ND	3.47	1.42	1.37
19	A1	809	CLA	C1D-ND	3.47	1.42	1.37
19	BB	816	CLA	C1D-ND	3.47	1.42	1.37
23	L1	201	BCR	C1-C6	-3.47	1.49	1.53
19	B2	824	CLA	C1D-ND	3.47	1.42	1.37
19	A1	834	CLA	C1D-ND	3.46	1.42	1.37
19	A	825	CLA	C1D-ND	3.46	1.42	1.37
19	A	810	CLA	C1D-ND	3.46	1.42	1.37
19	AA	806	CLA	C1D-ND	3.46	1.42	1.37
19	B	819	CLA	C1D-ND	3.46	1.42	1.37
19	AA	828	CLA	C1D-ND	3.46	1.42	1.37
19	BB	834	CLA	C1D-ND	3.45	1.42	1.37
19	A2	830	CLA	C1D-ND	3.45	1.42	1.37
19	B	824	CLA	C1D-ND	3.45	1.42	1.37
23	F1	306	BCR	C1-C6	-3.45	1.49	1.53
19	A	820	CLA	C1D-ND	3.45	1.42	1.37
19	A2	821	CLA	C1D-ND	3.44	1.42	1.37
19	A	834	CLA	C1D-ND	3.44	1.42	1.37
19	B1	821	CLA	C1D-ND	3.44	1.42	1.37
19	BB	802	CLA	C1D-ND	3.44	1.42	1.37
19	A1	819	CLA	C1D-ND	3.44	1.42	1.37
19	AA	835	CLA	C1D-ND	3.44	1.42	1.37
19	A2	835	CLA	C1D-ND	3.44	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	834	CLA	C1D-ND	3.43	1.42	1.37
19	B1	827	CLA	C1D-ND	3.43	1.42	1.37
19	BB	824	CLA	C1D-ND	3.43	1.42	1.37
19	A2	834	CLA	C1D-ND	3.43	1.42	1.37
23	B	848	BCR	C30-C25	-3.43	1.49	1.53
23	F2	305	BCR	C1-C6	-3.43	1.49	1.53
19	A1	820	CLA	C1D-ND	3.43	1.42	1.37
19	B	821	CLA	C1D-ND	3.43	1.42	1.37
19	FF	301	CLA	C1D-ND	3.42	1.42	1.37
19	B	802	CLA	C1D-ND	3.42	1.42	1.37
19	B	829	CLA	C1D-ND	3.42	1.42	1.37
19	B2	826	CLA	C1D-ND	3.42	1.42	1.37
23	I2	102	BCR	C1-C6	-3.42	1.49	1.53
19	L1	206	CLA	C4D-ND	-3.42	1.33	1.37
23	BB	847	BCR	C30-C25	-3.42	1.49	1.53
19	AA	820	CLA	C1D-ND	3.42	1.42	1.37
23	II	101	BCR	C30-C25	-3.41	1.49	1.53
23	F1	303	BCR	C1-C6	-3.41	1.49	1.53
19	BB	806	CLA	C1D-ND	3.41	1.42	1.37
19	B2	827	CLA	C1D-ND	3.41	1.42	1.37
19	FF	305	CLA	C1D-ND	3.41	1.42	1.37
23	AA	854	BCR	C1-C6	-3.40	1.49	1.53
19	A2	831	CLA	C1D-ND	3.40	1.42	1.37
23	I	101	BCR	C30-C25	-3.40	1.49	1.53
23	LL	204	BCR	C30-C25	-3.40	1.49	1.53
19	AA	801	CLA	C1D-ND	3.40	1.42	1.37
19	BB	814	CLA	C1D-ND	3.40	1.42	1.37
19	B2	830	CLA	C4D-ND	-3.40	1.33	1.37
19	BB	805	CLA	C1D-ND	3.40	1.42	1.37
23	I	102	BCR	C1-C6	-3.39	1.49	1.53
19	A1	830	CLA	C1D-ND	3.39	1.42	1.37
19	B1	824	CLA	CHC-C1C	3.39	1.43	1.35
23	A	853	BCR	C1-C6	-3.39	1.49	1.53
19	B2	806	CLA	C1D-ND	3.39	1.41	1.37
19	BB	810	CLA	C1D-ND	3.38	1.41	1.37
19	BB	820	CLA	C1D-ND	3.38	1.41	1.37
19	B2	821	CLA	C1D-ND	3.38	1.41	1.37
19	B	854	CLA	C1D-ND	3.38	1.41	1.37
19	A2	805	CLA	C1D-ND	3.38	1.41	1.37
19	B1	805	CLA	C1D-ND	3.38	1.41	1.37
19	AA	831	CLA	C1D-ND	3.38	1.41	1.37
19	B1	829	CLA	C4D-ND	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	828	CLA	C1D-ND	3.38	1.41	1.37
19	BB	829	CLA	C4D-ND	-3.38	1.33	1.37
19	BB	818	CLA	C1D-ND	3.37	1.41	1.37
23	AA	851	BCR	C1-C6	-3.37	1.49	1.53
19	AA	804	CLA	C1D-ND	3.37	1.41	1.37
19	B2	820	CLA	CHC-C1C	3.37	1.43	1.35
19	B2	834	CLA	CHC-C1C	3.37	1.43	1.35
23	A	851	BCR	C1-C6	-3.37	1.49	1.53
19	AA	829	CLA	C1D-ND	3.37	1.41	1.37
19	AA	834	CLA	C1D-ND	3.37	1.41	1.37
19	B	816	CLA	C1D-ND	3.37	1.41	1.37
19	L2	205	CLA	C4D-ND	-3.37	1.33	1.37
23	B1	842	BCR	C30-C25	-3.37	1.49	1.53
23	LL	204	BCR	C1-C6	-3.37	1.49	1.53
19	B	823	CLA	C4D-ND	-3.36	1.33	1.37
19	A2	829	CLA	C4D-ND	-3.36	1.33	1.37
19	B	810	CLA	C1D-ND	3.36	1.41	1.37
19	A	831	CLA	C1D-ND	3.36	1.41	1.37
23	A	850	BCR	C1-C6	-3.36	1.49	1.53
23	M	101	BCR	C30-C25	-3.36	1.49	1.53
19	B	835	CLA	C1D-ND	3.36	1.41	1.37
19	B1	824	CLA	C1D-ND	3.36	1.41	1.37
23	L1	208	BCR	C1-C6	-3.36	1.49	1.53
19	B	827	CLA	C1D-ND	3.36	1.41	1.37
23	B2	843	BCR	C30-C25	-3.35	1.49	1.53
23	L2	207	BCR	C30-C25	-3.35	1.49	1.53
19	A	801	CLA	C1D-ND	3.35	1.41	1.37
23	A2	851	BCR	C1-C6	-3.35	1.49	1.53
23	K2	103	BCR	C30-C25	-3.35	1.49	1.53
23	B	842	BCR	C1-C6	-3.35	1.49	1.53
19	B2	805	CLA	C1D-ND	3.35	1.41	1.37
23	BB	841	BCR	C1-C6	-3.35	1.49	1.53
23	K1	104	BCR	C30-C25	-3.34	1.49	1.53
19	B	830	CLA	C4D-ND	-3.34	1.33	1.37
19	B	822	CLA	C1D-ND	3.34	1.41	1.37
23	A1	853	BCR	C1-C6	-3.34	1.49	1.53
23	FF	303	BCR	C1-C6	-3.34	1.49	1.53
23	A1	851	BCR	C1-C6	-3.34	1.49	1.53
19	A2	801	CLA	C1D-ND	3.33	1.41	1.37
19	A1	852	CLA	C4D-ND	-3.33	1.33	1.37
19	A	829	CLA	C1D-ND	3.32	1.41	1.37
23	B1	841	BCR	C1-C6	-3.32	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	303	BCR	C1-C6	-3.32	1.49	1.53
19	B	806	CLA	C1D-ND	3.32	1.41	1.37
23	L1	209	BCR	C30-C25	-3.32	1.49	1.53
19	B2	850	CLA	C4D-ND	-3.32	1.33	1.37
19	A2	815	CLA	CHC-C1C	3.31	1.43	1.35
23	A2	853	BCR	C1-C6	-3.31	1.49	1.53
19	L	204	CLA	C1D-ND	3.31	1.41	1.37
19	AA	805	CLA	C1D-ND	3.31	1.41	1.37
19	A	829	CLA	C4D-ND	-3.30	1.33	1.37
19	A2	806	CLA	CHC-C1C	3.30	1.43	1.35
19	A	805	CLA	C1D-ND	3.30	1.41	1.37
19	BB	823	CLA	C4D-ND	-3.30	1.33	1.37
23	J	104	BCR	C30-C25	-3.30	1.49	1.53
19	A	804	CLA	CHC-C1C	3.30	1.43	1.35
19	A	810	CLA	CHC-C1C	3.29	1.43	1.35
19	LL	202	CLA	C1D-ND	3.29	1.41	1.37
19	BB	834	CLA	C4D-ND	-3.29	1.33	1.37
19	B	820	CLA	C1D-ND	3.29	1.41	1.37
19	BB	836	CLA	C1D-ND	3.29	1.41	1.37
19	A1	828	CLA	C4D-ND	-3.29	1.33	1.37
19	AA	829	CLA	C4D-ND	-3.29	1.33	1.37
19	B2	829	CLA	CHC-C1C	3.29	1.43	1.35
19	B1	849	CLA	C4D-ND	-3.29	1.33	1.37
19	B2	820	CLA	C1D-ND	3.29	1.41	1.37
23	B	843	BCR	C30-C25	-3.28	1.49	1.53
19	BB	821	CLA	C1D-ND	3.28	1.41	1.37
19	A1	814	CLA	CHC-C1C	3.28	1.43	1.35
19	B1	850	CLA	CHC-C1C	3.28	1.43	1.35
19	L	204	CLA	C4D-ND	-3.28	1.33	1.37
19	BB	821	CLA	CHC-C1C	3.28	1.43	1.35
19	B	826	CLA	CMB-C2B	-3.27	1.44	1.51
19	A2	804	CLA	CHC-C1C	3.27	1.43	1.35
19	B1	834	CLA	C4D-ND	-3.27	1.33	1.37
19	FF	305	CLA	CHC-C1C	3.27	1.43	1.35
19	BB	810	CLA	C4D-ND	-3.27	1.33	1.37
19	A2	829	CLA	C1D-ND	3.27	1.41	1.37
23	F2	303	BCR	C1-C6	-3.26	1.49	1.53
19	B1	848	CLA	C1D-ND	3.26	1.41	1.37
19	B	858	CLA	C4D-ND	-3.26	1.33	1.37
19	BB	827	CLA	C1D-ND	3.26	1.41	1.37
19	AA	806	CLA	CHC-C1C	3.26	1.43	1.35
19	AA	804	CLA	CHC-C1C	3.26	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	104	BCR	C1-C6	-3.26	1.49	1.53
19	L	203	CLA	C1D-ND	3.26	1.41	1.37
19	B2	849	CLA	C1D-ND	3.26	1.41	1.37
19	B1	820	CLA	CHC-C1C	3.26	1.43	1.35
19	B	835	CLA	C4D-ND	-3.25	1.33	1.37
19	B1	828	CLA	CHC-C1C	3.25	1.43	1.35
23	BB	842	BCR	C30-C25	-3.25	1.49	1.53
19	B2	827	CLA	CHC-C1C	3.25	1.43	1.35
19	AA	816	CLA	CHC-C1C	3.25	1.43	1.35
19	A	826	CLA	C4D-ND	-3.24	1.33	1.37
19	B	805	CLA	C1D-ND	3.24	1.41	1.37
23	I	102	BCR	C30-C25	-3.24	1.49	1.53
19	A	852	CLA	C4D-ND	-3.24	1.33	1.37
19	A1	806	CLA	CHC-C1C	3.24	1.43	1.35
19	A	806	CLA	CHC-C1C	3.24	1.43	1.35
19	B	833	CLA	C4D-ND	-3.24	1.33	1.37
19	B2	851	CLA	CHC-C1C	3.24	1.43	1.35
19	AA	823	CLA	CHC-C1C	3.24	1.43	1.35
19	BB	818	CLA	CHC-C1C	3.24	1.43	1.35
19	BB	822	CLA	C1D-ND	3.24	1.41	1.37
19	AA	810	CLA	CHC-C1C	3.24	1.43	1.35
19	A	823	CLA	CHC-C1C	3.23	1.43	1.35
23	B1	838	BCR	C30-C25	-3.23	1.49	1.53
19	AA	853	CLA	C4D-ND	-3.23	1.33	1.37
19	B2	816	CLA	CHC-C1C	3.23	1.43	1.35
19	A	841	CLA	C4D-ND	-3.23	1.33	1.37
19	B	822	CLA	CHC-C1C	3.23	1.43	1.35
19	BB	824	CLA	C4D-ND	-3.23	1.33	1.37
23	B2	839	BCR	C30-C25	-3.23	1.49	1.53
19	A2	807	CLA	CHC-C1C	3.23	1.43	1.35
23	J2	104	BCR	C30-C25	-3.22	1.49	1.53
19	A1	805	CLA	C4D-ND	-3.22	1.33	1.37
25	I1	102	LMG	C4-C5	3.22	1.59	1.53
19	B	813	CLA	CHC-C1C	3.22	1.43	1.35
19	A1	828	CLA	C1D-ND	3.22	1.41	1.37
19	L1	206	CLA	C1D-ND	3.22	1.41	1.37
19	A2	852	CLA	C4D-ND	-3.22	1.33	1.37
19	B2	852	CLA	C1D-ND	3.22	1.41	1.37
19	B2	802	CLA	CHC-C1C	3.22	1.43	1.35
19	B	810	CLA	C4D-ND	-3.22	1.33	1.37
19	AA	841	CLA	C4D-ND	-3.22	1.33	1.37
19	BB	856	CLA	CHC-C1C	3.22	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	849	BCR	C30-C25	-3.21	1.49	1.53
19	A2	810	CLA	CHC-C1C	3.21	1.43	1.35
19	B	860	CLA	C1D-ND	3.21	1.41	1.37
19	B1	813	CLA	CHC-C1C	3.21	1.43	1.35
23	A1	850	BCR	C30-C25	-3.21	1.49	1.53
23	B2	842	BCR	C1-C6	-3.21	1.49	1.53
19	A2	823	CLA	CHC-C1C	3.21	1.43	1.35
19	B2	811	CLA	CHC-C1C	3.21	1.43	1.35
19	B1	827	CLA	CHC-C1C	3.21	1.43	1.35
19	A2	830	CLA	C4D-ND	-3.20	1.33	1.37
19	B	859	CLA	CHC-C1C	3.20	1.43	1.35
19	A1	805	CLA	CHC-C1C	3.20	1.43	1.35
19	A1	815	CLA	CHC-C1C	3.20	1.43	1.35
19	B1	811	CLA	CHC-C1C	3.20	1.43	1.35
19	BB	822	CLA	CHC-C1C	3.20	1.43	1.35
23	J1	104	BCR	C30-C25	-3.20	1.49	1.53
19	BB	852	CLA	C1D-ND	3.20	1.41	1.37
19	BB	855	CLA	C4D-ND	-3.20	1.33	1.37
19	B	829	CLA	CHC-C1C	3.20	1.43	1.35
19	A2	841	CLA	C4D-ND	-3.20	1.33	1.37
23	A	848	BCR	C30-C25	-3.20	1.49	1.53
19	B2	833	CLA	C4D-ND	-3.20	1.33	1.37
19	B1	802	CLA	CHC-C1C	3.20	1.43	1.35
19	B2	813	CLA	CHC-C1C	3.20	1.43	1.35
19	B2	809	CLA	CHC-C1C	3.20	1.43	1.35
19	A	830	CLA	C4D-ND	-3.19	1.33	1.37
19	AA	820	CLA	C4D-ND	-3.19	1.33	1.37
19	B	829	CLA	C4D-ND	-3.19	1.33	1.37
19	B	816	CLA	CHC-C1C	3.19	1.43	1.35
19	B1	809	CLA	CHC-C1C	3.19	1.43	1.35
19	A2	835	CLA	CHC-C1C	3.19	1.43	1.35
19	B	824	CLA	C4D-ND	-3.19	1.33	1.37
19	AA	826	CLA	C4D-ND	-3.19	1.33	1.37
19	A2	829	CLA	CHC-C1C	3.19	1.43	1.35
19	B	811	CLA	CHC-C1C	3.19	1.43	1.35
19	A2	820	CLA	C4D-ND	-3.19	1.33	1.37
19	B1	816	CLA	CHC-C1C	3.18	1.43	1.35
19	A1	820	CLA	C4D-ND	-3.18	1.33	1.37
19	B	808	CLA	C4D-ND	-3.18	1.33	1.37
19	AA	811	CLA	C4D-ND	-3.18	1.33	1.37
19	A2	816	CLA	CHC-C1C	3.18	1.43	1.35
19	AA	815	CLA	CHC-C1C	3.18	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	826	CLA	CMB-C2B	-3.18	1.45	1.51
19	A	815	CLA	CHC-C1C	3.18	1.43	1.35
19	BB	813	CLA	CHC-C1C	3.18	1.43	1.35
19	BB	827	CLA	CHC-C1C	3.18	1.43	1.35
19	AA	843	CLA	C1D-ND	3.18	1.41	1.37
19	B1	823	CLA	C4D-ND	-3.18	1.33	1.37
19	J1	101	CLA	CHC-C1C	3.18	1.43	1.35
19	A	816	CLA	CHC-C1C	3.18	1.43	1.35
19	BB	820	CLA	CHC-C1C	3.18	1.43	1.35
23	A2	850	BCR	C30-C25	-3.18	1.49	1.53
19	A2	826	CLA	C4D-ND	-3.18	1.33	1.37
19	AA	834	CLA	C4D-ND	-3.18	1.33	1.37
23	II	102	BCR	C30-C25	-3.18	1.49	1.53
19	A1	809	CLA	C4D-ND	-3.18	1.33	1.37
23	I2	102	BCR	C30-C25	-3.18	1.49	1.53
19	A1	822	CLA	CHC-C1C	3.18	1.43	1.35
19	A	814	CLA	CHC-C1C	3.18	1.43	1.35
19	AA	842	CLA	CHC-C1C	3.18	1.43	1.35
19	J2	101	CLA	CHC-C1C	3.18	1.43	1.35
19	A	842	CLA	CHC-C1C	3.18	1.43	1.35
19	BB	802	CLA	CHC-C1C	3.17	1.43	1.35
19	A1	810	CLA	C4D-ND	-3.17	1.33	1.37
19	B	815	CLA	C4D-ND	-3.17	1.33	1.37
19	A1	801	CLA	C4D-ND	-3.17	1.33	1.37
19	A1	825	CLA	C4D-ND	-3.17	1.33	1.37
19	A1	840	CLA	C4D-ND	-3.17	1.33	1.37
19	A	807	CLA	CHC-C1C	3.17	1.43	1.35
19	A1	812	CLA	C4D-ND	-3.17	1.33	1.37
19	BB	832	CLA	C4D-ND	-3.17	1.33	1.37
19	K	101	CLA	CHC-C1C	3.17	1.43	1.35
19	A2	804	CLA	C1D-ND	3.17	1.41	1.37
19	A	804	CLA	C1D-ND	3.17	1.41	1.37
19	B1	810	CLA	C4D-ND	-3.17	1.33	1.37
19	A2	821	CLA	C4D-ND	-3.17	1.33	1.37
19	A	835	CLA	CHC-C1C	3.17	1.43	1.35
19	AA	835	CLA	CHC-C1C	3.17	1.43	1.35
19	A2	811	CLA	C4D-ND	-3.16	1.33	1.37
19	AA	814	CLA	CHC-C1C	3.16	1.43	1.35
19	B1	819	CLA	CHC-C1C	3.16	1.43	1.35
19	BB	811	CLA	CHC-C1C	3.16	1.43	1.35
23	L1	201	BCR	C30-C25	-3.16	1.49	1.53
23	BB	838	BCR	C30-C25	-3.16	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	807	CLA	CHC-C1C	3.16	1.43	1.35
19	BB	823	CLA	CHC-C1C	3.16	1.43	1.35
19	A	834	CLA	C4D-ND	-3.16	1.33	1.37
19	K2	102	CLA	CHC-C1C	3.16	1.43	1.35
19	B	804	CLA	CHC-C1C	3.16	1.43	1.35
19	B2	824	CLA	C4D-ND	-3.16	1.33	1.37
19	A1	842	CLA	C1D-ND	3.16	1.41	1.37
19	B1	833	CLA	CHC-C1C	3.16	1.43	1.35
19	A	840	CLA	C4D-ND	-3.16	1.33	1.37
19	A1	839	CLA	C4D-ND	-3.16	1.33	1.37
19	B2	810	CLA	C4D-ND	-3.16	1.33	1.37
19	BB	808	CLA	C4D-ND	-3.16	1.33	1.37
19	A	822	CLA	C4D-ND	-3.16	1.33	1.37
19	A1	834	CLA	CHC-C1C	3.16	1.43	1.35
19	B	802	CLA	CHC-C1C	3.15	1.43	1.35
19	KK	101	CLA	CHC-C1C	3.15	1.43	1.35
19	B2	846	CLA	CHC-C1C	3.15	1.43	1.35
19	B	820	CLA	CHC-C1C	3.15	1.43	1.35
19	A2	817	CLA	CHC-C1C	3.15	1.43	1.35
19	B1	845	CLA	CHC-C1C	3.15	1.43	1.35
19	A1	837	CLA	CHC-C1C	3.15	1.43	1.35
19	A1	807	CLA	C4D-ND	-3.15	1.33	1.37
19	A1	809	CLA	CHC-C1C	3.15	1.43	1.35
19	B2	849	CLA	CMB-C2B	-3.15	1.45	1.51
19	B1	807	CLA	CHC-C1C	3.15	1.43	1.35
19	B	809	CLA	CHC-C1C	3.15	1.43	1.35
19	A1	824	CLA	C4D-ND	-3.15	1.33	1.37
19	B	802	CLA	C4D-ND	-3.15	1.33	1.37
19	A2	801	CLA	C4D-ND	-3.15	1.33	1.37
19	AA	801	CLA	C4D-ND	-3.15	1.33	1.37
19	AA	807	CLA	CHC-C1C	3.15	1.43	1.35
19	A1	819	CLA	C4D-ND	-3.15	1.33	1.37
19	A2	813	CLA	C4D-ND	-3.15	1.33	1.37
23	B	839	BCR	C30-C25	-3.15	1.49	1.53
19	A	811	CLA	C4D-ND	-3.14	1.33	1.37
19	AA	820	CLA	CHC-C1C	3.14	1.43	1.35
19	B1	828	CLA	C4D-ND	-3.14	1.33	1.37
19	A2	834	CLA	C4D-ND	-3.14	1.33	1.37
19	BB	829	CLA	CHC-C1C	3.14	1.43	1.35
19	B1	823	CLA	CHC-C1C	3.14	1.43	1.35
19	FF	301	CLA	CHC-C1C	3.14	1.43	1.35
19	A2	840	CLA	C4D-ND	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	801	CLA	C4D-ND	-3.14	1.33	1.37
19	AA	840	CLA	C4D-ND	-3.14	1.33	1.37
19	A2	809	CLA	CHC-C1C	3.14	1.43	1.35
19	B	805	CLA	CHC-C1C	3.14	1.43	1.35
19	A1	816	CLA	CHC-C1C	3.14	1.43	1.35
19	A1	841	CLA	CHC-C1C	3.14	1.43	1.35
19	BB	816	CLA	CHC-C1C	3.14	1.43	1.35
19	A1	838	CLA	C4D-ND	-3.14	1.33	1.37
19	AA	842	CLA	C4D-ND	-3.14	1.33	1.37
19	FF	305	CLA	C4D-ND	-3.14	1.33	1.37
23	MM	101	BCR	C30-C25	-3.14	1.49	1.53
19	F1	301	CLA	CHC-C1C	3.14	1.43	1.35
19	A	852	CLA	CHC-C1C	3.14	1.43	1.35
19	AA	813	CLA	C4D-ND	-3.14	1.33	1.37
19	AA	825	CLA	C4D-ND	-3.14	1.33	1.37
19	A2	839	CLA	C4D-ND	-3.13	1.33	1.37
19	B	831	CLA	CHC-C1C	3.13	1.43	1.35
19	BB	809	CLA	CHC-C1C	3.13	1.43	1.35
19	AA	809	CLA	CHC-C1C	3.13	1.43	1.35
19	B	846	CLA	CHC-C1C	3.13	1.43	1.35
19	A1	803	CLA	CHC-C1C	3.13	1.43	1.35
19	B1	818	CLA	CHC-C1C	3.13	1.43	1.35
19	A1	817	CLA	CHC-C1C	3.13	1.43	1.35
19	A1	803	CLA	C1D-ND	3.13	1.41	1.37
19	A2	833	CLA	C4D-ND	-3.13	1.33	1.37
19	A2	812	CLA	C4D-ND	-3.13	1.33	1.37
19	L2	205	CLA	C1D-ND	3.13	1.41	1.37
19	B2	818	CLA	CHC-C1C	3.13	1.43	1.35
19	B1	829	CLA	CHC-C1C	3.12	1.43	1.35
19	BB	804	CLA	CHC-C1C	3.12	1.43	1.35
19	B	830	CLA	C1D-ND	3.12	1.41	1.37
19	AA	816	CLA	C4D-ND	-3.12	1.33	1.37
19	B1	832	CLA	C4D-ND	-3.12	1.33	1.37
19	B2	823	CLA	C4D-ND	-3.12	1.33	1.37
19	BB	845	CLA	CHC-C1C	3.12	1.43	1.35
19	A1	833	CLA	C4D-ND	-3.12	1.33	1.37
19	B	828	CLA	C4D-ND	-3.12	1.33	1.37
19	B1	814	CLA	CHC-C1C	3.12	1.43	1.35
19	K2	102	CLA	C4D-ND	-3.12	1.33	1.37
19	B	823	CLA	CHC-C1C	3.12	1.43	1.35
19	B1	848	CLA	CMB-C2B	-3.12	1.45	1.51
19	B2	827	CLA	C4D-ND	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	826	CLA	CHC-C1C	3.12	1.43	1.35
19	BB	831	CLA	CHC-C1C	3.12	1.43	1.35
19	B1	824	CLA	C4D-ND	-3.12	1.33	1.37
19	B2	822	CLA	CHC-C1C	3.12	1.43	1.35
19	AA	819	CLA	CHC-C1C	3.12	1.43	1.35
19	K1	102	CLA	C4D-ND	-3.12	1.33	1.37
19	A	808	CLA	C4D-ND	-3.12	1.33	1.37
19	B	816	CLA	C4D-ND	-3.12	1.33	1.37
19	AA	839	CLA	C4D-ND	-3.12	1.33	1.37
19	F1	305	CLA	CHC-C1C	3.12	1.43	1.35
19	BB	808	CLA	CHC-C1C	3.12	1.43	1.35
19	B	860	CLA	C4D-ND	-3.12	1.33	1.37
19	BB	807	CLA	CHC-C1C	3.12	1.43	1.35
19	B	828	CLA	CHC-C1C	3.11	1.42	1.35
19	AA	801	CLA	CHC-C1C	3.11	1.42	1.35
19	AA	806	CLA	C4D-ND	-3.11	1.33	1.37
19	K1	102	CLA	CHC-C1C	3.11	1.42	1.35
19	B	827	CLA	CHC-C1C	3.11	1.42	1.35
19	BB	805	CLA	CHC-C1C	3.11	1.42	1.35
19	A1	811	CLA	C4D-ND	-3.11	1.33	1.37
19	A2	810	CLA	C4D-ND	-3.11	1.33	1.37
19	A	842	CLA	C4D-ND	-3.11	1.33	1.37
19	BB	824	CLA	CHC-C1C	3.11	1.42	1.35
23	AA	851	BCR	C30-C25	-3.11	1.49	1.53
19	A2	835	CLA	C4D-ND	-3.11	1.33	1.37
19	BB	815	CLA	C4D-ND	-3.11	1.33	1.37
19	A2	818	CLA	CHC-C1C	3.11	1.42	1.35
19	JJ	101	CLA	CHC-C1C	3.11	1.42	1.35
19	B	820	CLA	C4D-ND	-3.11	1.33	1.37
19	AA	830	CLA	C4D-ND	-3.11	1.33	1.37
19	A1	837	CLA	C4D-ND	-3.11	1.33	1.37
19	BB	820	CLA	C4D-ND	-3.11	1.33	1.37
19	B2	826	CLA	CMB-C2B	-3.11	1.45	1.51
19	A1	808	CLA	CHC-C1C	3.11	1.42	1.35
19	A2	838	CLA	CHC-C1C	3.11	1.42	1.35
19	A	844	CLA	CHC-C1C	3.11	1.42	1.35
19	B	832	CLA	CHC-C1C	3.11	1.42	1.35
19	A2	814	CLA	CHC-C1C	3.11	1.42	1.35
19	B	807	CLA	CHC-C1C	3.11	1.42	1.35
19	A2	825	CLA	C4D-ND	-3.11	1.33	1.37
19	A	806	CLA	C4D-ND	-3.11	1.33	1.37
19	B	808	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	822	CLA	C4D-ND	-3.11	1.33	1.37
19	AA	812	CLA	C4D-ND	-3.11	1.33	1.37
19	BB	806	CLA	C4D-ND	-3.11	1.33	1.37
19	A1	813	CLA	CHC-C1C	3.11	1.42	1.35
19	F2	301	CLA	CHC-C1C	3.11	1.42	1.35
19	B1	810	CLA	CHC-C1C	3.10	1.42	1.35
19	B2	829	CLA	C4D-ND	-3.10	1.33	1.37
19	AA	853	CLA	CHC-C1C	3.10	1.42	1.35
19	B1	827	CLA	C4D-ND	-3.10	1.33	1.37
19	B	806	CLA	C4D-ND	-3.10	1.33	1.37
19	BB	802	CLA	C4D-ND	-3.10	1.33	1.37
19	A	813	CLA	C4D-ND	-3.10	1.33	1.37
19	A	825	CLA	C4D-ND	-3.10	1.33	1.37
19	B2	823	CLA	CHC-C1C	3.10	1.42	1.35
19	J	101	CLA	CHC-C1C	3.10	1.42	1.35
19	B	819	CLA	CHC-C1C	3.10	1.42	1.35
19	B	817	CLA	CHC-C1C	3.10	1.42	1.35
19	BB	828	CLA	CHC-C1C	3.10	1.42	1.35
19	B1	822	CLA	CHC-C1C	3.10	1.42	1.35
23	A	850	BCR	C30-C25	-3.10	1.49	1.53
19	A1	810	CLA	CHC-C1C	3.10	1.42	1.35
19	A1	812	CLA	CHC-C1C	3.10	1.42	1.35
19	A	817	CLA	CHC-C1C	3.10	1.42	1.35
19	A1	821	CLA	C4D-ND	-3.10	1.33	1.37
19	A2	807	CLA	C4D-ND	-3.10	1.33	1.37
19	A	812	CLA	C4D-ND	-3.10	1.33	1.37
19	AA	815	CLA	C4D-ND	-3.10	1.33	1.37
19	AA	817	CLA	CHC-C1C	3.10	1.42	1.35
19	BB	817	CLA	CHC-C1C	3.10	1.42	1.35
19	B2	828	CLA	CHC-C1C	3.10	1.42	1.35
19	B1	817	CLA	CHC-C1C	3.09	1.42	1.35
19	K1	103	CLA	CHC-C1C	3.09	1.42	1.35
19	A	811	CLA	CHC-C1C	3.09	1.42	1.35
19	A1	830	CLA	C4D-ND	-3.09	1.33	1.37
19	BB	831	CLA	C4D-ND	-3.09	1.33	1.37
19	F1	305	CLA	C4D-ND	-3.09	1.33	1.37
19	B1	804	CLA	CHC-C1C	3.09	1.42	1.35
19	KK	102	CLA	CHC-C1C	3.09	1.42	1.35
19	BB	803	CLA	C4D-ND	-3.09	1.33	1.37
19	B2	804	CLA	CHC-C1C	3.09	1.42	1.35
19	A2	852	CLA	CHC-C1C	3.09	1.42	1.35
19	K2	104	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	JJ	104	BCR	C30-C25	-3.09	1.49	1.53
19	B2	817	CLA	CHC-C1C	3.09	1.42	1.35
19	A1	852	CLA	CHC-C1C	3.09	1.42	1.35
19	B2	802	CLA	C4D-ND	-3.09	1.33	1.37
19	A2	802	CLA	CHC-C1C	3.09	1.42	1.35
19	A1	815	CLA	C4D-ND	-3.09	1.33	1.37
19	A	828	CLA	C4D-ND	-3.09	1.33	1.37
19	A2	840	CLA	CHC-C1C	3.09	1.42	1.35
19	A	801	CLA	CHC-C1C	3.09	1.42	1.35
19	A2	831	CLA	C4D-ND	-3.09	1.33	1.37
19	B2	836	CLA	C4D-ND	-3.09	1.33	1.37
19	A2	806	CLA	C4D-ND	-3.09	1.33	1.37
19	A2	838	CLA	C4D-ND	-3.09	1.33	1.37
19	BB	828	CLA	C4D-ND	-3.09	1.33	1.37
19	A1	801	CLA	CHC-C1C	3.09	1.42	1.35
19	A2	827	CLA	C4D-ND	-3.09	1.33	1.37
19	B2	819	CLA	CHC-C1C	3.08	1.42	1.35
19	A	821	CLA	C4D-ND	-3.08	1.33	1.37
19	BB	826	CLA	C1D-ND	3.08	1.41	1.37
19	A1	839	CLA	CHC-C1C	3.08	1.42	1.35
19	A2	813	CLA	CHC-C1C	3.08	1.42	1.35
19	BB	852	CLA	CMB-C2B	-3.08	1.45	1.51
19	A	815	CLA	C4D-ND	-3.08	1.33	1.37
19	B1	830	CLA	CHC-C1C	3.08	1.42	1.35
19	AA	838	CLA	CHC-C1C	3.08	1.42	1.35
19	A	809	CLA	CHC-C1C	3.08	1.42	1.35
19	B2	810	CLA	CHC-C1C	3.08	1.42	1.35
19	A2	828	CLA	C4D-ND	-3.08	1.33	1.37
19	B2	828	CLA	C4D-ND	-3.08	1.33	1.37
19	A	818	CLA	CHC-C1C	3.08	1.42	1.35
19	AA	818	CLA	CHC-C1C	3.08	1.42	1.35
19	A	827	CLA	CHC-C1C	3.08	1.42	1.35
19	A1	818	CLA	CHC-C1C	3.08	1.42	1.35
23	M1	101	BCR	C30-C25	-3.08	1.49	1.53
19	A2	808	CLA	C4D-ND	-3.08	1.33	1.37
23	A1	848	BCR	C30-C25	-3.08	1.49	1.53
19	A1	814	CLA	C4D-ND	-3.08	1.33	1.37
19	B	836	CLA	CHC-C1C	3.08	1.42	1.35
19	LL	202	CLA	CHC-C1C	3.08	1.42	1.35
19	A2	842	CLA	CHC-C1C	3.08	1.42	1.35
19	A	838	CLA	CHC-C1C	3.07	1.42	1.35
19	AA	827	CLA	C4D-ND	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	837	CLA	CHC-C1C	3.07	1.42	1.35
19	BB	835	CLA	CHC-C1C	3.07	1.42	1.35
19	B1	802	CLA	C4D-ND	-3.07	1.33	1.37
19	A	827	CLA	C4D-ND	-3.07	1.33	1.37
19	B2	824	CLA	CHC-C1C	3.07	1.42	1.35
19	AA	828	CLA	C4D-ND	-3.07	1.33	1.37
19	A2	801	CLA	CHC-C1C	3.07	1.42	1.35
19	A1	811	CLA	CHC-C1C	3.07	1.42	1.35
19	B1	803	CLA	C4D-ND	-3.07	1.33	1.37
19	B	805	CLA	C4D-ND	-3.07	1.33	1.37
19	A	839	CLA	C4D-ND	-3.07	1.33	1.37
19	AA	824	CLA	C4D-ND	-3.07	1.33	1.37
19	J1	103	CLA	CHC-C1C	3.07	1.42	1.35
19	A1	827	CLA	CHC-C1C	3.07	1.42	1.35
19	AA	845	CLA	CHC-C1C	3.07	1.42	1.35
19	A1	816	CLA	C4D-ND	-3.07	1.33	1.37
19	A	805	CLA	C4D-ND	-3.07	1.33	1.37
19	J2	103	CLA	CHC-C1C	3.07	1.42	1.35
19	A1	826	CLA	C4D-ND	-3.07	1.33	1.37
19	A	837	CLA	C4D-ND	-3.07	1.33	1.37
19	B1	808	CLA	CHC-C1C	3.07	1.42	1.35
19	BB	810	CLA	CHC-C1C	3.07	1.42	1.35
19	A2	811	CLA	CHC-C1C	3.07	1.42	1.35
19	AA	831	CLA	C4D-ND	-3.07	1.33	1.37
19	K	102	CLA	CHC-C1C	3.06	1.42	1.35
19	AA	837	CLA	CHC-C1C	3.06	1.42	1.35
19	A2	842	CLA	C4D-ND	-3.06	1.33	1.37
23	A2	848	BCR	C30-C25	-3.06	1.49	1.53
19	B1	808	CLA	C4D-ND	-3.06	1.33	1.37
19	B1	848	CLA	C4D-ND	-3.06	1.33	1.37
19	A2	818	CLA	C4D-ND	-3.06	1.33	1.37
19	AA	821	CLA	C4D-ND	-3.06	1.33	1.37
19	B2	808	CLA	C4D-ND	-3.06	1.33	1.37
19	A	807	CLA	C4D-ND	-3.06	1.33	1.37
19	B	810	CLA	CHC-C1C	3.06	1.42	1.35
19	A2	805	CLA	CHC-C1C	3.06	1.42	1.35
19	AA	822	CLA	C4D-ND	-3.06	1.33	1.37
19	BB	805	CLA	C4D-ND	-3.06	1.33	1.37
19	AA	828	CLA	CHC-C1C	3.06	1.42	1.35
19	A	831	CLA	C4D-ND	-3.06	1.33	1.37
19	B	836	CLA	C4D-ND	-3.06	1.33	1.37
19	KK	101	CLA	C4D-ND	-3.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	827	CLA	CHC-C1C	3.06	1.42	1.35
19	B2	831	CLA	CHC-C1C	3.06	1.42	1.35
19	AA	810	CLA	C4D-ND	-3.06	1.33	1.37
19	B2	849	CLA	C4D-ND	-3.06	1.33	1.37
23	F	303	BCR	C30-C25	-3.06	1.49	1.53
19	A1	806	CLA	C4D-ND	-3.06	1.33	1.37
19	A2	819	CLA	CHC-C1C	3.06	1.42	1.35
19	AA	807	CLA	C4D-ND	-3.06	1.33	1.37
19	L	203	CLA	CHC-C1C	3.06	1.42	1.35
19	A1	841	CLA	C4D-ND	-3.06	1.33	1.37
19	BB	814	CLA	C4D-ND	-3.06	1.33	1.37
19	KK	102	CLA	C4D-ND	-3.06	1.33	1.37
19	B1	812	CLA	CHC-C1C	3.06	1.42	1.35
19	A1	803	CLA	C4D-ND	-3.06	1.33	1.37
19	A1	817	CLA	C4D-ND	-3.06	1.33	1.37
19	B2	815	CLA	C4D-ND	-3.06	1.33	1.37
19	A2	819	CLA	C4D-ND	-3.06	1.33	1.37
19	B2	830	CLA	CHC-C1C	3.05	1.42	1.35
19	A1	834	CLA	C4D-ND	-3.05	1.33	1.37
19	A2	822	CLA	C4D-ND	-3.05	1.33	1.37
19	JJ	103	CLA	CHC-C1C	3.05	1.42	1.35
19	B1	835	CLA	C4D-ND	-3.05	1.33	1.37
19	B	803	CLA	C4D-ND	-3.05	1.33	1.37
19	B1	815	CLA	CHC-C1C	3.05	1.42	1.35
19	AA	811	CLA	CHC-C1C	3.05	1.42	1.35
19	A	810	CLA	C4D-ND	-3.05	1.33	1.37
19	B	854	CLA	C4D-ND	-3.05	1.33	1.37
19	B	837	CLA	CHC-C1C	3.05	1.42	1.35
19	A2	822	CLA	CHC-C1C	3.05	1.42	1.35
19	FF	301	CLA	C4D-ND	-3.05	1.33	1.37
19	L1	206	CLA	CHC-C1C	3.05	1.42	1.35
19	A	826	CLA	CHC-C1C	3.05	1.42	1.35
19	AA	827	CLA	CHC-C1C	3.05	1.42	1.35
19	B	819	CLA	C4D-ND	-3.05	1.33	1.37
19	A1	824	CLA	CHC-C1C	3.05	1.42	1.35
19	AA	835	CLA	C4D-ND	-3.05	1.33	1.37
19	AA	837	CLA	C4D-ND	-3.05	1.33	1.37
19	BB	835	CLA	C4D-ND	-3.05	1.33	1.37
19	B2	812	CLA	CHC-C1C	3.05	1.42	1.35
19	A2	812	CLA	CHC-C1C	3.04	1.42	1.35
19	B2	837	CLA	CHC-C1C	3.04	1.42	1.35
19	L2	205	CLA	CHC-C1C	3.04	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K1	105	CLA	CHC-C1C	3.04	1.42	1.35
19	B2	815	CLA	CHC-C1C	3.04	1.42	1.35
19	A	828	CLA	CHC-C1C	3.04	1.42	1.35
19	A1	813	CLA	C4D-ND	-3.04	1.33	1.37
19	A	818	CLA	C4D-ND	-3.04	1.33	1.37
19	B2	819	CLA	C4D-ND	-3.04	1.33	1.37
19	AA	843	CLA	C4D-ND	-3.04	1.33	1.37
19	F2	302	CLA	CHC-C1C	3.04	1.42	1.35
19	AA	818	CLA	C4D-ND	-3.04	1.33	1.37
19	B1	829	CLA	C1D-ND	3.04	1.41	1.37
19	A	812	CLA	CHC-C1C	3.04	1.42	1.35
19	B2	808	CLA	CHC-C1C	3.04	1.42	1.35
19	K1	103	CLA	C4D-ND	-3.04	1.33	1.37
19	AA	805	CLA	C4D-ND	-3.04	1.33	1.37
19	BB	827	CLA	C4D-ND	-3.04	1.33	1.37
19	A1	821	CLA	CHC-C1C	3.04	1.42	1.35
19	A1	804	CLA	CHC-C1C	3.04	1.42	1.35
19	B1	836	CLA	CHC-C1C	3.04	1.42	1.35
19	A2	815	CLA	C4D-ND	-3.04	1.33	1.37
19	A1	844	CLA	C4D-ND	-3.04	1.33	1.37
19	A2	837	CLA	C4D-ND	-3.04	1.33	1.37
19	AA	833	CLA	C4D-ND	-3.04	1.33	1.37
19	A1	827	CLA	C4D-ND	-3.04	1.33	1.37
19	AA	823	CLA	C4D-ND	-3.04	1.33	1.37
19	X1	101	CLA	CHC-C1C	3.03	1.42	1.35
19	AA	812	CLA	CHC-C1C	3.03	1.42	1.35
19	A2	817	CLA	C4D-ND	-3.03	1.33	1.37
19	B	832	CLA	C4D-ND	-3.03	1.33	1.37
19	K	101	CLA	C4D-ND	-3.03	1.33	1.37
19	BB	829	CLA	C1D-ND	3.03	1.41	1.37
23	M2	102	BCR	C30-C25	-3.03	1.49	1.53
19	B2	852	CLA	C4D-ND	-3.03	1.33	1.37
19	B	826	CLA	C4D-ND	-3.03	1.33	1.37
19	BB	819	CLA	C4D-ND	-3.03	1.33	1.37
19	A	840	CLA	CHC-C1C	3.03	1.42	1.35
19	B	824	CLA	CHC-C1C	3.03	1.42	1.35
19	AA	813	CLA	CHC-C1C	3.03	1.42	1.35
19	B1	820	CLA	C4D-ND	-3.03	1.33	1.37
19	A2	814	CLA	C4D-ND	-3.03	1.33	1.37
19	F	301	CLA	CHC-C1C	3.03	1.42	1.35
19	X2	101	CLA	CHC-C1C	3.03	1.42	1.35
19	A	822	CLA	CHC-C1C	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	832	CLA	C4D-ND	-3.03	1.33	1.37
19	A1	838	CLA	CHC-C1C	3.03	1.42	1.35
19	B1	801	CLA	CHC-C1C	3.03	1.42	1.35
19	A2	805	CLA	C4D-ND	-3.03	1.33	1.37
19	BB	852	CLA	C4D-ND	-3.03	1.33	1.37
19	A1	836	CLA	CHC-C1C	3.03	1.42	1.35
19	A2	828	CLA	CHC-C1C	3.03	1.42	1.35
19	A1	836	CLA	C4D-ND	-3.03	1.33	1.37
19	BB	816	CLA	C4D-ND	-3.03	1.33	1.37
19	B2	830	CLA	C1D-ND	3.03	1.41	1.37
19	A	808	CLA	CHC-C1C	3.03	1.42	1.35
19	B	814	CLA	CHC-C1C	3.03	1.42	1.35
19	B	821	CLA	C4D-ND	-3.03	1.33	1.37
23	A1	849	BCR	C30-C25	-3.03	1.49	1.53
19	B2	814	CLA	CHC-C1C	3.02	1.42	1.35
19	X	101	CLA	CHC-C1C	3.02	1.42	1.35
19	A1	818	CLA	C4D-ND	-3.02	1.33	1.37
19	L2	204	CLA	C4D-ND	-3.02	1.33	1.37
19	L	202	CLA	C4D-ND	-3.02	1.33	1.37
19	XX	101	CLA	C4D-ND	-3.02	1.33	1.37
19	B2	803	CLA	C4D-ND	-3.02	1.33	1.37
19	BB	811	CLA	C4D-ND	-3.02	1.33	1.37
19	B2	801	CLA	CHC-C1C	3.02	1.42	1.35
19	A	805	CLA	CHC-C1C	3.02	1.42	1.35
19	AA	819	CLA	C4D-ND	-3.02	1.33	1.37
19	FF	302	CLA	CHC-C1C	3.02	1.42	1.35
19	B	827	CLA	C4D-ND	-3.02	1.33	1.37
19	A	824	CLA	C4D-ND	-3.02	1.33	1.37
23	KK	103	BCR	C30-C25	-3.02	1.49	1.53
19	B2	836	CLA	CHC-C1C	3.02	1.42	1.35
19	B	834	CLA	CHC-C1C	3.02	1.42	1.35
19	XX	101	CLA	CHC-C1C	3.02	1.42	1.35
19	B2	805	CLA	CHC-C1C	3.02	1.42	1.35
19	A	833	CLA	CHC-C1C	3.02	1.42	1.35
19	A	820	CLA	C4D-ND	-3.02	1.33	1.37
19	AA	825	CLA	CHC-C1C	3.02	1.42	1.35
19	B	818	CLA	CHC-C1C	3.02	1.42	1.35
19	J	103	CLA	CHC-C1C	3.01	1.42	1.35
23	K	103	BCR	C30-C25	-3.01	1.49	1.53
19	A2	837	CLA	CHC-C1C	3.01	1.42	1.35
19	B2	832	CLA	CHC-C1C	3.01	1.42	1.35
19	A2	833	CLA	CHC-C1C	3.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	805	CLA	CHC-C1C	3.01	1.42	1.35
19	A	825	CLA	CHC-C1C	3.01	1.42	1.35
19	L1	205	CLA	C4D-ND	-3.01	1.33	1.37
19	A	814	CLA	C4D-ND	-3.01	1.33	1.37
19	A	835	CLA	C4D-ND	-3.01	1.33	1.37
19	B2	820	CLA	C4D-ND	-3.01	1.33	1.37
19	B1	805	CLA	CHC-C1C	3.01	1.42	1.35
19	A1	804	CLA	C4D-ND	-3.01	1.33	1.37
19	B1	821	CLA	CHC-C1C	3.01	1.42	1.35
19	AA	840	CLA	CHC-C1C	3.01	1.42	1.35
19	A2	802	CLA	C4D-ND	-3.01	1.33	1.37
19	A2	804	CLA	C4D-ND	-3.01	1.33	1.37
19	B	804	CLA	C4D-ND	-3.01	1.33	1.37
19	AA	833	CLA	CHC-C1C	3.01	1.42	1.35
19	A2	820	CLA	CHC-C1C	3.01	1.42	1.35
19	BB	836	CLA	CHC-C1C	3.01	1.42	1.35
19	A1	832	CLA	C4D-ND	-3.01	1.33	1.37
19	B1	805	CLA	C4D-ND	-3.01	1.33	1.37
19	A2	836	CLA	C4D-ND	-3.01	1.33	1.37
19	B2	805	CLA	C4D-ND	-3.01	1.33	1.37
19	A	821	CLA	CHC-C1C	3.00	1.42	1.35
19	A2	844	CLA	C4D-ND	-3.00	1.33	1.37
19	A	823	CLA	C4D-ND	-3.00	1.33	1.37
19	BB	804	CLA	C4D-ND	-3.00	1.33	1.37
19	A2	825	CLA	CHC-C1C	3.00	1.42	1.35
19	A	804	CLA	C4D-ND	-3.00	1.33	1.37
19	A	844	CLA	C4D-ND	-3.00	1.33	1.37
19	F1	302	CLA	CHC-C1C	3.00	1.42	1.35
19	A	819	CLA	CHC-C1C	3.00	1.42	1.35
19	B2	806	CLA	C4D-ND	-3.00	1.33	1.37
19	A2	834	CLA	CHC-C1C	3.00	1.42	1.35
19	B2	821	CLA	C4D-ND	-3.00	1.33	1.37
19	AA	808	CLA	CHC-C1C	3.00	1.42	1.35
19	X	101	CLA	C4D-ND	-3.00	1.33	1.37
19	F	302	CLA	CHC-C1C	3.00	1.42	1.35
19	A	819	CLA	C4D-ND	-3.00	1.33	1.37
23	A1	849	BCR	C1-C6	-3.00	1.49	1.53
23	II	104	BCR	C30-C25	-3.00	1.49	1.53
19	K	102	CLA	C4D-ND	-3.00	1.33	1.37
19	AA	814	CLA	C4D-ND	-3.00	1.33	1.37
23	F2	305	BCR	C30-C25	-3.00	1.49	1.53
19	B2	816	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	816	CLA	C4D-ND	-3.00	1.33	1.37
19	B	846	CLA	C4D-ND	-3.00	1.33	1.37
19	A1	829	CLA	CHC-C1C	3.00	1.42	1.35
19	A2	839	CLA	CHC-C1C	3.00	1.42	1.35
19	A	813	CLA	CHC-C1C	3.00	1.42	1.35
19	A2	809	CLA	C4D-ND	-3.00	1.33	1.37
19	A	820	CLA	CHC-C1C	3.00	1.42	1.35
19	AA	826	CLA	CHC-C1C	3.00	1.42	1.35
19	A1	833	CLA	CHC-C1C	3.00	1.42	1.35
19	A1	828	CLA	CHC-C1C	3.00	1.42	1.35
19	A2	844	CLA	CHC-C1C	3.00	1.42	1.35
19	B1	821	CLA	C4D-ND	-3.00	1.33	1.37
19	B	831	CLA	C4D-ND	-3.00	1.33	1.37
19	B1	835	CLA	CHC-C1C	2.99	1.42	1.35
23	A2	849	BCR	C30-C25	-2.99	1.49	1.53
19	B1	804	CLA	C4D-ND	-2.99	1.33	1.37
19	B1	819	CLA	C4D-ND	-2.99	1.33	1.37
19	B	814	CLA	C4D-ND	-2.99	1.33	1.37
23	A	849	BCR	C30-C25	-2.99	1.49	1.53
19	AA	822	CLA	CHC-C1C	2.99	1.42	1.35
23	AA	850	BCR	C30-C25	-2.99	1.49	1.53
19	B	812	CLA	CHC-C1C	2.99	1.42	1.35
19	A	832	CLA	C4D-ND	-2.99	1.33	1.37
23	F1	306	BCR	C30-C25	-2.99	1.49	1.53
19	B1	811	CLA	C4D-ND	-2.99	1.33	1.37
19	B	811	CLA	C4D-ND	-2.99	1.33	1.37
19	A2	821	CLA	CHC-C1C	2.99	1.42	1.35
19	AA	808	CLA	C4D-ND	-2.99	1.33	1.37
19	BB	825	CLA	CHC-C1C	2.99	1.42	1.35
19	B1	834	CLA	CHC-C1C	2.99	1.42	1.35
19	A1	844	CLA	CHC-C1C	2.99	1.42	1.35
19	BB	819	CLA	CHC-C1C	2.99	1.42	1.35
23	FF	303	BCR	C30-C25	-2.99	1.49	1.53
19	BB	814	CLA	CHC-C1C	2.99	1.42	1.35
19	AA	809	CLA	C4D-ND	-2.99	1.33	1.37
19	J1	101	CLA	C4D-ND	-2.99	1.33	1.37
19	AA	845	CLA	C4D-ND	-2.99	1.33	1.37
19	AA	821	CLA	CHC-C1C	2.99	1.42	1.35
19	B1	822	CLA	C4D-ND	-2.99	1.33	1.37
19	BB	817	CLA	C4D-ND	-2.99	1.33	1.37
19	BB	826	CLA	CMD-C2D	-2.98	1.44	1.50
19	AA	839	CLA	CHC-C1C	2.98	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	836	CLA	C4D-ND	-2.98	1.33	1.37
19	A1	825	CLA	CHC-C1C	2.98	1.42	1.35
19	B	801	CLA	CHC-C1C	2.98	1.42	1.35
19	AA	824	CLA	CHC-C1C	2.98	1.42	1.35
19	BB	803	CLA	CHC-C1C	2.98	1.42	1.35
19	A	836	CLA	C4D-ND	-2.98	1.33	1.37
19	B	803	CLA	CHC-C1C	2.98	1.42	1.35
19	AA	838	CLA	C4D-ND	-2.98	1.33	1.37
19	A1	819	CLA	CHC-C1C	2.98	1.42	1.35
19	B	825	CLA	CHC-C1C	2.98	1.42	1.35
19	B1	816	CLA	C4D-ND	-2.98	1.33	1.37
19	B2	811	CLA	C4D-ND	-2.98	1.33	1.37
19	A	834	CLA	CHC-C1C	2.98	1.42	1.35
19	BB	830	CLA	CHC-C1C	2.98	1.42	1.35
19	B2	804	CLA	C4D-ND	-2.98	1.33	1.37
19	AA	830	CLA	CHC-C1C	2.98	1.42	1.35
19	JJ	103	CLA	C4D-ND	-2.98	1.33	1.37
19	A2	824	CLA	CHC-C1C	2.98	1.42	1.35
20	A1	802	CL0	C3D-C2D	2.98	1.47	1.39
19	A	824	CLA	CHC-C1C	2.98	1.42	1.35
19	A	839	CLA	CHC-C1C	2.98	1.42	1.35
19	B	812	CLA	C4D-ND	-2.97	1.33	1.37
19	A1	832	CLA	CHC-C1C	2.97	1.42	1.35
19	A	838	CLA	C4D-ND	-2.97	1.33	1.37
19	BB	822	CLA	C4D-ND	-2.97	1.33	1.37
19	BB	845	CLA	C4D-ND	-2.97	1.33	1.37
19	BB	856	CLA	C4D-ND	-2.97	1.33	1.37
19	A1	820	CLA	CHC-C1C	2.97	1.42	1.35
19	L1	205	CLA	CHC-C1C	2.97	1.42	1.35
19	B2	834	CLA	CMB-C2B	-2.97	1.45	1.51
19	AA	834	CLA	CHC-C1C	2.97	1.42	1.35
19	A2	824	CLA	C4D-ND	-2.97	1.33	1.37
19	L2	204	CLA	CHC-C1C	2.97	1.42	1.35
19	A1	808	CLA	C4D-ND	-2.97	1.33	1.37
19	B1	814	CLA	C4D-ND	-2.97	1.33	1.37
19	A1	823	CLA	CHC-C1C	2.97	1.42	1.35
19	A2	808	CLA	CHC-C1C	2.97	1.42	1.35
19	AA	836	CLA	CHC-C1C	2.97	1.42	1.35
19	B1	825	CLA	CHC-C1C	2.96	1.42	1.35
19	L2	206	CLA	CHC-C1C	2.96	1.42	1.35
19	BB	812	CLA	CHC-C1C	2.96	1.42	1.35
19	B	813	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	204	CLA	CHC-C1C	2.96	1.42	1.35
23	A	849	BCR	C1-C6	-2.96	1.49	1.53
19	A1	842	CLA	C4D-ND	-2.96	1.33	1.37
19	B1	831	CLA	C4D-ND	-2.96	1.33	1.37
19	A1	807	CLA	CHC-C1C	2.96	1.42	1.35
19	B1	806	CLA	CHC-C1C	2.96	1.42	1.35
19	B1	849	CLA	CHC-C1C	2.96	1.42	1.35
19	B	806	CLA	CHC-C1C	2.96	1.42	1.35
19	B	815	CLA	CHC-C1C	2.96	1.42	1.35
19	B2	835	CLA	CHC-C1C	2.96	1.42	1.35
19	B	859	CLA	C4D-ND	-2.96	1.33	1.37
19	J	103	CLA	C4D-ND	-2.96	1.33	1.37
19	A2	830	CLA	CHC-C1C	2.96	1.42	1.35
19	B2	818	CLA	C4D-ND	-2.96	1.33	1.37
19	B2	803	CLA	CHC-C1C	2.96	1.42	1.35
19	J	101	CLA	C4D-ND	-2.96	1.33	1.37
19	B	821	CLA	CHC-C1C	2.96	1.42	1.35
19	X1	101	CLA	C4D-ND	-2.96	1.33	1.37
19	J2	101	CLA	C4D-ND	-2.95	1.33	1.37
19	BB	815	CLA	CHC-C1C	2.95	1.42	1.35
19	A	809	CLA	C4D-ND	-2.95	1.33	1.37
19	A1	831	CLA	C4D-ND	-2.95	1.33	1.37
19	B2	832	CLA	C4D-ND	-2.95	1.33	1.37
19	B1	831	CLA	CHC-C1C	2.95	1.42	1.35
19	L1	207	CLA	CHC-C1C	2.95	1.42	1.35
23	AA	848	BCR	C30-C25	-2.95	1.49	1.53
19	LL	201	CLA	C4D-ND	-2.95	1.33	1.37
19	BB	830	CLA	C4D-ND	-2.95	1.33	1.37
19	B2	850	CLA	CHC-C1C	2.95	1.42	1.35
19	BB	834	CLA	CHC-C1C	2.95	1.42	1.35
19	A2	816	CLA	C4D-ND	-2.95	1.33	1.37
19	B1	815	CLA	C4D-ND	-2.95	1.33	1.37
19	B	822	CLA	C4D-ND	-2.95	1.33	1.37
19	BB	836	CLA	C4D-ND	-2.95	1.33	1.37
20	AA	803	CL0	C3D-C2D	2.95	1.47	1.39
19	BB	821	CLA	C4D-ND	-2.95	1.33	1.37
23	L	205	BCR	C30-C25	-2.95	1.49	1.53
19	B1	818	CLA	C4D-ND	-2.94	1.33	1.37
19	BB	806	CLA	CHC-C1C	2.94	1.42	1.35
20	A2	803	CL0	C3D-C2D	2.94	1.47	1.39
19	B2	821	CLA	CHC-C1C	2.94	1.42	1.35
19	B1	806	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	JJ	101	CLA	C4D-ND	-2.94	1.33	1.37
19	B1	803	CLA	CHC-C1C	2.94	1.42	1.35
23	A	847	BCR	C30-C25	-2.94	1.49	1.53
19	A	833	CLA	C4D-ND	-2.94	1.33	1.37
19	B2	812	CLA	C4D-ND	-2.94	1.33	1.37
19	B2	814	CLA	C4D-ND	-2.94	1.33	1.37
19	A	836	CLA	CHC-C1C	2.93	1.42	1.35
19	B1	812	CLA	C4D-ND	-2.93	1.33	1.37
19	A2	832	CLA	C4D-ND	-2.93	1.33	1.37
23	F2	303	BCR	C30-C25	-2.93	1.49	1.53
19	A2	826	CLA	CHC-C1C	2.93	1.42	1.35
19	B	830	CLA	CHC-C1C	2.93	1.42	1.35
19	A	817	CLA	C4D-ND	-2.93	1.33	1.37
19	B	817	CLA	C4D-ND	-2.93	1.33	1.37
19	BB	812	CLA	C4D-ND	-2.93	1.33	1.37
19	B	835	CLA	CHC-C1C	2.93	1.42	1.35
19	AA	831	CLA	CHC-C1C	2.93	1.42	1.35
19	L	202	CLA	CHC-C1C	2.92	1.42	1.35
23	B	842	BCR	C30-C25	-2.92	1.49	1.53
19	BB	833	CLA	CHC-C1C	2.92	1.42	1.35
19	J1	103	CLA	C4D-ND	-2.92	1.33	1.37
19	A2	823	CLA	C4D-ND	-2.92	1.33	1.37
19	J2	103	CLA	C4D-ND	-2.92	1.33	1.37
19	B1	830	CLA	C4D-ND	-2.92	1.33	1.37
19	L1	207	CLA	C4D-ND	-2.92	1.33	1.37
19	A	829	CLA	CHC-C1C	2.92	1.42	1.35
19	B2	825	CLA	CHC-C1C	2.92	1.42	1.35
19	B1	817	CLA	C4D-ND	-2.92	1.33	1.37
19	X2	101	CLA	C4D-ND	-2.92	1.33	1.37
19	B2	813	CLA	C4D-ND	-2.92	1.33	1.37
19	K2	104	CLA	C4D-ND	-2.91	1.33	1.37
19	AA	804	CLA	C4D-ND	-2.91	1.33	1.37
19	A2	831	CLA	CHC-C1C	2.91	1.42	1.35
19	B2	822	CLA	C4D-ND	-2.91	1.33	1.37
19	A1	829	CLA	C4D-ND	-2.91	1.33	1.37
19	B2	826	CLA	C4D-ND	-2.91	1.33	1.37
19	AA	817	CLA	C4D-ND	-2.91	1.33	1.37
19	B1	826	CLA	C4D-ND	-2.91	1.33	1.37
19	B	837	CLA	C4D-ND	-2.91	1.33	1.37
20	A	803	CL0	C3D-C2D	2.91	1.47	1.39
19	L	203	CLA	CMB-C2B	-2.91	1.45	1.51
19	B	818	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	813	CLA	C4D-ND	-2.91	1.33	1.37
19	BB	801	CLA	CHC-C1C	2.91	1.42	1.35
19	A1	823	CLA	C4D-ND	-2.90	1.33	1.37
19	A	831	CLA	CHC-C1C	2.90	1.42	1.35
23	BB	841	BCR	C30-C25	-2.90	1.49	1.53
19	B1	801	CLA	C4D-ND	-2.90	1.33	1.37
19	BB	818	CLA	C4D-ND	-2.90	1.33	1.37
19	LL	201	CLA	CHC-C1C	2.90	1.42	1.35
19	A1	835	CLA	C4D-ND	-2.90	1.33	1.37
19	B2	837	CLA	C4D-ND	-2.90	1.33	1.37
19	B	807	CLA	C4D-ND	-2.90	1.33	1.37
19	A	830	CLA	CHC-C1C	2.90	1.42	1.35
19	B	858	CLA	CHC-C1C	2.90	1.42	1.35
19	A1	830	CLA	CHC-C1C	2.90	1.42	1.35
19	B1	813	CLA	C4D-ND	-2.90	1.33	1.37
19	A1	842	CLA	CHC-C1C	2.90	1.42	1.35
19	A1	835	CLA	CHC-C1C	2.89	1.42	1.35
19	B1	836	CLA	C4D-ND	-2.89	1.33	1.37
19	BB	833	CLA	CMB-C2B	-2.89	1.45	1.51
19	FF	302	CLA	C4D-ND	-2.89	1.33	1.37
19	B2	817	CLA	C4D-ND	-2.89	1.33	1.37
19	AA	829	CLA	CHC-C1C	2.89	1.42	1.35
19	B2	852	CLA	CHC-C1C	2.89	1.42	1.35
19	B2	806	CLA	CHC-C1C	2.89	1.42	1.35
19	B	809	CLA	C4D-ND	-2.88	1.33	1.37
19	A2	837	CLA	CMB-C2B	-2.88	1.45	1.51
19	B1	850	CLA	C4D-ND	-2.88	1.33	1.37
19	BB	826	CLA	CHC-C1C	2.88	1.42	1.35
19	A2	832	CLA	CHC-C1C	2.88	1.42	1.35
19	BB	809	CLA	C4D-ND	-2.88	1.33	1.37
19	B2	826	CLA	CHC-C1C	2.88	1.42	1.35
23	A1	847	BCR	C30-C25	-2.87	1.49	1.53
19	B2	851	CLA	C4D-ND	-2.87	1.33	1.37
19	B1	845	CLA	C4D-ND	-2.87	1.33	1.37
19	B	834	CLA	CMB-C2B	-2.87	1.45	1.51
19	BB	807	CLA	C4D-ND	-2.87	1.33	1.37
23	I2	103	BCR	C30-C25	-2.87	1.49	1.53
19	B2	831	CLA	C4D-ND	-2.87	1.33	1.37
19	B2	801	CLA	C4D-ND	-2.87	1.33	1.37
19	B2	846	CLA	C4D-ND	-2.87	1.33	1.37
19	AA	832	CLA	CHC-C1C	2.86	1.42	1.35
19	BB	825	CLA	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	847	BCR	C30-C25	-2.86	1.49	1.53
19	B1	825	CLA	C4D-ND	-2.86	1.33	1.37
19	F	302	CLA	C4D-ND	-2.85	1.33	1.37
19	AA	843	CLA	CHC-C1C	2.85	1.42	1.35
19	A1	840	CLA	CHC-C1C	2.85	1.42	1.35
19	B1	807	CLA	C4D-ND	-2.85	1.33	1.37
19	BB	816	CLA	CMB-C2B	-2.85	1.45	1.51
23	B1	841	BCR	C30-C25	-2.85	1.49	1.53
19	B2	825	CLA	C4D-ND	-2.85	1.33	1.37
19	LL	203	CLA	CHC-C1C	2.85	1.42	1.35
19	A2	836	CLA	CHC-C1C	2.84	1.42	1.35
19	A	841	CLA	CHC-C1C	2.84	1.42	1.35
19	B1	833	CLA	CMB-C2B	-2.84	1.45	1.51
19	AA	841	CLA	CHC-C1C	2.84	1.42	1.35
23	FF	306	BCR	C30-C25	-2.84	1.49	1.53
19	B1	809	CLA	C4D-ND	-2.84	1.33	1.37
19	A2	836	CLA	CMB-C2B	-2.84	1.45	1.51
19	A2	841	CLA	CHC-C1C	2.83	1.42	1.35
19	B	860	CLA	CHC-C1C	2.83	1.42	1.35
19	BB	826	CLA	C4D-ND	-2.83	1.33	1.37
19	B2	807	CLA	C4D-ND	-2.83	1.33	1.37
19	BB	855	CLA	CHC-C1C	2.83	1.42	1.35
19	B	834	CLA	C4D-ND	-2.83	1.33	1.37
23	L1	208	BCR	C30-C25	-2.82	1.49	1.53
19	BB	833	CLA	C4D-ND	-2.82	1.33	1.37
19	B1	826	CLA	CHC-C1C	2.82	1.42	1.35
19	B2	809	CLA	C4D-ND	-2.82	1.33	1.37
19	L2	206	CLA	C4D-ND	-2.82	1.33	1.37
19	B	825	CLA	C4D-ND	-2.82	1.33	1.37
23	F	305	BCR	C30-C25	-2.81	1.49	1.53
19	F1	302	CLA	C4D-ND	-2.81	1.33	1.37
19	B	826	CLA	CHC-C1C	2.81	1.42	1.35
19	B	833	CLA	CHC-C1C	2.80	1.42	1.35
19	A1	831	CLA	CHC-C1C	2.80	1.42	1.35
19	B	816	CLA	CMB-C2B	-2.80	1.45	1.51
23	F1	303	BCR	C30-C25	-2.79	1.49	1.53
19	BB	852	CLA	CHC-C1C	2.79	1.42	1.35
19	A1	836	CLA	CMB-C2B	-2.79	1.45	1.51
19	B2	833	CLA	CHC-C1C	2.78	1.42	1.35
19	BB	832	CLA	CHC-C1C	2.78	1.42	1.35
19	A	832	CLA	CHC-C1C	2.78	1.42	1.35
19	BB	808	CLA	CMB-C2B	-2.78	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F2	302	CLA	C4D-ND	-2.78	1.33	1.37
19	K1	105	CLA	C4D-ND	-2.77	1.33	1.37
23	AA	850	BCR	C1-C6	-2.77	1.50	1.53
19	F2	301	CLA	C4D-ND	-2.76	1.33	1.37
19	B	854	CLA	CMB-C2B	-2.76	1.45	1.51
19	B2	834	CLA	C3B-C2B	-2.76	1.36	1.40
19	B2	850	CLA	CMB-C2B	-2.75	1.45	1.51
19	AA	837	CLA	CMB-C2B	-2.75	1.45	1.51
19	A	831	CLA	CMB-C2B	-2.75	1.45	1.51
19	B	854	CLA	CHC-C1C	2.75	1.42	1.35
19	B	801	CLA	C4D-ND	-2.74	1.33	1.37
19	BB	801	CLA	C4D-ND	-2.74	1.33	1.37
19	AA	820	CLA	CMB-C2B	-2.74	1.45	1.51
19	F	301	CLA	C4D-ND	-2.74	1.33	1.37
19	BB	802	CLA	CMB-C2B	-2.74	1.46	1.51
19	A	837	CLA	CMB-C2B	-2.73	1.46	1.51
19	AA	832	CLA	CMB-C2B	-2.73	1.46	1.51
19	L2	205	CLA	CMB-C2B	-2.72	1.46	1.51
19	L1	206	CLA	CMB-C2B	-2.72	1.46	1.51
19	B2	852	CLA	CMB-C2B	-2.72	1.46	1.51
19	B	860	CLA	CMB-C2B	-2.72	1.46	1.51
19	A2	827	CLA	CMB-C2B	-2.72	1.46	1.51
19	B2	814	CLA	CMB-C2B	-2.72	1.46	1.51
19	B	802	CLA	CMB-C2B	-2.72	1.46	1.51
19	F1	301	CLA	C4D-ND	-2.71	1.34	1.37
23	B1	839	BCR	C30-C25	-2.71	1.50	1.53
19	BB	831	CLA	C3B-C2B	-2.70	1.36	1.40
19	B2	834	CLA	C4D-ND	-2.70	1.34	1.37
19	B1	832	CLA	CHC-C1C	2.70	1.41	1.35
19	A1	824	CLA	CMB-C2B	-2.70	1.46	1.51
19	A	820	CLA	CMB-C2B	-2.70	1.46	1.51
19	A2	831	CLA	CMB-C2B	-2.70	1.46	1.51
19	AA	831	CLA	CMB-C2B	-2.69	1.46	1.51
19	A2	825	CLA	CMB-C2B	-2.69	1.46	1.51
19	B1	816	CLA	CMB-C2B	-2.69	1.46	1.51
19	LL	202	CLA	CMB-C2B	-2.69	1.46	1.51
19	A1	830	CLA	CMB-C2B	-2.68	1.46	1.51
23	A2	849	BCR	C1-C6	-2.68	1.50	1.53
19	B2	849	CLA	CHC-C1C	2.67	1.41	1.35
19	A1	831	CLA	CMB-C2B	-2.67	1.46	1.51
19	A2	820	CLA	CMB-C2B	-2.67	1.46	1.51
23	K1	106	BCR	C30-C25	-2.67	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	832	CLA	CMB-C2B	-2.67	1.46	1.51
20	A	803	CL0	C1D-C2D	2.67	1.50	1.45
19	A2	820	CLA	C3B-CAB	-2.67	1.42	1.47
23	BB	839	BCR	C30-C25	-2.66	1.50	1.53
19	A2	823	CLA	CMB-C2B	-2.66	1.46	1.51
19	F2	302	CLA	CMB-C2B	-2.66	1.46	1.51
19	LL	203	CLA	C4D-ND	-2.66	1.34	1.37
19	B1	803	CLA	CMB-C2B	-2.66	1.46	1.51
23	B	840	BCR	C30-C25	-2.65	1.50	1.53
19	A1	819	CLA	CMB-C2B	-2.65	1.46	1.51
19	B	814	CLA	CMB-C2B	-2.65	1.46	1.51
19	A2	824	CLA	CMB-C2B	-2.65	1.46	1.51
19	FF	301	CLA	CMB-C2B	-2.65	1.46	1.51
19	B1	807	CLA	CMD-C2D	-2.65	1.45	1.50
19	BB	855	CLA	CMB-C2B	-2.64	1.46	1.51
19	BB	814	CLA	CMB-C2B	-2.64	1.46	1.51
19	A2	811	CLA	CMB-C2B	-2.64	1.46	1.51
19	LL	201	CLA	CMB-C2B	-2.64	1.46	1.51
19	A	822	CLA	CMB-C2B	-2.64	1.46	1.51
19	B	803	CLA	CMB-C2B	-2.63	1.46	1.51
19	A1	819	CLA	C3B-CAB	-2.63	1.42	1.47
19	B1	833	CLA	C4D-ND	-2.63	1.34	1.37
19	AA	812	CLA	CMB-C2B	-2.63	1.46	1.51
19	B2	803	CLA	CMB-C2B	-2.63	1.46	1.51
19	A1	823	CLA	CMB-C2B	-2.63	1.46	1.51
19	F1	302	CLA	CMB-C2B	-2.63	1.46	1.51
19	B	829	CLA	CMB-C2B	-2.63	1.46	1.51
19	A	836	CLA	CMB-C2B	-2.62	1.46	1.51
19	F	302	CLA	CMB-C2B	-2.62	1.46	1.51
19	AA	835	CLA	CMB-C2B	-2.62	1.46	1.51
19	A	832	CLA	CMB-C2B	-2.62	1.46	1.51
19	B2	805	CLA	CMB-C2B	-2.62	1.46	1.51
19	B	858	CLA	CMB-C2B	-2.62	1.46	1.51
19	BB	803	CLA	CMB-C2B	-2.62	1.46	1.51
19	AA	834	CLA	CMB-C2B	-2.62	1.46	1.51
19	AA	836	CLA	CMB-C2B	-2.62	1.46	1.51
19	B2	816	CLA	CMB-C2B	-2.62	1.46	1.51
19	B	832	CLA	C3B-C2B	-2.62	1.36	1.40
19	BB	805	CLA	CMB-C2B	-2.62	1.46	1.51
19	B	836	CLA	CMB-C2B	-2.61	1.46	1.51
19	B1	848	CLA	CHC-C1C	2.61	1.41	1.35
19	A1	811	CLA	CMB-C2B	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	824	CLA	CMB-C2B	-2.61	1.46	1.51
19	B1	805	CLA	CMB-C2B	-2.61	1.46	1.51
19	LL	203	CLA	CMD-C2D	-2.61	1.45	1.50
19	A	824	CLA	CMB-C2B	-2.61	1.46	1.51
19	B	832	CLA	CMB-C2B	-2.61	1.46	1.51
19	B	825	CLA	CMB-C2B	-2.61	1.46	1.51
19	A	812	CLA	CMB-C2B	-2.61	1.46	1.51
19	A	823	CLA	CMB-C2B	-2.61	1.46	1.51
19	A2	852	CLA	CMB-C2B	-2.60	1.46	1.51
19	AA	829	CLA	CMB-C2B	-2.60	1.46	1.51
19	B	805	CLA	CMB-C2B	-2.60	1.46	1.51
19	A	834	CLA	CMB-C2B	-2.60	1.46	1.51
19	BB	825	CLA	CMB-C2B	-2.60	1.46	1.51
19	A1	810	CLA	CMB-C2B	-2.60	1.46	1.51
19	AA	823	CLA	CMB-C2B	-2.60	1.46	1.51
19	A1	832	CLA	CMB-C2B	-2.60	1.46	1.51
19	A	805	CLA	CMB-C2B	-2.60	1.46	1.51
19	A	840	CLA	CMB-C2B	-2.60	1.46	1.51
19	B2	807	CLA	CMD-C2D	-2.60	1.45	1.50
19	AA	805	CLA	CMB-C2B	-2.59	1.46	1.51
19	B2	829	CLA	CMB-C2B	-2.59	1.46	1.51
19	A2	833	CLA	CMB-C2B	-2.59	1.46	1.51
19	B2	825	CLA	CMB-C2B	-2.59	1.46	1.51
19	A1	822	CLA	CMB-C2B	-2.59	1.46	1.51
19	A	829	CLA	CMB-C2B	-2.59	1.46	1.51
19	A2	835	CLA	CMB-C2B	-2.59	1.46	1.51
19	A	835	CLA	CMB-C2B	-2.59	1.46	1.51
19	B2	807	CLA	CMB-C2B	-2.59	1.46	1.51
19	B	813	CLA	CMB-C2B	-2.59	1.46	1.51
23	AA	855	BCR	C30-C25	-2.59	1.50	1.53
19	A2	834	CLA	CMB-C2B	-2.58	1.46	1.51
19	FF	302	CLA	CMB-C2B	-2.58	1.46	1.51
19	L	202	CLA	CMB-C2B	-2.58	1.46	1.51
19	B1	828	CLA	CMB-C2B	-2.58	1.46	1.51
22	L1	211	LHG	P-O3	2.58	1.69	1.59
23	B2	840	BCR	C30-C25	-2.58	1.50	1.53
19	A1	833	CLA	CMB-C2B	-2.58	1.46	1.51
19	BB	836	CLA	CMB-C2B	-2.58	1.46	1.51
23	B2	842	BCR	C30-C25	-2.58	1.50	1.53
19	A2	820	CLA	C3B-C2B	-2.58	1.36	1.40
19	F	301	CLA	CMB-C2B	-2.58	1.46	1.51
19	BB	809	CLA	CMB-C2B	-2.58	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	822	CLA	CMB-C2B	-2.58	1.46	1.51
19	B	859	CLA	CMB-C2B	-2.58	1.46	1.51
19	L2	204	CLA	CMB-C2B	-2.57	1.46	1.51
19	BB	831	CLA	CMB-C2B	-2.57	1.46	1.51
19	B1	804	CLA	CMB-C2B	-2.57	1.46	1.51
19	B1	807	CLA	CMB-C2B	-2.57	1.46	1.51
19	A	820	CLA	C3B-CAB	-2.57	1.42	1.47
19	BB	813	CLA	CMB-C2B	-2.57	1.46	1.51
23	K2	105	BCR	C30-C25	-2.57	1.50	1.53
19	A1	821	CLA	CMB-C2B	-2.57	1.46	1.51
19	A1	834	CLA	CMB-C2B	-2.57	1.46	1.51
19	A2	818	CLA	CMB-C2B	-2.57	1.46	1.51
19	B1	814	CLA	CMB-C2B	-2.57	1.46	1.51
19	B2	804	CLA	CMB-C2B	-2.57	1.46	1.51
19	AA	811	CLA	CMB-C2B	-2.57	1.46	1.51
20	A2	803	CL0	C1D-C2D	2.57	1.50	1.45
19	B2	851	CLA	CMB-C2B	-2.56	1.46	1.51
19	A	811	CLA	CMB-C2B	-2.56	1.46	1.51
19	B	809	CLA	CMB-C2B	-2.56	1.46	1.51
19	BB	835	CLA	CMB-C2B	-2.56	1.46	1.51
19	A1	842	CLA	CMB-C2B	-2.56	1.46	1.51
19	BB	812	CLA	CMB-C2B	-2.56	1.46	1.51
19	B1	831	CLA	CMB-C2B	-2.56	1.46	1.51
19	L1	205	CLA	CMB-C2B	-2.56	1.46	1.51
19	B1	824	CLA	CMB-C2B	-2.56	1.46	1.51
19	A	807	CLA	CMB-C2B	-2.56	1.46	1.51
19	LL	203	CLA	CMB-C2B	-2.56	1.46	1.51
19	FF	305	CLA	CMB-C2B	-2.56	1.46	1.51
19	AA	843	CLA	CMB-C2B	-2.55	1.46	1.51
19	B1	849	CLA	CMB-C2B	-2.55	1.46	1.51
19	A2	805	CLA	CMB-C2B	-2.55	1.46	1.51
19	BB	824	CLA	CMB-C2B	-2.55	1.46	1.51
19	B1	825	CLA	CMB-C2B	-2.55	1.46	1.51
19	A2	842	CLA	CMB-C2B	-2.54	1.46	1.51
19	BB	856	CLA	CMB-C2B	-2.54	1.46	1.51
19	B2	802	CLA	CMB-C2B	-2.54	1.46	1.51
19	AA	822	CLA	CMB-C2B	-2.54	1.46	1.51
19	BB	829	CLA	CMB-C2B	-2.54	1.46	1.51
19	A	842	CLA	CMB-C2B	-2.54	1.46	1.51
19	AA	807	CLA	CMB-C2B	-2.54	1.46	1.51
19	BB	820	CLA	CMB-C2B	-2.54	1.46	1.51
19	A1	825	CLA	CMB-C2B	-2.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	815	CLA	CMB-C2B	-2.54	1.46	1.51
19	BB	818	CLA	CMD-C2D	-2.54	1.45	1.50
19	AA	842	CLA	CMB-C2B	-2.54	1.46	1.51
19	A2	826	CLA	CMB-C2B	-2.54	1.46	1.51
19	A	814	CLA	CMB-C2B	-2.54	1.46	1.51
19	AA	838	CLA	CMB-C2B	-2.53	1.46	1.51
19	B	833	CLA	CMB-C2B	-2.53	1.46	1.51
19	BB	832	CLA	CMB-C2B	-2.53	1.46	1.51
19	B	820	CLA	CMB-C2B	-2.53	1.46	1.51
19	A2	829	CLA	CMB-C2B	-2.53	1.46	1.51
20	A1	802	CL0	C1D-C2D	2.53	1.50	1.45
19	B1	801	CLA	CMB-C2B	-2.53	1.46	1.51
19	B2	822	CLA	CMB-C2B	-2.53	1.46	1.51
19	B2	808	CLA	CMB-C2B	-2.53	1.46	1.51
19	A1	819	CLA	C3B-C2B	-2.53	1.36	1.40
19	A	838	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	826	CLA	C3B-C2B	-2.52	1.36	1.40
19	B2	824	CLA	CMB-C2B	-2.52	1.46	1.51
19	A1	807	CLA	CMB-C2B	-2.52	1.46	1.51
19	A	825	CLA	CMB-C2B	-2.52	1.46	1.51
19	B1	850	CLA	CMB-C2B	-2.52	1.46	1.51
19	BB	807	CLA	CMB-C2B	-2.52	1.46	1.51
19	A2	817	CLA	CMB-C2B	-2.52	1.46	1.51
19	F1	301	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	827	CLA	CMB-C2B	-2.52	1.46	1.51
19	B1	802	CLA	CMB-C2B	-2.52	1.46	1.51
19	B1	808	CLA	CMB-C2B	-2.52	1.46	1.51
19	AA	825	CLA	CMB-C2B	-2.52	1.46	1.51
19	A2	807	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	808	CLA	CMB-C2B	-2.52	1.46	1.51
19	A2	819	CLA	CMB-C2B	-2.52	1.46	1.51
19	A1	816	CLA	CMB-C2B	-2.51	1.46	1.51
19	A2	828	CLA	CMB-C2B	-2.51	1.46	1.51
19	BB	827	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	806	CLA	CMB-C2B	-2.51	1.46	1.51
19	B2	830	CLA	CMB-C2B	-2.51	1.46	1.51
19	B1	829	CLA	CMB-C2B	-2.51	1.46	1.51
19	B2	826	CLA	CMD-C2D	-2.51	1.45	1.50
19	A1	818	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	835	CLA	CMB-C2B	-2.51	1.46	1.51
19	F2	301	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	803	CLA	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	844	CLA	CMB-C2B	-2.51	1.46	1.51
19	B1	826	CLA	CMD-C2D	-2.51	1.45	1.50
19	B1	820	CLA	CMB-C2B	-2.51	1.46	1.51
19	AA	816	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	808	CLA	CMB-C2B	-2.51	1.46	1.51
19	AA	845	CLA	CMB-C2B	-2.51	1.46	1.51
19	B2	837	CLA	CMB-C2B	-2.51	1.46	1.51
19	B1	836	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	840	CLA	CMB-C2B	-2.50	1.46	1.51
19	A1	844	CLA	CMB-C2B	-2.50	1.46	1.51
19	B	834	CLA	CMD-C2D	-2.50	1.45	1.50
19	A1	828	CLA	CMB-C2B	-2.50	1.46	1.51
19	L	204	CLA	CMB-C2B	-2.50	1.46	1.51
19	AA	853	CLA	CMB-C2B	-2.50	1.46	1.51
19	B2	836	CLA	CMB-C2B	-2.50	1.46	1.51
19	BB	834	CLA	CMB-C2B	-2.50	1.46	1.51
19	K1	102	CLA	CMB-C2B	-2.50	1.46	1.51
19	B	807	CLA	CMB-C2B	-2.50	1.46	1.51
19	A1	827	CLA	CMB-C2B	-2.50	1.46	1.51
19	B2	801	CLA	CMB-C2B	-2.50	1.46	1.51
19	BB	845	CLA	CMB-C2B	-2.50	1.46	1.51
19	A2	808	CLA	CMB-C2B	-2.50	1.46	1.51
19	AA	808	CLA	CMB-C2B	-2.50	1.46	1.51
19	A	804	CLA	CMB-C2B	-2.50	1.46	1.51
19	AA	814	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	804	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	841	CLA	CMB-C2B	-2.49	1.46	1.51
19	BB	807	CLA	CMD-C2D	-2.49	1.45	1.50
19	A1	838	CLA	CMB-C2B	-2.49	1.46	1.51
19	A1	839	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	817	CLA	CMB-C2B	-2.49	1.46	1.51
19	BB	804	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	835	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	846	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	807	CLA	CMD-C2D	-2.49	1.45	1.50
19	A	808	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	826	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	841	CLA	CMB-C2B	-2.49	1.46	1.51
19	BB	806	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	813	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	820	CLA	C3B-CAB	-2.49	1.42	1.47
19	AA	826	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	833	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	833	CLA	CMB-C2B	-2.49	1.46	1.51
23	A	854	BCR	C30-C25	-2.49	1.50	1.53
19	B2	823	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	816	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	810	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	813	CLA	CMB-C2B	-2.49	1.46	1.51
19	B2	832	CLA	CMB-C2B	-2.49	1.46	1.51
19	A2	844	CLA	CMB-C2B	-2.48	1.46	1.51
19	A	819	CLA	CMB-C2B	-2.48	1.46	1.51
19	A1	817	CLA	CMB-C2B	-2.48	1.46	1.51
19	BB	817	CLA	CMB-C2B	-2.48	1.46	1.51
19	A	820	CLA	C3B-C2B	-2.48	1.36	1.40
19	BB	815	CLA	CMB-C2B	-2.48	1.46	1.51
19	B1	823	CLA	CMB-C2B	-2.48	1.46	1.51
19	AA	818	CLA	CMB-C2B	-2.48	1.46	1.51
19	A1	852	CLA	CMB-C2B	-2.48	1.46	1.51
19	A2	841	CLA	CMB-C2B	-2.48	1.46	1.51
19	AA	819	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	801	CLA	CMB-C2B	-2.48	1.46	1.51
19	B2	813	CLA	CMB-C2B	-2.48	1.46	1.51
19	K2	102	CLA	CMB-C2B	-2.48	1.46	1.51
19	A	828	CLA	CMB-C2B	-2.48	1.46	1.51
19	A2	812	CLA	CMB-C2B	-2.48	1.46	1.51
19	B2	827	CLA	CMB-C2B	-2.48	1.46	1.51
19	B1	813	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	823	CLA	CMB-C2B	-2.47	1.46	1.51
19	AA	828	CLA	CMB-C2B	-2.47	1.46	1.51
19	A2	814	CLA	CMB-C2B	-2.47	1.46	1.51
19	A1	812	CLA	CMB-C2B	-2.47	1.46	1.51
19	AA	806	CLA	CMB-C2B	-2.47	1.46	1.51
19	BB	823	CLA	CMB-C2B	-2.47	1.46	1.51
19	A	806	CLA	CMB-C2B	-2.47	1.46	1.51
19	A	810	CLA	CMB-C2B	-2.47	1.46	1.51
19	AA	804	CLA	CMB-C2B	-2.47	1.46	1.51
19	A	852	CLA	CMB-C2B	-2.47	1.46	1.51
19	BB	818	CLA	CMB-C2B	-2.47	1.46	1.51
19	BB	821	CLA	CMD-C2D	-2.47	1.45	1.50
19	A1	841	CLA	CMB-C2B	-2.47	1.46	1.51
19	B2	820	CLA	CMB-C2B	-2.47	1.46	1.51
19	BB	801	CLA	CMB-C2B	-2.46	1.46	1.51
19	A1	826	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	812	CLA	CMB-C2B	-2.46	1.46	1.51
19	A2	813	CLA	CMB-C2B	-2.46	1.46	1.51
19	AA	840	CLA	CMB-C2B	-2.46	1.46	1.51
19	B1	809	CLA	CMB-C2B	-2.46	1.46	1.51
19	A1	819	CLA	CMD-C2D	-2.46	1.45	1.50
19	JJ	101	CLA	CMB-C2B	-2.46	1.46	1.51
19	L1	207	CLA	CMB-C2B	-2.46	1.46	1.51
19	A2	839	CLA	CMB-C2B	-2.46	1.46	1.51
19	A1	805	CLA	CMB-C2B	-2.45	1.46	1.51
19	A2	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	A	839	CLA	CMB-C2B	-2.45	1.46	1.51
19	J	101	CLA	CMB-C2B	-2.45	1.46	1.51
19	B2	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	A1	829	CLA	CMD-C2D	-2.45	1.45	1.50
19	A	818	CLA	CMB-C2B	-2.45	1.46	1.51
19	A1	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	A	820	CLA	CMD-C2D	-2.45	1.45	1.50
19	A1	837	CLA	CMB-C2B	-2.45	1.46	1.51
19	BB	826	CLA	C3B-C2B	-2.45	1.37	1.40
19	A2	801	CLA	CMC-C2C	-2.45	1.45	1.50
19	B	824	CLA	CMD-C2D	-2.45	1.45	1.50
19	A	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	A2	838	CLA	CMB-C2B	-2.45	1.46	1.51
19	B1	827	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	824	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	806	CLA	CMB-C2B	-2.45	1.46	1.51
19	A2	820	CLA	CMD-C2D	-2.45	1.45	1.50
19	A2	804	CLA	CMD-C2D	-2.45	1.45	1.50
19	K	101	CLA	CMB-C2B	-2.45	1.46	1.51
19	A	811	CLA	C3B-CAB	-2.44	1.43	1.47
19	B	827	CLA	CMD-C2D	-2.44	1.45	1.50
19	A	804	CLA	CMD-C2D	-2.44	1.45	1.50
19	B1	817	CLA	CMB-C2B	-2.44	1.46	1.51
19	A1	801	CLA	CMC-C2C	-2.44	1.45	1.50
19	A1	832	CLA	CMD-C2D	-2.44	1.45	1.50
19	AA	839	CLA	CMB-C2B	-2.44	1.46	1.51
19	A2	840	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	822	CLA	CMB-C2B	-2.44	1.46	1.51
19	B1	812	CLA	CMB-C2B	-2.44	1.46	1.51
19	B2	817	CLA	CMB-C2B	-2.44	1.46	1.51
19	A1	813	CLA	CMB-C2B	-2.44	1.46	1.51
19	B2	835	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	810	CLA	CMB-C2B	-2.43	1.46	1.51
19	BB	824	CLA	CMD-C2D	-2.43	1.45	1.50
22	X1	102	LHG	P-O3	2.43	1.69	1.59
19	BB	802	CLA	C3B-C2B	-2.43	1.37	1.40
19	B1	835	CLA	CMB-C2B	-2.43	1.46	1.51
19	KK	101	CLA	CMB-C2B	-2.43	1.46	1.51
19	B1	830	CLA	CMB-C2B	-2.43	1.46	1.51
19	A	827	CLA	CMB-C2B	-2.43	1.46	1.51
19	A1	826	CLA	C3B-C2B	-2.43	1.37	1.40
19	BB	833	CLA	CMD-C2D	-2.43	1.45	1.50
19	B1	833	CLA	CMD-C2D	-2.43	1.45	1.50
19	A	805	CLA	CMD-C2D	-2.43	1.45	1.50
19	A2	811	CLA	C3B-CAB	-2.43	1.43	1.47
19	B	810	CLA	CMB-C2B	-2.43	1.46	1.51
19	B2	850	CLA	C3B-C2B	-2.43	1.37	1.40
19	B1	826	CLA	C3B-C2B	-2.42	1.37	1.40
19	B	801	CLA	CMD-C2D	-2.42	1.45	1.50
19	AA	801	CLA	CMB-C2B	-2.42	1.46	1.51
19	BB	832	CLA	C3B-C2B	-2.42	1.37	1.40
19	AA	820	CLA	C3B-C2B	-2.42	1.37	1.40
19	A2	806	CLA	CMB-C2B	-2.42	1.46	1.51
19	B1	831	CLA	C3B-C2B	-2.42	1.37	1.40
19	J2	101	CLA	CMB-C2B	-2.42	1.46	1.51
19	A	815	CLA	CMB-C2B	-2.42	1.46	1.51
19	BB	833	CLA	C3B-CAB	-2.42	1.43	1.47
19	A1	815	CLA	CMB-C2B	-2.42	1.46	1.51
19	AA	809	CLA	CMB-C2B	-2.42	1.46	1.51
22	X2	102	LHG	P-O3	2.42	1.69	1.59
19	J1	101	CLA	CMB-C2B	-2.42	1.46	1.51
19	B1	834	CLA	CMB-C2B	-2.41	1.46	1.51
19	A1	801	CLA	CMB-C2B	-2.41	1.46	1.51
19	BB	827	CLA	CMD-C2D	-2.41	1.45	1.50
19	B	834	CLA	C3B-CAB	-2.41	1.43	1.47
19	AA	820	CLA	CMD-C2D	-2.41	1.45	1.50
19	B1	848	CLA	CMD-C2D	-2.41	1.45	1.50
19	B1	822	CLA	CMB-C2B	-2.41	1.46	1.51
19	B2	812	CLA	CMB-C2B	-2.41	1.46	1.51
22	B2	848	LHG	P-O3	2.41	1.69	1.59
22	A1	845	LHG	O7-C5	-2.41	1.40	1.46
19	LL	202	CLA	C3B-C2B	-2.41	1.37	1.40
19	XX	101	CLA	CMB-C2B	-2.41	1.46	1.51
19	L2	206	CLA	CMD-C2D	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A1	802	CL0	C4B-CHC	2.41	1.47	1.41
19	B	815	CLA	CMB-C2B	-2.40	1.46	1.51
19	B2	834	CLA	C3B-CAB	-2.40	1.43	1.47
19	BB	830	CLA	CMB-C2B	-2.40	1.46	1.51
19	A	801	CLA	CMB-C2B	-2.40	1.46	1.51
19	B	821	CLA	CMD-C2D	-2.40	1.45	1.50
19	B1	848	CLA	C3B-C2B	-2.40	1.37	1.40
19	B1	815	CLA	CMB-C2B	-2.40	1.46	1.51
19	A2	816	CLA	CMB-C2B	-2.40	1.46	1.51
19	B	831	CLA	CMB-C2B	-2.40	1.46	1.51
19	AA	815	CLA	CMB-C2B	-2.40	1.46	1.51
19	BB	810	CLA	CMB-C2B	-2.40	1.46	1.51
19	A1	807	CLA	CMD-C2D	-2.40	1.45	1.50
19	B1	845	CLA	CMB-C2B	-2.39	1.46	1.51
19	AA	804	CLA	CMD-C2D	-2.39	1.45	1.50
19	X	101	CLA	CMB-C2B	-2.39	1.46	1.51
19	B1	810	CLA	CMB-C2B	-2.39	1.46	1.51
19	X1	101	CLA	CMB-C2B	-2.39	1.46	1.51
19	AA	817	CLA	CMB-C2B	-2.39	1.46	1.51
19	B2	824	CLA	CMD-C2D	-2.39	1.45	1.50
19	JJ	103	CLA	CMB-C2B	-2.39	1.46	1.51
19	L	202	CLA	CMD-C2D	-2.39	1.45	1.50
19	B1	833	CLA	C3B-C2B	-2.39	1.37	1.40
19	A	801	CLA	CMC-C2C	-2.39	1.45	1.50
19	BB	828	CLA	CMB-C2B	-2.39	1.46	1.51
20	AA	803	CL0	C1D-C2D	2.39	1.50	1.45
19	X2	101	CLA	CMB-C2B	-2.39	1.46	1.51
19	B2	806	CLA	CMB-C2B	-2.39	1.46	1.51
19	A	817	CLA	CMB-C2B	-2.39	1.46	1.51
19	AA	827	CLA	CMB-C2B	-2.39	1.46	1.51
19	B2	819	CLA	CMB-C2B	-2.39	1.46	1.51
19	B	828	CLA	CMB-C2B	-2.38	1.46	1.51
22	XX	102	LHG	P-O3	2.38	1.68	1.59
19	AA	843	CLA	C3B-C2B	-2.38	1.37	1.40
19	K1	103	CLA	CMB-C2B	-2.38	1.46	1.51
19	B2	831	CLA	CMB-C2B	-2.38	1.46	1.51
19	K1	105	CLA	CMB-C2B	-2.38	1.46	1.51
19	B	830	CLA	CMB-C2B	-2.38	1.46	1.51
22	L	207	LHG	C6-C5	2.38	1.58	1.50
19	B2	846	CLA	CMB-C2B	-2.38	1.46	1.51
19	B1	833	CLA	C3B-CAB	-2.38	1.43	1.47
19	J1	103	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	810	CLA	CMB-C2B	-2.38	1.46	1.51
19	B1	818	CLA	CMB-C2B	-2.37	1.46	1.51
19	BB	852	CLA	CMD-C2D	-2.37	1.45	1.50
19	BB	811	CLA	CMB-C2B	-2.37	1.46	1.51
22	LL	205	LHG	C6-C5	2.37	1.58	1.50
19	B1	824	CLA	CMD-C2D	-2.37	1.45	1.50
19	AA	805	CLA	CMD-C2D	-2.37	1.45	1.50
19	B2	818	CLA	CMB-C2B	-2.37	1.46	1.51
19	A1	828	CLA	CMD-C2D	-2.37	1.45	1.50
19	B2	822	CLA	CMD-C2D	-2.37	1.45	1.50
19	A2	801	CLA	CMB-C2B	-2.37	1.46	1.51
19	A	827	CLA	CMD-C2D	-2.37	1.45	1.50
20	A	803	CL0	C4B-CHC	2.37	1.47	1.41
19	B	819	CLA	CMB-C2B	-2.37	1.46	1.51
19	KK	102	CLA	CMB-C2B	-2.37	1.46	1.51
19	BB	819	CLA	CMB-C2B	-2.37	1.46	1.51
19	A2	802	CLA	CMB-C2B	-2.36	1.46	1.51
22	A	845	LHG	O7-C5	-2.36	1.40	1.46
19	A1	830	CLA	CMD-C2D	-2.36	1.45	1.50
20	AA	803	CL0	C4B-CHC	2.36	1.47	1.41
19	K2	104	CLA	CMB-C2B	-2.36	1.46	1.51
19	L1	207	CLA	CMD-C2D	-2.36	1.45	1.50
19	A2	831	CLA	CMD-C2D	-2.36	1.45	1.50
19	J	103	CLA	CMB-C2B	-2.36	1.46	1.51
19	A2	827	CLA	C3B-C2B	-2.36	1.37	1.40
20	A1	802	CL0	C1C-C2C	2.35	1.49	1.44
19	F1	305	CLA	CMB-C2B	-2.35	1.46	1.51
19	B2	801	CLA	CMD-C2D	-2.35	1.45	1.50
19	BB	822	CLA	CMB-C2B	-2.35	1.46	1.51
22	X	102	LHG	P-O3	2.35	1.68	1.59
19	A	821	CLA	CMB-C2B	-2.35	1.46	1.51
19	A	827	CLA	C3B-C2B	-2.35	1.37	1.40
19	A1	829	CLA	CMB-C2B	-2.34	1.46	1.51
19	B2	828	CLA	CMB-C2B	-2.34	1.46	1.51
19	K	102	CLA	CMB-C2B	-2.34	1.46	1.51
19	J2	103	CLA	CMB-C2B	-2.34	1.46	1.51
22	AA	846	LHG	O7-C5	-2.34	1.40	1.46
19	LL	201	CLA	CMD-C2D	-2.34	1.45	1.50
19	BB	855	CLA	C3B-C2B	-2.34	1.37	1.40
19	B1	806	CLA	CMB-C2B	-2.34	1.46	1.51
19	A1	810	CLA	C3B-CAB	-2.34	1.43	1.47
19	AA	827	CLA	CMD-C2D	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	803	CLA	CMD-C2D	-2.34	1.45	1.50
19	A1	840	CLA	CMD-C2D	-2.34	1.45	1.50
19	L	204	CLA	CMD-C2D	-2.34	1.45	1.50
19	AA	811	CLA	C3B-CAB	-2.34	1.43	1.47
20	AA	803	CL0	C4C-C3C	2.33	1.49	1.45
19	A1	804	CLA	CMB-C2B	-2.33	1.46	1.51
19	A2	830	CLA	CMB-C2B	-2.33	1.46	1.51
19	B	834	CLA	C3B-C2B	-2.33	1.37	1.40
19	B1	824	CLA	C3B-C2B	-2.33	1.37	1.40
19	B1	811	CLA	CMB-C2B	-2.33	1.46	1.51
19	A2	804	CLA	CMB-C2B	-2.33	1.46	1.51
19	A2	833	CLA	C3B-C2B	-2.33	1.37	1.40
20	A2	803	CL0	C1C-C2C	2.33	1.49	1.44
19	B1	819	CLA	CMB-C2B	-2.33	1.46	1.51
19	BB	833	CLA	C3B-C2B	-2.32	1.37	1.40
19	B	811	CLA	CMB-C2B	-2.32	1.46	1.51
19	A	808	CLA	CMD-C2D	-2.32	1.45	1.50
19	A2	852	CLA	C3B-C2B	-2.32	1.37	1.40
19	B2	821	CLA	CMD-C2D	-2.31	1.45	1.50
19	A1	825	CLA	CMD-C2D	-2.31	1.45	1.50
19	A	831	CLA	CMD-C2D	-2.31	1.45	1.50
19	B2	811	CLA	CMB-C2B	-2.31	1.46	1.51
19	BB	801	CLA	CMD-C2D	-2.31	1.45	1.50
19	A2	833	CLA	CMD-C2D	-2.31	1.45	1.50
19	B	835	CLA	CMD-C2D	-2.31	1.45	1.50
19	AA	831	CLA	CMD-C2D	-2.31	1.45	1.50
19	B2	834	CLA	CMD-C2D	-2.31	1.45	1.50
19	A1	814	CLA	CMB-C2B	-2.31	1.46	1.51
19	A	830	CLA	CMB-C2B	-2.31	1.46	1.51
19	B2	827	CLA	C3B-C2B	-2.31	1.37	1.40
22	L	207	LHG	P-O3	2.30	1.68	1.59
22	BB	850	LHG	P-O3	2.30	1.68	1.59
22	LL	205	LHG	P-O3	2.30	1.68	1.59
19	AA	801	CLA	CMC-C2C	-2.30	1.45	1.50
19	A2	805	CLA	CMD-C2D	-2.30	1.45	1.50
19	B	805	CLA	CMD-C2D	-2.30	1.45	1.50
19	A1	836	CLA	CMD-C2D	-2.30	1.45	1.50
19	A2	842	CLA	CMC-C2C	-2.30	1.45	1.50
19	AA	853	CLA	C3B-C2B	-2.30	1.37	1.40
19	B2	832	CLA	C3B-C2B	-2.29	1.37	1.40
19	B	816	CLA	CMD-C2D	-2.29	1.45	1.50
19	A2	829	CLA	CMD-C2D	-2.29	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	849	CLA	C3B-C2B	-2.29	1.37	1.40
19	BB	827	CLA	C3B-C2B	-2.29	1.37	1.40
19	B1	832	CLA	CMB-C2B	-2.29	1.46	1.51
19	B1	821	CLA	CMD-C2D	-2.29	1.45	1.50
19	B1	836	CLA	CMD-C2D	-2.29	1.46	1.50
19	B2	849	CLA	CMD-C2D	-2.29	1.46	1.50
19	BB	816	CLA	C3B-C2B	-2.29	1.37	1.40
19	B1	801	CLA	CMD-C2D	-2.29	1.46	1.50
19	A2	837	CLA	CMD-C2D	-2.28	1.46	1.50
19	B2	833	CLA	CMB-C2B	-2.28	1.46	1.51
19	B2	852	CLA	C3B-C2B	-2.28	1.37	1.40
19	BB	814	CLA	CMD-C2D	-2.28	1.46	1.50
19	B1	816	CLA	CMD-C2D	-2.28	1.46	1.50
19	B2	826	CLA	C3B-C2B	-2.28	1.37	1.40
19	A2	801	CLA	CMD-C2D	-2.28	1.46	1.50
19	AA	833	CLA	CMD-C2D	-2.28	1.46	1.50
19	B	837	CLA	CMB-C2B	-2.28	1.46	1.51
19	AA	853	CLA	C3B-CAB	-2.28	1.43	1.47
19	B	822	CLA	CMD-C2D	-2.28	1.46	1.50
19	BB	829	CLA	C3B-CAB	-2.28	1.43	1.47
19	A2	827	CLA	CMD-C2D	-2.28	1.46	1.50
19	BB	836	CLA	CMD-C2D	-2.28	1.46	1.50
19	A	842	CLA	CMD-C2D	-2.28	1.46	1.50
19	A	852	CLA	C3B-C2B	-2.28	1.37	1.40
19	B	816	CLA	C3B-C2B	-2.28	1.37	1.40
19	B	860	CLA	C3B-C2B	-2.28	1.37	1.40
19	AA	808	CLA	CMD-C2D	-2.28	1.46	1.50
22	X2	103	LHG	P-O3	2.27	1.68	1.59
19	A2	810	CLA	C3B-C2B	-2.27	1.37	1.40
19	A2	828	CLA	CMD-C2D	-2.27	1.46	1.50
19	B	814	CLA	CMD-C2D	-2.27	1.46	1.50
19	AA	827	CLA	C3B-C2B	-2.27	1.37	1.40
19	A1	842	CLA	CMD-C2D	-2.27	1.46	1.50
19	AA	801	CLA	CMD-C2D	-2.27	1.46	1.50
19	AA	821	CLA	CMB-C2B	-2.27	1.46	1.51
19	B	826	CLA	CMC-C2C	-2.27	1.46	1.50
19	A	829	CLA	CMD-C2D	-2.27	1.46	1.50
19	BB	823	CLA	CMD-C2D	-2.27	1.46	1.50
19	AA	810	CLA	C3B-C2B	-2.27	1.37	1.40
19	B2	837	CLA	CMD-C2D	-2.27	1.46	1.50
19	A	801	CLA	CMD-C2D	-2.27	1.46	1.50
22	B	852	LHG	P-O3	2.26	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	838	CLA	CMD-C2D	-2.26	1.46	1.50
19	B	854	CLA	CMD-C2D	-2.26	1.46	1.50
19	B	858	CLA	C3B-C2B	-2.26	1.37	1.40
19	L2	206	CLA	CMB-C2B	-2.26	1.46	1.51
19	B1	827	CLA	CMD-C2D	-2.26	1.46	1.50
19	B	827	CLA	C3B-C2B	-2.26	1.37	1.40
19	B	822	CLA	C3B-C2B	-2.26	1.37	1.40
19	A	833	CLA	C3B-C2B	-2.26	1.37	1.40
19	BB	822	CLA	C3B-C2B	-2.26	1.37	1.40
19	B	836	CLA	CMD-C2D	-2.26	1.46	1.50
19	A2	808	CLA	CMD-C2D	-2.26	1.46	1.50
19	AA	843	CLA	CMD-C2D	-2.26	1.46	1.50
19	FF	301	CLA	CMD-C2D	-2.26	1.46	1.50
19	BB	831	CLA	C3B-CAB	-2.25	1.43	1.47
19	B2	827	CLA	CMD-C2D	-2.25	1.46	1.50
22	X1	103	LHG	P-O3	2.25	1.68	1.59
19	AA	842	CLA	CMC-C2C	-2.25	1.46	1.50
19	A	835	CLA	CMD-C2D	-2.25	1.46	1.50
19	A2	806	CLA	C3B-C2B	-2.25	1.37	1.40
19	A2	836	CLA	CMD-C2D	-2.25	1.46	1.50
19	B	806	CLA	CMD-C2D	-2.25	1.46	1.50
19	A1	835	CLA	C3B-C2B	-2.25	1.37	1.40
19	L	203	CLA	C3B-C2B	-2.25	1.37	1.40
19	BB	834	CLA	CMD-C2D	-2.25	1.46	1.50
19	B1	824	CLA	C3B-CAB	-2.25	1.43	1.47
22	BB	851	LHG	P-O3	2.25	1.68	1.59
19	B	802	CLA	C3B-C2B	-2.25	1.37	1.40
19	A1	804	CLA	CMD-C2D	-2.25	1.46	1.50
19	A2	815	CLA	CMB-C2B	-2.25	1.47	1.51
19	B	837	CLA	CMD-C2D	-2.24	1.46	1.50
19	A1	841	CLA	CMD-C2D	-2.24	1.46	1.50
19	B	823	CLA	CMD-C2D	-2.24	1.46	1.50
19	B	837	CLA	C3B-C2B	-2.24	1.37	1.40
19	B	832	CLA	CMD-C2D	-2.24	1.46	1.50
19	A2	841	CLA	CMD-C2D	-2.24	1.46	1.50
19	B	811	CLA	CMD-C2D	-2.24	1.46	1.50
19	A1	832	CLA	C3B-C2B	-2.24	1.37	1.40
19	A2	842	CLA	CMD-C2D	-2.24	1.46	1.50
19	B1	827	CLA	C3B-C2B	-2.24	1.37	1.40
19	B2	852	CLA	CMD-C2D	-2.24	1.46	1.50
19	AA	829	CLA	CMD-C2D	-2.24	1.46	1.50
19	B2	816	CLA	CMD-C2D	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	835	CLA	CMD-C2D	-2.24	1.46	1.50
19	B2	850	CLA	C3B-CAB	-2.24	1.43	1.47
19	K1	105	CLA	CMD-C2D	-2.24	1.46	1.50
19	AA	833	CLA	C3B-C2B	-2.24	1.37	1.40
19	A2	839	CLA	CMD-C2D	-2.24	1.46	1.50
19	A	811	CLA	CMD-C2D	-2.24	1.46	1.50
19	B1	805	CLA	CMD-C2D	-2.24	1.46	1.50
19	AA	824	CLA	CMD-C2D	-2.24	1.46	1.50
19	A2	811	CLA	C3B-C2B	-2.24	1.37	1.40
19	A2	821	CLA	CMB-C2B	-2.24	1.47	1.51
19	A	852	CLA	C3B-CAB	-2.23	1.43	1.47
19	B1	835	CLA	CMD-C2D	-2.23	1.46	1.50
19	AA	842	CLA	CMD-C2D	-2.23	1.46	1.50
19	K2	102	CLA	CMD-C2D	-2.23	1.46	1.50
19	A1	827	CLA	CMD-C2D	-2.23	1.46	1.50
20	A2	803	CL0	C4C-C3C	2.23	1.48	1.45
19	B1	849	CLA	C3B-C2B	-2.23	1.37	1.40
19	A1	824	CLA	CMD-C2D	-2.23	1.46	1.50
19	A1	842	CLA	C3B-C2B	-2.23	1.37	1.40
19	B	860	CLA	CMD-C2D	-2.23	1.46	1.50
19	B1	849	CLA	CMD-C2D	-2.23	1.46	1.50
19	A1	801	CLA	CMD-C2D	-2.23	1.46	1.50
19	B	826	CLA	CMD-C2D	-2.23	1.46	1.50
19	A1	852	CLA	CMD-C2D	-2.22	1.46	1.50
19	B1	834	CLA	CMD-C2D	-2.22	1.46	1.50
19	A1	835	CLA	CMD-C2D	-2.22	1.46	1.50
19	A	836	CLA	CMD-C2D	-2.22	1.46	1.50
19	B	815	CLA	CMD-C2D	-2.22	1.46	1.50
19	A1	805	CLA	C3B-C2B	-2.22	1.37	1.40
19	A	811	CLA	C3B-C2B	-2.22	1.37	1.40
19	A1	826	CLA	CMD-C2D	-2.22	1.46	1.50
19	AA	836	CLA	CMD-C2D	-2.22	1.46	1.50
19	A1	841	CLA	CMC-C2C	-2.22	1.46	1.50
19	B2	850	CLA	CMD-C2D	-2.22	1.46	1.50
19	B2	805	CLA	CMD-C2D	-2.22	1.46	1.50
22	L2	208	LHG	P-O3	2.22	1.68	1.59
19	A2	837	CLA	C3B-C2B	-2.22	1.37	1.40
19	BB	832	CLA	CMD-C2D	-2.22	1.46	1.50
19	AA	830	CLA	CMB-C2B	-2.22	1.47	1.51
22	X2	102	LHG	P-O6	2.22	1.68	1.59
19	B1	814	CLA	CMD-C2D	-2.22	1.46	1.50
19	B	819	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	836	CLA	CMC-C2C	-2.21	1.46	1.50
19	A2	830	CLA	CMD-C2D	-2.21	1.46	1.50
19	L1	206	CLA	CMD-C2D	-2.21	1.46	1.50
19	AA	819	CLA	CMD-C2D	-2.21	1.46	1.50
19	B2	815	CLA	CMD-C2D	-2.21	1.46	1.50
19	AA	834	CLA	CMD-C2D	-2.21	1.46	1.50
19	K1	102	CLA	CMD-C2D	-2.21	1.46	1.50
19	B2	821	CLA	CMB-C2B	-2.21	1.47	1.51
19	L2	205	CLA	CMD-C2D	-2.21	1.46	1.50
22	AA	846	LHG	P-O3	2.21	1.68	1.59
19	B1	818	CLA	CMD-C2D	-2.21	1.46	1.50
19	BB	802	CLA	C3B-CAB	-2.21	1.43	1.47
19	A2	823	CLA	CMD-C2D	-2.21	1.46	1.50
19	A	828	CLA	CMD-C2D	-2.21	1.46	1.50
19	A1	822	CLA	CMD-C2D	-2.21	1.46	1.50
19	B2	827	CLA	C3B-CAB	-2.21	1.43	1.47
19	BB	856	CLA	C3B-C2B	-2.21	1.37	1.40
19	BB	829	CLA	CMD-C2D	-2.20	1.46	1.50
19	A1	821	CLA	CMD-C2D	-2.20	1.46	1.50
19	B2	836	CLA	CMD-C2D	-2.20	1.46	1.50
19	A	829	CLA	MG-ND	-2.20	2.01	2.05
19	A1	826	CLA	C3B-CAB	-2.20	1.43	1.47
19	B1	821	CLA	CMB-C2B	-2.20	1.47	1.51
19	A2	840	CLA	CMD-C2D	-2.20	1.46	1.50
19	B1	822	CLA	CMD-C2D	-2.20	1.46	1.50
19	A	841	CLA	CMD-C2D	-2.20	1.46	1.50
19	A2	852	CLA	C3B-CAB	-2.20	1.43	1.47
19	BB	835	CLA	CMD-C2D	-2.20	1.46	1.50
23	B1	843	BCR	C38-C26	-2.20	1.47	1.50
19	B2	814	CLA	C3B-C2B	-2.20	1.37	1.40
19	BB	829	CLA	C3B-C2B	-2.20	1.37	1.40
19	A1	810	CLA	CMD-C2D	-2.20	1.46	1.50
20	AA	803	CL0	C1C-C2C	2.20	1.48	1.44
19	A1	835	CLA	CMC-C2C	-2.20	1.46	1.50
19	BB	810	CLA	CMD-C2D	-2.20	1.46	1.50
19	BB	815	CLA	CMD-C2D	-2.20	1.46	1.50
19	B1	832	CLA	CMD-C2D	-2.20	1.46	1.50
19	A2	811	CLA	CMD-C2D	-2.20	1.46	1.50
19	A2	806	CLA	CMC-C2C	-2.20	1.46	1.50
19	AA	811	CLA	CMD-C2D	-2.20	1.46	1.50
19	B2	829	CLA	CMD-C2D	-2.20	1.46	1.50
19	B	817	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X1	102	LHG	P-O6	2.20	1.68	1.59
19	BB	822	CLA	CMD-C2D	-2.20	1.46	1.50
19	A2	829	CLA	C3B-CAB	-2.20	1.43	1.47
19	A1	809	CLA	C3B-C2B	-2.20	1.37	1.40
19	A	834	CLA	CMD-C2D	-2.19	1.46	1.50
19	A1	820	CLA	CMB-C2B	-2.19	1.47	1.51
19	A2	836	CLA	C3B-C2B	-2.19	1.37	1.40
19	B	833	CLA	CMD-C2D	-2.19	1.46	1.50
23	B2	844	BCR	C38-C26	-2.19	1.47	1.50
19	AA	830	CLA	CMD-C2D	-2.19	1.46	1.50
19	B1	811	CLA	CMD-C2D	-2.19	1.46	1.50
19	AA	836	CLA	CMC-C2C	-2.19	1.46	1.50
19	AA	839	CLA	CMD-C2D	-2.19	1.46	1.50
19	B	802	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	853	LHG	P-O3	2.19	1.68	1.59
19	A1	834	CLA	CMD-C2D	-2.19	1.46	1.50
19	B2	818	CLA	CMD-C2D	-2.19	1.46	1.50
19	B	804	CLA	CMD-C2D	-2.19	1.46	1.50
19	BB	804	CLA	CMD-C2D	-2.19	1.46	1.50
19	A2	827	CLA	C3B-CAB	-2.19	1.43	1.47
19	F	301	CLA	CMD-C2D	-2.19	1.46	1.50
19	AA	806	CLA	C3B-C2B	-2.19	1.37	1.40
19	B2	814	CLA	CMD-C2D	-2.19	1.46	1.50
19	LL	202	CLA	CMD-C2D	-2.19	1.46	1.50
19	A	833	CLA	CMD-C2D	-2.19	1.46	1.50
19	B	859	CLA	C3B-C2B	-2.19	1.37	1.40
19	A2	835	CLA	CMD-C2D	-2.19	1.46	1.50
19	FF	302	CLA	CMD-C2D	-2.19	1.46	1.50
19	B1	829	CLA	C3B-CAB	-2.18	1.43	1.47
19	A2	822	CLA	CMD-C2D	-2.18	1.46	1.50
19	A2	821	CLA	CMC-C2C	-2.18	1.46	1.50
19	A1	810	CLA	C3B-C2B	-2.18	1.37	1.40
19	A2	826	CLA	CMD-C2D	-2.18	1.46	1.50
19	AA	841	CLA	CMD-C2D	-2.18	1.46	1.50
19	B1	804	CLA	CMD-C2D	-2.18	1.46	1.50
19	A2	824	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	830	CLA	CMD-C2D	-2.18	1.46	1.50
19	BB	806	CLA	CMD-C2D	-2.18	1.46	1.50
19	BB	811	CLA	CMD-C2D	-2.18	1.46	1.50
19	BB	816	CLA	CMD-C2D	-2.18	1.46	1.50
19	A2	825	CLA	CMD-C2D	-2.18	1.46	1.50
19	BB	812	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F1	301	CLA	C3B-C2B	-2.18	1.37	1.40
19	B2	823	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	836	CLA	CMC-C2C	-2.18	1.46	1.50
19	AA	811	CLA	C3B-C2B	-2.18	1.37	1.40
19	B1	803	CLA	CMD-C2D	-2.18	1.46	1.50
22	A1	845	LHG	P-O3	2.18	1.68	1.59
19	B	832	CLA	C3B-CAB	-2.18	1.43	1.47
19	B	810	CLA	CMD-C2D	-2.18	1.46	1.50
19	AA	828	CLA	CMD-C2D	-2.18	1.46	1.50
19	B2	804	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	806	CLA	CMD-C2D	-2.18	1.46	1.50
19	B	828	CLA	CMD-C2D	-2.18	1.46	1.50
22	B1	847	LHG	P-O3	2.17	1.68	1.59
19	L1	207	CLA	MG-ND	-2.17	2.01	2.05
19	A1	839	CLA	CMD-C2D	-2.17	1.46	1.50
19	BB	805	CLA	CMD-C2D	-2.17	1.46	1.50
19	BB	828	CLA	CMD-C2D	-2.17	1.46	1.50
19	A2	810	CLA	CMD-C2D	-2.17	1.46	1.50
19	AA	806	CLA	CMD-C2D	-2.17	1.46	1.50
19	A	842	CLA	C3B-C2B	-2.17	1.37	1.40
19	B	803	CLA	CMD-C2D	-2.17	1.46	1.50
19	B	812	CLA	CMD-C2D	-2.17	1.46	1.50
19	B	823	CLA	CMC-C2C	-2.17	1.46	1.50
19	BB	836	CLA	C3B-C2B	-2.17	1.37	1.40
19	A2	844	CLA	CMD-C2D	-2.16	1.46	1.50
19	FF	305	CLA	CMD-C2D	-2.16	1.46	1.50
19	B1	815	CLA	CMD-C2D	-2.16	1.46	1.50
19	A1	810	CLA	CMC-C2C	-2.16	1.46	1.50
19	F2	302	CLA	CMD-C2D	-2.16	1.46	1.50
19	AA	810	CLA	CMD-C2D	-2.16	1.46	1.50
22	A	845	LHG	P-O3	2.16	1.68	1.59
19	A1	809	CLA	CMD-C2D	-2.16	1.46	1.50
19	F	302	CLA	CMD-C2D	-2.16	1.46	1.50
19	B	821	CLA	CMB-C2B	-2.16	1.47	1.51
19	A1	805	CLA	CMD-C2D	-2.16	1.46	1.50
19	A	839	CLA	CMD-C2D	-2.16	1.46	1.50
19	B	829	CLA	CMD-C2D	-2.16	1.46	1.50
19	AA	809	CLA	CMD-C2D	-2.16	1.46	1.50
19	B2	835	CLA	CMD-C2D	-2.16	1.46	1.50
19	BB	802	CLA	CMD-C2D	-2.16	1.46	1.50
19	B2	803	CLA	CMD-C2D	-2.16	1.46	1.50
19	AA	837	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	852	CLA	C3B-CAB	-2.16	1.43	1.47
19	A	810	CLA	CMD-C2D	-2.16	1.46	1.50
19	A	837	CLA	CMD-C2D	-2.16	1.46	1.50
19	B	809	CLA	CMD-C2D	-2.16	1.46	1.50
19	BB	856	CLA	CMD-C2D	-2.15	1.46	1.50
19	KK	101	CLA	CMD-C2D	-2.15	1.46	1.50
19	A1	820	CLA	CMC-C2C	-2.15	1.46	1.50
19	A1	814	CLA	CMD-C2D	-2.15	1.46	1.50
19	BB	803	CLA	CMD-C2D	-2.15	1.46	1.50
19	A2	825	CLA	C3B-C2B	-2.15	1.37	1.40
19	K	101	CLA	CMD-C2D	-2.15	1.46	1.50
19	BB	832	CLA	C3B-CAB	-2.15	1.43	1.47
19	B2	811	CLA	CMD-C2D	-2.15	1.46	1.50
19	B1	828	CLA	CMD-C2D	-2.15	1.46	1.50
19	A	815	CLA	CMD-C2D	-2.15	1.46	1.50
19	BB	809	CLA	CMD-C2D	-2.15	1.46	1.50
19	BB	855	CLA	CMD-C2D	-2.15	1.46	1.50
19	B	858	CLA	CMD-C2D	-2.15	1.46	1.50
19	AA	821	CLA	CMD-C2D	-2.15	1.46	1.50
19	B2	822	CLA	C3B-C2B	-2.15	1.37	1.40
19	A	810	CLA	C3B-C2B	-2.15	1.37	1.40
19	A	821	CLA	CMD-C2D	-2.15	1.46	1.50
19	B	806	CLA	CMC-C2C	-2.15	1.46	1.50
19	A2	852	CLA	CMD-C2D	-2.15	1.46	1.50
19	A	814	CLA	CMD-C2D	-2.15	1.46	1.50
19	AA	822	CLA	CMD-C2D	-2.15	1.46	1.50
19	BB	817	CLA	CMD-C2D	-2.15	1.46	1.50
20	A2	803	CL0	C4B-CHC	2.15	1.47	1.41
22	A2	846	LHG	P-O3	2.15	1.68	1.59
19	A	806	CLA	C3B-C2B	-2.15	1.37	1.40
23	B	844	BCR	C38-C26	-2.15	1.47	1.50
19	BB	803	CLA	CMC-C2C	-2.14	1.46	1.50
19	A2	806	CLA	CMD-C2D	-2.14	1.46	1.50
19	B	825	CLA	CMD-C2D	-2.14	1.46	1.50
19	BB	825	CLA	CMD-C2D	-2.14	1.46	1.50
19	AA	829	CLA	MG-ND	-2.14	2.01	2.05
19	BB	852	CLA	C3B-C2B	-2.14	1.37	1.40
19	B2	830	CLA	C3B-CAB	-2.14	1.43	1.47
19	A	819	CLA	CMD-C2D	-2.14	1.46	1.50
19	B	859	CLA	CMD-C2D	-2.14	1.46	1.50
19	AA	815	CLA	CMD-C2D	-2.14	1.46	1.50
19	BB	813	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	815	CLA	CMD-C2D	-2.14	1.46	1.50
19	B2	810	CLA	CMD-C2D	-2.14	1.46	1.50
19	AA	823	CLA	CMD-C2D	-2.14	1.46	1.50
19	B1	850	CLA	CMD-C2D	-2.14	1.46	1.50
19	B2	851	CLA	CMD-C2D	-2.14	1.46	1.50
19	A	823	CLA	CMD-C2D	-2.14	1.46	1.50
19	A2	814	CLA	CMD-C2D	-2.14	1.46	1.50
19	BB	830	CLA	CMD-C2D	-2.14	1.46	1.50
19	B1	810	CLA	CMD-C2D	-2.14	1.46	1.50
19	B	803	CLA	CMC-C2C	-2.14	1.46	1.50
19	A1	820	CLA	CMD-C2D	-2.14	1.46	1.50
19	B2	806	CLA	CMD-C2D	-2.14	1.46	1.50
19	F1	302	CLA	CMD-C2D	-2.14	1.46	1.50
19	B2	830	CLA	CMD-C2D	-2.14	1.46	1.50
19	BB	819	CLA	CMD-C2D	-2.14	1.46	1.50
19	AA	814	CLA	CMD-C2D	-2.14	1.46	1.50
19	A2	821	CLA	CMD-C2D	-2.14	1.46	1.50
19	A	842	CLA	CMC-C2C	-2.14	1.46	1.50
19	B1	817	CLA	CMD-C2D	-2.14	1.46	1.50
19	B1	823	CLA	CMD-C2D	-2.14	1.46	1.50
19	B2	833	CLA	CMD-C2D	-2.14	1.46	1.50
19	A1	823	CLA	CMD-C2D	-2.13	1.46	1.50
20	A	803	CL0	C1C-C2C	2.13	1.48	1.44
22	A2	845	LHG	P-O3	2.13	1.67	1.59
19	AA	840	CLA	CMD-C2D	-2.13	1.46	1.50
19	AA	813	CLA	CMD-C2D	-2.13	1.46	1.50
19	A2	823	CLA	C3B-C2B	-2.13	1.37	1.40
19	A1	837	CLA	CMD-C2D	-2.13	1.46	1.50
19	B1	816	CLA	C3B-C2B	-2.13	1.37	1.40
19	B1	805	CLA	CMC-C2C	-2.13	1.46	1.50
19	A2	820	CLA	CMC-C2C	-2.13	1.46	1.50
19	A	807	CLA	C3B-C2B	-2.13	1.37	1.40
19	B	804	CLA	C3B-C2B	-2.13	1.37	1.40
19	A2	817	CLA	CMD-C2D	-2.13	1.46	1.50
19	A	825	CLA	CMD-C2D	-2.13	1.46	1.50
19	A	821	CLA	CMC-C2C	-2.13	1.46	1.50
22	A1	846	LHG	P-O3	2.13	1.67	1.59
19	A1	816	CLA	CMD-C2D	-2.13	1.46	1.50
19	B	808	CLA	CMD-C2D	-2.13	1.46	1.50
19	B1	819	CLA	CMD-C2D	-2.13	1.46	1.50
19	AA	825	CLA	CMD-C2D	-2.13	1.46	1.50
19	A2	829	CLA	MG-ND	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	XX	101	CLA	CMD-C2D	-2.13	1.46	1.50
19	BB	856	CLA	C3B-CAB	-2.13	1.43	1.47
19	B	830	CLA	CMD-C2D	-2.13	1.46	1.50
19	A1	818	CLA	CMD-C2D	-2.12	1.46	1.50
19	B1	845	CLA	CBD-CAD	2.12	1.56	1.51
19	A	809	CLA	CMD-C2D	-2.12	1.46	1.50
19	AA	830	CLA	CMC-C2C	-2.12	1.46	1.50
19	B2	846	CLA	CBD-CAD	2.12	1.56	1.51
19	A	813	CLA	CMD-C2D	-2.12	1.46	1.50
19	A	840	CLA	CMD-C2D	-2.12	1.46	1.50
19	A2	804	CLA	CMC-C2C	-2.12	1.46	1.50
19	A2	834	CLA	CMD-C2D	-2.12	1.46	1.50
19	AA	836	CLA	C3B-C2B	-2.12	1.37	1.40
19	B2	819	CLA	CMC-C2C	-2.12	1.46	1.50
19	B	831	CLA	CMD-C2D	-2.12	1.46	1.50
22	AA	847	LHG	P-O3	2.12	1.67	1.59
19	A1	812	CLA	CMD-C2D	-2.12	1.46	1.50
19	B1	808	CLA	CMD-C2D	-2.12	1.46	1.50
19	X	101	CLA	CMD-C2D	-2.12	1.46	1.50
19	A2	838	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	841	ECH	C1-C6	-2.12	1.50	1.53
19	B1	822	CLA	C3B-C2B	-2.12	1.37	1.40
19	A1	833	CLA	CMD-C2D	-2.12	1.46	1.50
19	B2	819	CLA	CMD-C2D	-2.12	1.46	1.50
19	A1	828	CLA	MG-ND	-2.12	2.01	2.05
19	BB	826	CLA	CMC-C2C	-2.12	1.46	1.50
19	A2	833	CLA	CMC-C2C	-2.12	1.46	1.50
19	A	844	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	813	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	830	CLA	CMC-C2C	-2.12	1.46	1.50
19	L	203	CLA	CMD-C2D	-2.12	1.46	1.50
19	AA	833	CLA	CMC-C2C	-2.12	1.46	1.50
19	BB	804	CLA	C3B-C2B	-2.11	1.37	1.40
19	F	301	CLA	C3B-C2B	-2.11	1.37	1.40
19	AA	807	CLA	C3B-C2B	-2.11	1.37	1.40
19	AA	842	CLA	C3B-C2B	-2.11	1.37	1.40
19	B1	809	CLA	CMD-C2D	-2.11	1.46	1.50
19	A	812	CLA	CMD-C2D	-2.11	1.46	1.50
19	LL	202	CLA	C3B-CAB	-2.11	1.43	1.47
19	A2	813	CLA	CMD-C2D	-2.11	1.46	1.50
19	BB	826	CLA	MG-ND	-2.11	2.01	2.05
19	K1	103	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	829	CLA	CMC-C2C	-2.11	1.46	1.50
19	A	832	CLA	CMC-C2C	-2.11	1.46	1.50
23	FF	306	BCR	C33-C5	-2.11	1.47	1.50
19	B1	826	CLA	CMC-C2C	-2.11	1.46	1.50
19	BB	820	CLA	C3B-C2B	-2.11	1.37	1.40
19	AA	812	CLA	CMD-C2D	-2.11	1.46	1.50
19	A1	811	CLA	CMD-C2D	-2.11	1.46	1.50
19	B	859	CLA	C3B-CAB	-2.11	1.43	1.47
19	B2	809	CLA	CMD-C2D	-2.11	1.46	1.50
19	B2	820	CLA	CMD-C2D	-2.11	1.46	1.50
19	BB	806	CLA	CMC-C2C	-2.11	1.46	1.50
19	B1	850	CLA	C3B-C2B	-2.11	1.37	1.40
19	B2	817	CLA	CMD-C2D	-2.11	1.46	1.50
19	B1	829	CLA	CMD-C2D	-2.11	1.46	1.50
19	A1	831	CLA	CMC-C2C	-2.10	1.46	1.50
19	B1	806	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	846	CLA	CMD-C2D	-2.10	1.46	1.50
19	BB	845	CLA	CBD-CAD	2.10	1.56	1.51
19	B2	825	CLA	CMD-C2D	-2.10	1.46	1.50
19	A	818	CLA	CMD-C2D	-2.10	1.46	1.50
19	BB	808	CLA	CMD-C2D	-2.10	1.46	1.50
23	F	305	BCR	C33-C5	-2.10	1.47	1.50
19	F1	301	CLA	CMD-C2D	-2.10	1.46	1.50
19	B2	850	CLA	CMC-C2C	-2.10	1.46	1.50
19	B2	836	CLA	C3B-C2B	-2.10	1.37	1.40
19	A	829	CLA	C3B-CAB	-2.10	1.43	1.47
19	A2	802	CLA	CMD-C2D	-2.10	1.46	1.50
19	A	826	CLA	CMD-C2D	-2.10	1.46	1.50
19	B1	829	CLA	C3B-C2B	-2.10	1.37	1.40
22	XX	102	LHG	P-O6	2.10	1.67	1.59
19	A2	819	CLA	CMD-C2D	-2.10	1.46	1.50
19	B2	808	CLA	CMD-C2D	-2.10	1.46	1.50
19	A1	824	CLA	C3B-C2B	-2.10	1.37	1.40
19	A2	831	CLA	C3B-CAB	-2.10	1.43	1.47
19	B1	805	CLA	C3B-C2B	-2.10	1.37	1.40
19	A2	812	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	816	CLA	C3B-CAB	-2.10	1.43	1.47
23	BB	843	BCR	C38-C26	-2.10	1.47	1.50
19	A2	811	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	836	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	813	CLA	C3B-C2B	-2.10	1.37	1.40
19	X1	101	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	828	CLA	CMD-C2D	-2.10	1.46	1.50
19	AA	818	CLA	CMD-C2D	-2.10	1.46	1.50
19	B1	820	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	846	CLA	CBD-CAD	2.10	1.56	1.51
19	F2	301	CLA	C3B-C2B	-2.10	1.37	1.40
19	KK	102	CLA	CMD-C2D	-2.09	1.46	1.50
19	L	204	CLA	C4B-CHC	-2.09	1.35	1.41
19	A1	836	CLA	C3B-C2B	-2.09	1.37	1.40
19	A	811	CLA	CMC-C2C	-2.09	1.46	1.50
19	B1	825	CLA	CMD-C2D	-2.09	1.46	1.50
19	B2	805	CLA	C3B-C2B	-2.09	1.37	1.40
22	A	846	LHG	P-O3	2.09	1.67	1.59
19	F1	305	CLA	CMD-C2D	-2.09	1.46	1.50
19	B1	821	CLA	C3B-CAB	-2.09	1.43	1.47
19	B	854	CLA	CMC-C2C	-2.09	1.46	1.50
19	AA	806	CLA	C3B-CAB	-2.09	1.43	1.47
19	A	833	CLA	CMC-C2C	-2.09	1.46	1.50
19	A2	829	CLA	CMC-C2C	-2.09	1.46	1.50
19	B	833	CLA	C3B-C2B	-2.09	1.37	1.40
19	BB	805	CLA	C3B-C2B	-2.09	1.37	1.40
19	AA	821	CLA	CMC-C2C	-2.09	1.46	1.50
19	B1	806	CLA	CMC-C2C	-2.08	1.46	1.50
19	JJ	103	CLA	CMD-C2D	-2.08	1.46	1.50
19	BB	816	CLA	C3B-CAB	-2.08	1.43	1.47
19	BB	808	CLA	C3B-C2B	-2.08	1.37	1.40
19	B2	830	CLA	CMC-C2C	-2.08	1.46	1.50
19	A	819	CLA	CMC-C2C	-2.08	1.46	1.50
19	BB	845	CLA	CMD-C2D	-2.08	1.46	1.50
19	A2	832	CLA	CMC-C2C	-2.08	1.46	1.50
19	A1	852	CLA	C3B-C2B	-2.08	1.37	1.40
19	B1	813	CLA	CMD-C2D	-2.08	1.46	1.50
19	B2	836	CLA	CMC-C2C	-2.08	1.46	1.50
19	AA	817	CLA	CMD-C2D	-2.08	1.46	1.50
22	L1	211	LHG	O7-C5	-2.08	1.41	1.46
19	X2	101	CLA	CMD-C2D	-2.08	1.46	1.50
19	L1	206	CLA	C3B-C2B	-2.08	1.37	1.40
19	A1	819	CLA	CMC-C2C	-2.08	1.46	1.50
19	B2	813	CLA	CMD-C2D	-2.08	1.46	1.50
19	B1	803	CLA	C3B-CAB	-2.08	1.43	1.47
19	B1	803	CLA	C3B-C2B	-2.08	1.37	1.40
19	B2	804	CLA	C3B-C2B	-2.08	1.37	1.40
19	A1	844	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	806	CLA	C3B-C2B	-2.08	1.37	1.40
19	B2	802	CLA	CMD-C2D	-2.08	1.46	1.50
19	BB	814	CLA	C3B-CAB	-2.08	1.43	1.47
19	B1	802	CLA	CMD-C2D	-2.07	1.46	1.50
19	B1	849	CLA	CMC-C2C	-2.07	1.46	1.50
19	J	101	CLA	CMD-C2D	-2.07	1.46	1.50
19	A2	818	CLA	CMD-C2D	-2.07	1.46	1.50
19	A2	825	CLA	CMC-C2C	-2.07	1.46	1.50
19	A2	826	CLA	CMC-C2C	-2.07	1.46	1.50
19	A	817	CLA	CMD-C2D	-2.07	1.46	1.50
19	JJ	101	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	805	CLA	C3B-C2B	-2.07	1.37	1.40
19	A1	832	CLA	CMC-C2C	-2.07	1.46	1.50
19	A	852	CLA	CMD-C2D	-2.07	1.46	1.50
19	A2	807	CLA	C3B-C2B	-2.07	1.37	1.40
19	A1	834	CLA	CMC-C2C	-2.07	1.46	1.50
19	A2	835	CLA	CMC-C2C	-2.07	1.46	1.50
19	K	102	CLA	CMD-C2D	-2.07	1.46	1.50
22	B2	848	LHG	P-O6	2.07	1.67	1.59
19	AA	845	CLA	CMD-C2D	-2.07	1.46	1.50
22	BB	851	LHG	P-O6	2.07	1.67	1.59
19	A2	816	CLA	CMD-C2D	-2.07	1.46	1.50
19	A1	815	CLA	CMD-C2D	-2.07	1.46	1.50
19	A2	819	CLA	CMC-C2C	-2.07	1.46	1.50
19	AA	820	CLA	CMC-C2C	-2.07	1.46	1.50
19	A1	817	CLA	CMD-C2D	-2.07	1.46	1.50
19	J	103	CLA	CMD-C2D	-2.07	1.46	1.50
19	A2	835	CLA	C3B-C2B	-2.07	1.37	1.40
19	B1	812	CLA	CMD-C2D	-2.07	1.46	1.50
19	F2	301	CLA	CMD-C2D	-2.07	1.46	1.50
19	AA	838	CLA	CMD-C2D	-2.07	1.46	1.50
19	B2	820	CLA	C3B-C2B	-2.07	1.37	1.40
19	A	816	CLA	CMD-C2D	-2.07	1.46	1.50
22	X	102	LHG	P-O6	2.07	1.67	1.59
19	BB	814	CLA	CMC-C2C	-2.07	1.46	1.50
19	BB	834	CLA	CMC-C2C	-2.07	1.46	1.50
19	B1	835	CLA	C3B-C2B	-2.07	1.37	1.40
19	A2	806	CLA	C3B-CAB	-2.07	1.43	1.47
19	B2	812	CLA	CMD-C2D	-2.07	1.46	1.50
19	J	103	CLA	C3B-C2B	-2.06	1.37	1.40
19	L1	205	CLA	CMD-C2D	-2.06	1.46	1.50
19	B	802	CLA	C3B-CAB	-2.06	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	813	CLA	CMD-C2D	-2.06	1.46	1.50
19	BB	820	CLA	CMD-C2D	-2.06	1.46	1.50
19	B	809	CLA	C3B-C2B	-2.06	1.37	1.40
19	BB	814	CLA	C3B-C2B	-2.06	1.37	1.40
19	A	838	CLA	CMD-C2D	-2.06	1.46	1.50
19	BB	823	CLA	CMC-C2C	-2.06	1.46	1.50
19	B2	851	CLA	C3B-C2B	-2.06	1.37	1.40
19	L2	204	CLA	CMD-C2D	-2.06	1.46	1.50
19	A1	808	CLA	CMD-C2D	-2.06	1.46	1.50
19	A	826	CLA	CMC-C2C	-2.06	1.46	1.50
19	BB	811	CLA	CMC-C2C	-2.06	1.46	1.50
23	MM	101	BCR	C33-C5	-2.06	1.47	1.50
19	B	805	CLA	CMC-C2C	-2.06	1.46	1.50
25	I2	105	LMG	C4-C5	2.06	1.57	1.53
19	AA	801	CLA	C3B-CAB	-2.06	1.43	1.47
19	B	811	CLA	CMC-C2C	-2.06	1.46	1.50
19	BB	824	CLA	C3B-C2B	-2.06	1.37	1.40
22	L	207	LHG	P-O6	2.06	1.67	1.59
19	A2	809	CLA	CMD-C2D	-2.06	1.46	1.50
19	L2	206	CLA	MG-ND	-2.06	2.01	2.05
22	LL	205	LHG	P-O6	2.06	1.67	1.59
26	B1	840	ECH	C1-C6	-2.05	1.50	1.53
19	B1	804	CLA	C3B-C2B	-2.05	1.37	1.40
19	A1	806	CLA	CMD-C2D	-2.05	1.46	1.50
19	AA	816	CLA	CMD-C2D	-2.05	1.46	1.50
19	A	807	CLA	CMD-C2D	-2.05	1.46	1.50
19	J1	103	CLA	CMD-C2D	-2.05	1.46	1.50
19	B1	831	CLA	C3B-CAB	-2.05	1.43	1.47
19	BB	804	CLA	CMC-C2C	-2.05	1.46	1.50
19	A1	806	CLA	C3B-CAB	-2.05	1.43	1.47
19	BB	827	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	805	CLA	CMC-C2C	-2.05	1.46	1.50
19	A1	834	CLA	C3B-C2B	-2.05	1.37	1.40
19	BB	828	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	835	CLA	C3B-C2B	-2.05	1.37	1.40
19	A	830	CLA	CMC-C2C	-2.05	1.46	1.50
19	AA	840	CLA	CMC-C2C	-2.05	1.46	1.50
19	A	806	CLA	C3B-CAB	-2.05	1.43	1.47
19	B2	803	CLA	CMC-C2C	-2.05	1.46	1.50
19	J2	103	CLA	CMD-C2D	-2.05	1.46	1.50
19	AA	853	CLA	CMC-C2C	-2.04	1.46	1.50
19	J1	101	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	824	CLA	CMD-C2D	-2.04	1.46	1.50
19	B	814	CLA	CMC-C2C	-2.04	1.46	1.50
19	K2	104	CLA	CMD-C2D	-2.04	1.46	1.50
19	A	827	CLA	CMC-C2C	-2.04	1.46	1.50
19	A	852	CLA	CMC-C2C	-2.04	1.46	1.50
19	AA	807	CLA	CMD-C2D	-2.04	1.46	1.50
23	K2	103	BCR	C33-C5	-2.04	1.47	1.50
23	M	101	BCR	C33-C5	-2.04	1.47	1.50
19	A2	834	CLA	CMC-C2C	-2.04	1.46	1.50
19	J2	101	CLA	CMD-C2D	-2.04	1.46	1.50
19	AA	834	CLA	CMC-C2C	-2.04	1.46	1.50
19	B2	803	CLA	C3B-CAB	-2.04	1.43	1.47
19	BB	831	CLA	CMD-C2D	-2.04	1.46	1.50
26	B2	841	ECH	C1-C6	-2.04	1.51	1.53
19	B1	802	CLA	C3B-C2B	-2.04	1.37	1.40
19	A2	832	CLA	CMD-C2D	-2.04	1.46	1.50
19	BB	822	CLA	CMC-C2C	-2.04	1.46	1.50
19	A1	833	CLA	CMC-C2C	-2.04	1.46	1.50
19	B1	848	CLA	CMC-C2C	-2.04	1.46	1.50
19	B2	849	CLA	MG-ND	-2.04	2.01	2.05
19	BB	835	CLA	C3B-CAB	-2.04	1.43	1.47
19	B1	803	CLA	CMC-C2C	-2.04	1.46	1.50
19	BB	855	CLA	CMC-C2C	-2.04	1.46	1.50
19	L2	205	CLA	CMC-C2C	-2.04	1.46	1.50
19	B	828	CLA	CMC-C2C	-2.04	1.46	1.50
19	B1	835	CLA	CMC-C2C	-2.04	1.46	1.50
19	A1	805	CLA	C3B-CAB	-2.04	1.43	1.47
25	BB	844	LMG	C7-C8	2.04	1.56	1.50
19	AA	853	CLA	CMD-C2D	-2.04	1.46	1.50
19	A2	807	CLA	CMD-C2D	-2.04	1.46	1.50
19	BB	855	CLA	C3B-CAB	-2.04	1.43	1.47
19	AA	832	CLA	CMD-C2D	-2.04	1.46	1.50
19	A1	805	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	836	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	854	CLA	C3B-C2B	-2.03	1.37	1.40
19	A1	822	CLA	CMC-C2C	-2.03	1.46	1.50
19	B1	831	CLA	CMD-C2D	-2.03	1.46	1.50
19	AA	826	CLA	CMC-C2C	-2.03	1.46	1.50
19	BB	827	CLA	C3B-CAB	-2.03	1.43	1.47
19	B2	816	CLA	C3B-C2B	-2.03	1.37	1.40
20	A1	802	CL0	C4C-C3C	2.03	1.48	1.45
19	K2	104	CLA	CBD-CAD	2.03	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	840	CLA	CMC-C2C	-2.03	1.46	1.50
19	L	202	CLA	CMC-C2C	-2.03	1.46	1.50
19	A	801	CLA	C3B-CAB	-2.03	1.43	1.47
19	A1	841	CLA	C3B-C2B	-2.03	1.37	1.40
19	A2	807	CLA	C3B-CAB	-2.03	1.43	1.47
23	M1	101	BCR	C33-C5	-2.03	1.47	1.50
19	BB	820	CLA	C3B-CAB	-2.03	1.43	1.47
19	L	203	CLA	CMC-C2C	-2.03	1.46	1.50
19	AA	832	CLA	CMC-C2C	-2.03	1.46	1.50
19	B2	804	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	810	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	820	CLA	CMD-C2D	-2.03	1.46	1.50
19	A2	842	CLA	C3B-C2B	-2.03	1.37	1.40
19	B2	830	CLA	C3B-C2B	-2.03	1.37	1.40
19	A	827	CLA	C3B-CAB	-2.03	1.43	1.47
23	K1	104	BCR	C33-C5	-2.03	1.47	1.50
19	AA	826	CLA	CMD-C2D	-2.03	1.46	1.50
22	L1	211	LHG	P-O6	2.03	1.67	1.59
19	B	833	CLA	C3B-CAB	-2.03	1.43	1.47
19	AA	837	CLA	C3B-C2B	-2.03	1.37	1.40
23	II	102	BCR	C33-C5	-2.03	1.47	1.50
19	B2	806	CLA	C3B-CAB	-2.03	1.43	1.47
19	BB	809	CLA	C3B-C2B	-2.03	1.37	1.40
23	K	103	BCR	C33-C5	-2.02	1.47	1.50
19	A2	836	CLA	C3B-CAB	-2.02	1.43	1.47
23	BB	843	BCR	C33-C5	-2.02	1.47	1.50
19	AA	801	CLA	C3B-C2B	-2.02	1.37	1.40
19	B2	832	CLA	CMD-C2D	-2.02	1.46	1.50
19	A	820	CLA	CMC-C2C	-2.02	1.46	1.50
19	A2	844	CLA	CMC-C2C	-2.02	1.46	1.50
19	A1	822	CLA	C3B-C2B	-2.02	1.37	1.40
19	A2	808	CLA	CMC-C2C	-2.02	1.46	1.50
19	A2	829	CLA	C3B-C2B	-2.02	1.37	1.40
19	L2	205	CLA	C3B-C2B	-2.02	1.37	1.40
25	II	105	LMG	C7-C8	2.02	1.56	1.50
19	A	834	CLA	CMC-C2C	-2.02	1.46	1.50
19	AA	816	CLA	C3B-C2B	-2.02	1.37	1.40
19	A	804	CLA	C3B-CAB	-2.02	1.43	1.47
23	JJ	104	BCR	C33-C5	-2.02	1.47	1.50
19	L1	206	CLA	CMC-C2C	-2.02	1.46	1.50
19	B1	805	CLA	C3B-CAB	-2.02	1.43	1.47
19	A	832	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	842	CLA	C4C-C3C	2.02	1.48	1.45
19	B	858	CLA	C3B-CAB	-2.02	1.43	1.47
19	B2	806	CLA	CMC-C2C	-2.02	1.46	1.50
19	A1	816	CLA	C3B-C2B	-2.02	1.37	1.40
19	F1	302	CLA	C3B-C2B	-2.02	1.37	1.40
19	A2	820	CLA	MG-ND	-2.02	2.01	2.05
19	B2	832	CLA	C3B-CAB	-2.02	1.43	1.47
23	M2	102	BCR	C33-C5	-2.02	1.47	1.50
19	B1	827	CLA	C3B-CAB	-2.02	1.43	1.47
19	A2	835	CLA	C3B-CAB	-2.02	1.43	1.47
19	LL	202	CLA	CMC-C2C	-2.02	1.46	1.50
19	B	827	CLA	C3B-CAB	-2.02	1.43	1.47
19	A2	826	CLA	C3B-C2B	-2.01	1.37	1.40
19	AA	816	CLA	C3B-CAB	-2.01	1.43	1.47
19	AA	827	CLA	C3B-CAB	-2.01	1.43	1.47
19	F2	302	CLA	C3B-C2B	-2.01	1.37	1.40
19	A1	842	CLA	MG-ND	-2.01	2.01	2.05
19	BB	814	CLA	MG-ND	-2.01	2.01	2.05
19	A2	812	CLA	C3B-CAB	-2.01	1.43	1.47
19	BB	821	CLA	CMB-C2B	-2.01	1.47	1.51
19	BB	835	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	818	CLA	CMD-C2D	-2.01	1.46	1.50
19	A	838	CLA	C3B-CAB	-2.01	1.43	1.47
23	B	844	BCR	C33-C5	-2.01	1.47	1.50
19	A2	840	CLA	CMC-C2C	-2.01	1.46	1.50
19	AA	806	CLA	CMC-C2C	-2.01	1.46	1.50
19	A	844	CLA	C3B-CAB	-2.01	1.43	1.47
19	AA	838	CLA	C3B-CAB	-2.01	1.43	1.47
19	B2	805	CLA	CMC-C2C	-2.01	1.46	1.50
19	B2	827	CLA	CMC-C2C	-2.01	1.46	1.50
19	A2	812	CLA	C3B-C2B	-2.01	1.37	1.40
19	B1	804	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	819	CLA	CMC-C2C	-2.01	1.46	1.50
19	AA	811	CLA	CMC-C2C	-2.01	1.46	1.50
19	B1	849	CLA	C3B-CAB	-2.01	1.43	1.47
19	B	827	CLA	CMC-C2C	-2.01	1.46	1.50
25	B2	847	LMG	O7-C8	-2.01	1.41	1.46
19	A1	831	CLA	CMD-C2D	-2.01	1.46	1.50
19	A2	831	CLA	C3B-C2B	-2.01	1.37	1.40
19	A1	823	CLA	CMC-C2C	-2.01	1.46	1.50
19	A1	819	CLA	MG-ND	-2.01	2.01	2.05
19	A	823	CLA	C3B-C2B	-2.01	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	807	CLA	CMC-C2C	-2.01	1.46	1.50
19	B1	827	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	826	CLA	C4B-CHC	-2.01	1.35	1.41
19	AA	823	CLA	C3B-C2B	-2.00	1.37	1.40
19	AA	831	CLA	C3B-CAB	-2.00	1.43	1.47
19	B2	846	CLA	CMD-C2D	-2.00	1.46	1.50
19	AA	805	CLA	CMC-C2C	-2.00	1.46	1.50
19	B2	831	CLA	CMD-C2D	-2.00	1.46	1.50
19	B	820	CLA	C3B-C2B	-2.00	1.37	1.40
19	A1	825	CLA	CMC-C2C	-2.00	1.46	1.50
19	A2	817	CLA	CMC-C2C	-2.00	1.46	1.50
19	LL	201	CLA	CMC-C2C	-2.00	1.46	1.50
19	A	806	CLA	CMC-C2C	-2.00	1.46	1.50
19	A	804	CLA	CMC-C2C	-2.00	1.46	1.50
19	B2	836	CLA	C3B-CAB	-2.00	1.43	1.47
19	A1	811	CLA	C3B-C2B	-2.00	1.37	1.40
19	F	302	CLA	C3B-C2B	-2.00	1.37	1.40
19	A1	839	CLA	CMC-C2C	-2.00	1.46	1.50

All (4106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	841	ECH	C16-C17-C18	-9.89	113.19	127.31
26	B1	840	ECH	C16-C17-C18	-9.84	113.27	127.31
26	B2	841	ECH	C16-C17-C18	-9.81	113.30	127.31
26	BB	840	ECH	C16-C17-C18	-9.54	113.70	127.31
20	A	803	CL0	CMD-C2D-C1D	8.52	139.72	124.71
19	BB	801	CLA	C4A-NA-C1A	8.33	110.45	106.71
20	A2	803	CL0	CMD-C2D-C1D	8.22	139.21	124.71
20	AA	803	CL0	O2D-CGD-CBD	8.18	125.81	111.27
20	A1	802	CL0	CMD-C2D-C1D	8.17	139.12	124.71
19	B	801	CLA	C4A-NA-C1A	8.09	110.34	106.71
19	B1	848	CLA	C4A-NA-C1A	8.02	110.31	106.71
20	AA	803	CL0	CMD-C2D-C1D	7.96	138.74	124.71
19	L2	205	CLA	C4A-NA-C1A	7.85	110.23	106.71
19	B2	801	CLA	C4A-NA-C1A	7.84	110.23	106.71
19	B1	801	CLA	C4A-NA-C1A	7.77	110.20	106.71
19	B	805	CLA	C4A-NA-C1A	7.75	110.19	106.71
19	A2	836	CLA	C4A-NA-C1A	7.68	110.16	106.71
19	BB	852	CLA	C4A-NA-C1A	7.62	110.13	106.71
20	A	803	CL0	O2D-CGD-CBD	7.57	124.73	111.27
19	B	854	CLA	C4A-NA-C1A	7.56	110.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	805	CLA	C4A-NA-C1A	7.56	110.11	106.71
19	L1	206	CLA	C4A-NA-C1A	7.47	110.07	106.71
19	B2	805	CLA	C4A-NA-C1A	7.46	110.06	106.71
19	LL	202	CLA	C4A-NA-C1A	7.41	110.04	106.71
19	L	204	CLA	C4A-NA-C1A	7.37	110.02	106.71
19	A2	801	CLA	C4A-NA-C1A	7.36	110.02	106.71
19	A	836	CLA	C4A-NA-C1A	7.36	110.01	106.71
19	B1	805	CLA	C4A-NA-C1A	7.35	110.01	106.71
19	A1	835	CLA	C4A-NA-C1A	7.35	110.01	106.71
19	B	859	CLA	C4A-NA-C1A	7.34	110.01	106.71
19	A	832	CLA	C4A-NA-C1A	7.31	109.99	106.71
19	BB	856	CLA	C4A-NA-C1A	7.30	109.99	106.71
19	A2	842	CLA	C4A-NA-C1A	7.27	109.97	106.71
20	A2	803	CL0	C2C-C1C-NC	7.27	116.78	109.97
19	A2	813	CLA	C4A-NA-C1A	7.25	109.96	106.71
19	AA	813	CLA	C4A-NA-C1A	7.24	109.96	106.71
19	B2	849	CLA	C4A-NA-C1A	7.22	109.95	106.71
19	A1	829	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	B	817	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	A1	801	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	AA	836	CLA	C4A-NA-C1A	7.19	109.94	106.71
19	B2	851	CLA	C4A-NA-C1A	7.19	109.94	106.71
19	A	825	CLA	C4A-NA-C1A	7.18	109.93	106.71
19	B1	826	CLA	C4A-NA-C1A	7.16	109.92	106.71
19	B2	826	CLA	C4A-NA-C1A	7.14	109.92	106.71
19	B1	836	CLA	C4A-NA-C1A	7.14	109.92	106.71
19	A	801	CLA	C4A-NA-C1A	7.14	109.92	106.71
19	A1	841	CLA	C4A-NA-C1A	7.13	109.91	106.71
19	A	813	CLA	C4A-NA-C1A	7.13	109.91	106.71
19	AA	801	CLA	C4A-NA-C1A	7.12	109.91	106.71
19	A2	838	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	B	833	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	BB	822	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	A1	831	CLA	C4A-NA-C1A	7.07	109.88	106.71
19	B2	837	CLA	C4A-NA-C1A	7.05	109.88	106.71
19	B1	850	CLA	C4A-NA-C1A	7.04	109.87	106.71
19	B	822	CLA	C4A-NA-C1A	7.03	109.86	106.71
19	B1	832	CLA	C4A-NA-C1A	6.97	109.84	106.71
19	A	830	CLA	C4A-NA-C1A	6.97	109.84	106.71
19	BB	817	CLA	C4A-NA-C1A	6.96	109.84	106.71
19	A2	832	CLA	C4A-NA-C1A	6.96	109.83	106.71
19	A2	823	CLA	C4A-NA-C1A	6.95	109.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	845	CLA	C4A-NA-C1A	6.95	109.83	106.71
19	A1	807	CLA	C4A-NA-C1A	6.95	109.83	106.71
19	AA	825	CLA	C4A-NA-C1A	6.94	109.83	106.71
19	A2	825	CLA	C4A-NA-C1A	6.94	109.82	106.71
20	A1	802	CL0	C2C-C1C-NC	6.92	116.46	109.97
19	K2	104	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	A	808	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	B	821	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	B	826	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	A	819	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	B2	821	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	A1	803	CLA	C4A-NA-C1A	6.89	109.80	106.71
19	B1	803	CLA	C4A-NA-C1A	6.88	109.80	106.71
19	B2	823	CLA	C4A-NA-C1A	6.88	109.80	106.71
20	AA	803	CL0	C2C-C1C-NC	6.87	116.41	109.97
19	AA	832	CLA	C4A-NA-C1A	6.87	109.80	106.71
19	A1	825	CLA	C4A-NA-C1A	6.87	109.79	106.71
19	AA	842	CLA	C4A-NA-C1A	6.87	109.79	106.71
19	B1	823	CLA	C4A-NA-C1A	6.86	109.79	106.71
19	A1	812	CLA	C4A-NA-C1A	6.85	109.79	106.71
19	A	828	CLA	C4A-NA-C1A	6.85	109.79	106.71
19	A1	822	CLA	C4A-NA-C1A	6.85	109.78	106.71
19	A1	837	CLA	C4A-NA-C1A	6.85	109.78	106.71
19	B2	833	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	B2	836	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	AA	828	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	B1	821	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	A2	822	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	A2	826	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	B	823	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	AA	822	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	AA	821	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	A2	808	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	B	812	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	AA	823	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	K	102	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A1	821	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	AA	818	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A2	827	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A1	823	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	A	817	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	B1	806	CLA	C4A-NA-C1A	6.77	109.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	803	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	A1	826	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	B2	817	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	X1	101	CLA	C4A-NA-C1A	6.76	109.74	106.71
19	F	301	CLA	C4A-NA-C1A	6.76	109.74	106.71
19	A2	828	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	A	844	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	B	802	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	B1	817	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	B1	804	CLA	C4A-NA-C1A	6.74	109.73	106.71
19	B1	835	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	B2	825	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	A	818	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	A	815	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	F1	302	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	B2	830	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	A	821	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	A1	838	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	BB	832	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	A	824	CLA	C4A-NA-C1A	6.72	109.72	106.71
19	B2	804	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	A	823	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	A2	802	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	B	830	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	AA	830	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	BB	823	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	AA	804	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	A2	841	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	B	809	CLA	C4A-NA-C1A	6.69	109.72	106.71
19	L	202	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	B2	824	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	A1	840	CLA	C4A-NA-C1A	6.67	109.71	106.71
19	AA	839	CLA	C4A-NA-C1A	6.67	109.71	106.71
19	BB	809	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	B1	815	CLA	C4A-NA-C1A	6.66	109.70	106.71
20	A	803	CL0	C2C-C1C-NC	6.66	116.21	109.97
19	B2	803	CLA	C4A-NA-C1A	6.66	109.70	106.71
19	A1	844	CLA	C4A-NA-C1A	6.65	109.70	106.71
19	BB	831	CLA	C4A-NA-C1A	6.65	109.70	106.71
20	A2	803	CL0	O2D-CGD-CBD	6.65	123.09	111.27
19	A1	808	CLA	C4A-NA-C1A	6.65	109.70	106.71
19	L1	205	CLA	C4A-NA-C1A	6.65	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	818	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	A2	809	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	B1	807	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	A2	830	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	AA	817	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	BB	828	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	XX	101	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	KK	102	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	A1	827	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	X	101	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	B1	812	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A2	819	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A2	824	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	L2	204	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	B	807	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A	838	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	A2	821	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	B2	831	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	B	836	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	AA	815	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	A2	852	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	B2	812	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	BB	812	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	A1	817	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	A	839	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	BB	803	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	BB	836	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	AA	805	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	AA	838	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	K1	103	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	A	805	CLA	C4A-NA-C1A	6.58	109.67	106.71
19	BB	807	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	BB	830	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	A2	818	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	B2	807	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	AA	841	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	A2	844	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	A2	839	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	A2	816	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	BB	813	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	A	841	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	AA	808	CLA	C4A-NA-C1A	6.55	109.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	842	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	BB	804	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	B1	822	CLA	C4A-NA-C1A	6.54	109.65	106.71
19	A	812	CLA	C4A-NA-C1A	6.54	109.64	106.71
19	F2	302	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	B2	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	B	806	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	A1	824	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	B1	825	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	JJ	101	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	J	101	CLA	C4A-NA-C1A	6.51	109.64	106.71
19	AA	824	CLA	C4A-NA-C1A	6.51	109.64	106.71
19	A2	805	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	X2	101	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	B1	808	CLA	C4A-NA-C1A	6.49	109.63	106.71
19	A	804	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	B	810	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	B	860	CLA	CAC-C3C-C4C	6.49	133.23	124.81
19	A2	817	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	A1	820	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	A1	832	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	A	829	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	B	829	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	B1	830	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	B1	802	CLA	C4A-NA-C1A	6.47	109.62	106.71
19	B	804	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	A	816	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	A1	828	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	BB	835	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	B1	809	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	FF	302	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	B2	809	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	B1	831	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	AA	829	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	A2	806	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	AA	843	CLA	CAC-C3C-C4C	6.43	133.15	124.81
19	AA	812	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	BB	821	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	B2	819	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	BB	806	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	LL	201	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	FF	301	CLA	C4A-NA-C1A	6.42	109.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	829	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	B	827	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	F1	301	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	A1	842	CLA	CAC-C3C-C4C	6.41	133.13	124.81
19	A1	815	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	B2	802	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	BB	845	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	F	302	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	B2	806	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	A	833	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	AA	819	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	A1	804	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	B2	828	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	A	831	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	BB	826	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	A	822	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	BB	824	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	B2	832	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	A1	814	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	A2	804	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	A2	807	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	A1	816	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	B	828	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	B	846	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	AA	809	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	B2	822	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	B	831	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	AA	831	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	B2	815	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	L	203	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	BB	827	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	A	809	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	A2	812	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	AA	827	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	K1	105	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	F2	301	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	B1	834	CLA	C4A-NA-C1A	6.29	109.53	106.71
19	B1	813	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	AA	826	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	K1	102	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	B	816	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	BB	825	CLA	C4A-NA-C1A	6.28	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	840	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	B	813	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	B	824	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	A	826	CLA	C4A-NA-C1A	6.27	109.52	106.71
19	B	825	CLA	C4A-NA-C1A	6.27	109.52	106.71
19	B	819	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	A2	835	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	A1	806	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	B	832	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	J1	103	CLA	C4A-NA-C1A	6.25	109.51	106.71
19	B	837	CLA	C4A-NA-C1A	6.25	109.51	106.71
19	A2	814	CLA	C4A-NA-C1A	6.24	109.51	106.71
19	A	840	CLA	C4A-NA-C1A	6.24	109.51	106.71
19	A2	811	CLA	C4A-NA-C1A	6.23	109.51	106.71
19	A	806	CLA	C4A-NA-C1A	6.23	109.51	106.71
19	FF	305	CLA	C4A-NA-C1A	6.23	109.51	106.71
19	B2	852	CLA	CAC-C3C-C4C	6.23	132.89	124.81
19	B2	814	CLA	C4A-NA-C1A	6.23	109.50	106.71
19	A1	833	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	A	827	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	B2	813	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	F1	305	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	BB	808	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	B2	810	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	B2	846	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	B2	835	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	A1	813	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	B1	845	CLA	C4A-NA-C1A	6.19	109.49	106.71
19	AA	833	CLA	C4A-NA-C1A	6.19	109.49	106.71
19	J1	101	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	J2	103	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	B	814	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	AA	814	CLA	C4A-NA-C1A	6.16	109.48	106.71
19	LL	203	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	B1	819	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	B	835	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	BB	810	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	BB	834	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	A1	830	CLA	C4A-NA-C1A	6.14	109.47	106.71
19	BB	814	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	A1	810	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	A1	836	CLA	C4A-NA-C1A	6.13	109.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	834	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	B	808	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	A	834	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	JJ	103	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	AA	837	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	B1	828	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	A	837	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	AA	806	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	A1	839	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	J	103	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	B1	827	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	AA	816	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	A	814	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	A1	834	CLA	C4A-NA-C1A	6.10	109.45	106.71
19	A2	820	CLA	C4A-NA-C1A	6.08	109.44	106.71
19	BB	819	CLA	C4A-NA-C1A	6.08	109.44	106.71
19	J2	101	CLA	C4A-NA-C1A	6.07	109.44	106.71
19	AA	807	CLA	C4A-NA-C1A	6.07	109.43	106.71
19	K2	102	CLA	C4A-NA-C1A	6.06	109.43	106.71
19	BB	802	CLA	C4A-NA-C1A	6.06	109.43	106.71
19	B1	810	CLA	C4A-NA-C1A	6.05	109.43	106.71
19	AA	834	CLA	C4A-NA-C1A	6.05	109.42	106.71
19	A2	837	CLA	C4A-NA-C1A	6.04	109.42	106.71
19	A	807	CLA	C4A-NA-C1A	6.02	109.41	106.71
19	B1	818	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	BB	816	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	L2	206	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	A2	840	CLA	C4A-NA-C1A	6.00	109.41	106.71
19	B2	816	CLA	C4A-NA-C1A	6.00	109.41	106.71
19	BB	855	CLA	C4A-NA-C1A	5.99	109.40	106.71
19	A2	815	CLA	C4A-NA-C1A	5.98	109.39	106.71
19	K	101	CLA	C4A-NA-C1A	5.98	109.39	106.71
19	B1	814	CLA	C4A-NA-C1A	5.97	109.39	106.71
19	B2	818	CLA	C4A-NA-C1A	5.96	109.39	106.71
19	KK	101	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	B2	850	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	BB	815	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	BB	836	CLA	CAC-C3C-C4C	5.95	132.53	124.81
19	A2	831	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	A	835	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	B	818	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	B1	849	CLA	C4A-NA-C1A	5.92	109.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	811	CLA	C4A-NA-C1A	5.92	109.37	106.71
19	B	815	CLA	C4A-NA-C1A	5.90	109.36	106.71
19	A	852	CLA	C4A-NA-C1A	5.88	109.35	106.71
19	A2	833	CLA	C4A-NA-C1A	5.87	109.35	106.71
19	BB	811	CLA	C4A-NA-C1A	5.87	109.35	106.71
19	A2	829	CLA	C4A-NA-C1A	5.87	109.34	106.71
19	A1	809	CLA	C4A-NA-C1A	5.87	109.34	106.71
19	B2	829	CLA	C4A-NA-C1A	5.85	109.33	106.71
19	A1	811	CLA	C4A-NA-C1A	5.84	109.33	106.71
19	B	860	CLA	C4A-NA-C1A	5.83	109.33	106.71
19	A1	852	CLA	C4A-NA-C1A	5.82	109.32	106.71
19	L1	207	CLA	C4A-NA-C1A	5.82	109.32	106.71
19	BB	829	CLA	C4A-NA-C1A	5.81	109.32	106.71
19	LL	201	CLA	C4-C3-C5	5.81	125.04	115.27
19	B2	827	CLA	C4A-NA-C1A	5.79	109.31	106.71
19	B2	811	CLA	C4A-NA-C1A	5.79	109.31	106.71
19	B1	816	CLA	C4A-NA-C1A	5.75	109.29	106.71
19	AA	820	CLA	C4A-NA-C1A	5.74	109.28	106.71
19	AA	843	CLA	C4A-NA-C1A	5.73	109.28	106.71
20	AA	803	CL0	CHB-C4A-NA	5.72	132.42	124.51
19	A	811	CLA	C4A-NA-C1A	5.72	109.28	106.71
19	BB	818	CLA	C4A-NA-C1A	5.72	109.28	106.71
19	B2	852	CLA	C4A-NA-C1A	5.71	109.27	106.71
19	AA	811	CLA	C4A-NA-C1A	5.69	109.26	106.71
19	AA	810	CLA	C4A-NA-C1A	5.65	109.25	106.71
20	A1	802	CL0	CHB-C4A-NA	5.64	132.32	124.51
19	B1	820	CLA	C4A-NA-C1A	5.64	109.24	106.71
26	B	841	ECH	C19-C18-C17	5.63	127.58	118.94
20	A	803	CL0	CHB-C4A-NA	5.62	132.29	124.51
19	B	820	CLA	C4A-NA-C1A	5.61	109.23	106.71
19	A1	805	CLA	C4A-NA-C1A	5.59	109.22	106.71
19	AA	853	CLA	C4A-NA-C1A	5.56	109.20	106.71
20	A1	802	CL0	O2D-CGD-CBD	5.54	121.11	111.27
19	AA	835	CLA	C4A-NA-C1A	5.54	109.20	106.71
19	A	810	CLA	C4A-NA-C1A	5.52	109.19	106.71
19	B	834	CLA	C4A-NA-C1A	5.52	109.19	106.71
19	A	820	CLA	C4A-NA-C1A	5.51	109.18	106.71
19	A1	842	CLA	C4A-NA-C1A	5.50	109.18	106.71
19	B1	811	CLA	C4A-NA-C1A	5.49	109.17	106.71
19	B	858	CLA	C4A-NA-C1A	5.46	109.16	106.71
26	B2	841	ECH	C19-C18-C17	5.38	127.20	118.94
19	L	202	CLA	C4-C3-C5	5.35	124.27	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	820	CLA	C4A-NA-C1A	5.35	109.11	106.71
19	A1	819	CLA	C4A-NA-C1A	5.33	109.10	106.71
20	AA	803	CL0	CAA-C2A-C1A	5.32	129.41	111.97
26	B1	840	ECH	C19-C18-C17	5.31	127.09	118.94
26	BB	840	ECH	C19-C18-C17	5.31	127.09	118.94
20	A1	802	CL0	CAA-C2A-C1A	5.31	129.36	111.97
19	BB	833	CLA	C4A-NA-C1A	5.30	109.09	106.71
19	B1	833	CLA	C4A-NA-C1A	5.28	109.08	106.71
19	B1	824	CLA	C4A-NA-C1A	5.27	109.08	106.71
19	A2	810	CLA	C4A-NA-C1A	5.27	109.08	106.71
19	B2	820	CLA	CAC-C3C-C4C	5.19	131.55	124.81
19	BB	820	CLA	CAC-C3C-C4C	5.18	131.53	124.81
19	B	820	CLA	CAC-C3C-C4C	5.16	131.50	124.81
20	A2	803	CL0	CHB-C4A-NA	5.15	131.63	124.51
20	A2	803	CL0	CMC-C2C-C1C	5.13	132.85	125.04
26	B1	840	ECH	C24-C23-C22	-5.01	118.66	126.23
26	B	841	ECH	C24-C23-C22	-4.98	118.71	126.23
19	LL	203	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
20	A2	803	CL0	O1D-CGD-CBD	-4.93	114.39	124.48
28	BB	854	DGD	O3G-C3G-C2G	-4.93	99.00	110.90
19	B	815	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
19	B2	834	CLA	C4A-NA-C1A	4.84	108.88	106.71
19	BB	826	CLA	CMB-C2B-C1B	-4.83	121.05	128.46
26	BB	840	ECH	C24-C23-C22	-4.82	118.95	126.23
19	B2	820	CLA	C4A-NA-C1A	4.81	108.87	106.71
28	B	856	DGD	O3G-C3G-C2G	-4.77	99.39	110.90
19	B1	833	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
19	BB	833	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
26	B	841	ECH	C36-C18-C19	-4.73	110.63	118.08
19	BB	815	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
26	B2	841	ECH	C24-C23-C22	-4.72	119.11	126.23
20	A2	803	CL0	C1C-C2C-C3C	-4.70	102.01	106.96
19	B	834	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
20	A2	803	CL0	CAA-C2A-C1A	4.63	127.14	111.97
19	A2	810	CLA	CAA-C2A-C1A	-4.60	96.91	111.97
19	AA	810	CLA	CAA-C2A-C1A	-4.56	97.02	111.97
20	A2	803	CL0	O2D-CGD-O1D	-4.49	115.07	123.84
19	B2	834	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
26	BB	840	ECH	C36-C18-C19	-4.42	111.11	118.08
26	B2	841	ECH	C36-C18-C19	-4.41	111.14	118.08
21	A1	843	PQN	C14-C13-C15	4.37	122.62	115.27
20	A	803	CL0	C1C-C2C-C3C	-4.36	102.37	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A1	802	CL0	C1C-C2C-C3C	-4.36	102.37	106.96
26	B1	840	ECH	C36-C18-C19	-4.36	111.21	118.08
19	B	860	CLA	CAC-C3C-C2C	-4.34	120.11	127.53
19	B1	815	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
20	A1	802	CL0	C3C-C4C-NC	4.33	115.43	110.57
20	AA	803	CL0	O2D-CGD-O1D	-4.30	115.43	123.84
21	A2	843	PQN	C14-C13-C15	4.30	122.50	115.27
26	BB	840	ECH	C16-C15-C14	-4.29	114.69	123.47
19	AA	843	CLA	CAC-C3C-C2C	-4.28	120.21	127.53
20	AA	803	CL0	O1D-CGD-CBD	-4.27	115.74	124.48
19	BB	833	CLA	CMB-C2B-C3B	4.26	132.65	124.68
19	A1	842	CLA	CAC-C3C-C2C	-4.26	120.25	127.53
19	B2	852	CLA	CAC-C3C-C2C	-4.24	120.28	127.53
20	A	803	CL0	O2A-CGA-CBA	4.24	125.21	111.91
19	B2	826	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
19	A	810	CLA	CAA-C2A-C1A	-4.23	98.13	111.97
21	A	843	PQN	C14-C13-C15	4.22	122.37	115.27
19	BB	803	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
19	L1	207	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
20	A2	803	CL0	CAC-C3C-C4C	4.19	130.25	124.81
19	B	815	CLA	CMB-C2B-C3B	4.19	132.51	124.68
19	B	834	CLA	CMB-C2B-C3B	4.16	132.45	124.68
19	AA	805	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
19	B	803	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
23	F1	306	BCR	C15-C16-C17	-4.14	114.99	123.47
19	B1	833	CLA	CMB-C2B-C3B	4.14	132.42	124.68
23	F2	305	BCR	C15-C16-C17	-4.14	115.00	123.47
19	B2	807	CLA	O2D-CGD-CBD	4.13	118.61	111.27
20	AA	803	CL0	CAC-C3C-C4C	4.13	130.17	124.81
19	B1	826	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
19	B2	803	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
19	L2	206	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
19	A	805	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
19	B	846	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
19	BB	845	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
20	AA	803	CL0	C1C-C2C-C3C	-4.05	102.70	106.96
19	L	204	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
19	A	852	CLA	C7-C6-C5	4.02	124.27	113.36
20	A2	803	CL0	C3D-C2D-C1D	-3.99	100.38	105.83
19	BB	815	CLA	CMB-C2B-C3B	3.99	132.14	124.68
19	B	814	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
19	B2	815	CLA	CMB-C2B-C1B	-3.98	122.35	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	807	CLA	O2D-CGD-CBD	3.97	118.32	111.27
19	BB	807	CLA	O2D-CGD-CBD	3.97	118.31	111.27
19	B1	828	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
19	B	829	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
20	AA	803	CL0	C3C-C4C-NC	3.91	114.96	110.57
19	A2	805	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
19	A2	837	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
19	B2	807	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
19	A2	852	CLA	C7-C6-C5	3.86	123.85	113.36
19	A2	823	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
19	KK	101	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
19	L	203	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	BB	834	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	B	807	CLA	O2D-CGD-CBD	3.84	118.08	111.27
19	FF	305	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
26	B	841	ECH	C33-C5-C6	-3.83	120.23	124.53
19	B2	846	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
19	B	826	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
19	B1	807	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
19	AA	824	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
19	AA	838	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
19	LL	203	CLA	CMB-C2B-C3B	3.81	131.80	124.68
19	BB	807	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
19	B1	845	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
19	B2	833	CLA	CGD-CBD-CAD	-3.79	98.44	110.73
19	A	837	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
20	A2	803	CL0	C3B-C4B-NB	3.79	114.11	109.21
19	B2	829	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	A	823	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	A1	837	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	J	104	BCR	C2-C1-C6	3.76	116.28	110.48
19	K	101	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
19	AA	829	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
19	B	807	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	BB	847	BCR	C15-C16-C17	-3.75	115.80	123.47
26	B1	840	ECH	C16-C15-C14	-3.75	115.80	123.47
20	A	803	CL0	C3C-C4C-NC	3.75	114.77	110.57
19	AA	837	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	AA	823	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	B1	825	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
19	A	824	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
21	AA	844	PQN	C14-C13-C15	3.73	121.55	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A1	802	CL0	C3D-C2D-C1D	-3.73	100.74	105.83
19	AA	835	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
19	AA	820	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
19	A2	832	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
19	A	831	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
19	BB	803	CLA	CMB-C2B-C3B	3.71	131.61	124.68
19	A1	836	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
23	BB	841	BCR	C15-C14-C13	-3.70	122.03	127.31
23	B	848	BCR	C15-C16-C17	-3.69	115.91	123.47
19	B2	834	CLA	CMB-C2B-C3B	3.69	131.59	124.68
23	B	842	BCR	C15-C14-C13	-3.69	122.04	127.31
19	B	821	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
19	BB	814	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
19	B	825	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
20	AA	803	CL0	C3B-C4B-NB	3.69	113.98	109.21
26	BB	840	ECH	C12-C13-C14	-3.68	113.29	118.94
20	A2	803	CL0	C3C-C4C-NC	3.68	114.70	110.57
19	B	801	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
20	A1	802	CL0	O1D-CGD-CBD	-3.67	116.97	124.48
26	B2	841	ECH	C33-C5-C6	-3.67	120.40	124.53
26	BB	840	ECH	C33-C5-C6	-3.67	120.41	124.53
26	B1	840	ECH	C33-C5-C6	-3.67	120.41	124.53
19	B1	815	CLA	CMB-C2B-C3B	3.67	131.54	124.68
19	B2	834	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
19	A2	823	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
19	A	839	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
23	F	305	BCR	C15-C16-C17	-3.67	115.96	123.47
19	A2	831	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
19	BB	825	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	F1	306	BCR	C15-C14-C13	-3.65	122.10	127.31
19	B2	825	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
23	F2	305	BCR	C15-C14-C13	-3.65	122.10	127.31
19	B	801	CLA	C4-C3-C2	-3.64	114.33	123.68
19	A	838	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
19	A1	823	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
19	B1	833	CLA	O2D-CGD-CBD	3.63	117.73	111.27
19	B	825	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	B2	841	ECH	C16-C15-C14	-3.63	116.03	123.47
19	B	812	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
19	B2	803	CLA	CMB-C2B-C3B	3.63	131.47	124.68
19	AA	839	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
19	B1	803	CLA	CMB-C2B-C1B	-3.61	122.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	803	CLA	CMB-C2B-C3B	3.61	131.44	124.68
19	A1	830	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
19	B2	801	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
20	A	803	CL0	CMD-C2D-C3D	-3.60	119.33	127.61
19	BB	825	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
20	AA	803	CL0	C3D-C2D-C1D	-3.59	100.93	105.83
19	BB	836	CLA	CAC-C3C-C2C	-3.59	121.38	127.53
20	A	803	CL0	C3B-C4B-NB	3.59	113.85	109.21
20	A	803	CL0	C3D-C2D-C1D	-3.59	100.93	105.83
19	A1	828	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
26	B1	840	ECH	C7-C8-C9	-3.59	120.82	126.23
23	J1	102	BCR	C15-C16-C17	-3.59	116.13	123.47
19	BB	816	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
23	FF	306	BCR	C15-C16-C17	-3.58	116.15	123.47
19	B2	825	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
23	B2	842	BCR	C1-C6-C5	-3.57	117.59	122.61
26	B2	841	ECH	C7-C8-C9	-3.56	120.86	126.23
19	A2	824	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
19	A	829	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	B2	834	CLA	O2D-CGD-CBD	3.55	117.58	111.27
20	A1	802	CL0	C3B-C4B-NB	3.55	113.80	109.21
23	J	102	BCR	C15-C16-C17	-3.55	116.20	123.47
19	A1	838	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	A2	839	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
26	B	841	ECH	C16-C15-C14	-3.54	116.22	123.47
19	L2	205	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
19	BB	801	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
23	A1	850	BCR	C15-C16-C17	-3.53	116.24	123.47
19	B1	801	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
23	FF	306	BCR	C15-C14-C13	-3.53	122.28	127.31
23	F1	304	BCR	C24-C23-C22	-3.52	120.91	126.23
23	B2	842	BCR	C15-C16-C17	-3.52	116.26	123.47
19	A	810	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
28	BB	854	DGD	O6D-C1D-O3G	-3.52	101.64	109.97
19	B	835	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
19	A1	819	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
19	AA	831	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
20	A	803	CL0	O1D-CGD-CBD	-3.51	117.31	124.48
19	L2	206	CLA	CMB-C2B-C3B	3.50	131.23	124.68
23	AA	854	BCR	C15-C16-C17	-3.50	116.30	123.47
19	B1	825	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
19	B2	850	CLA	CMB-C2B-C1B	-3.50	123.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	850	BCR	C15-C16-C17	-3.50	116.30	123.47
26	B	841	ECH	C7-C8-C9	-3.50	120.95	126.23
23	J2	102	BCR	C15-C16-C17	-3.50	116.31	123.47
19	F	302	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
19	BB	808	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
19	A	820	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
19	F2	302	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
23	A	853	BCR	C15-C16-C17	-3.49	116.33	123.47
19	B	836	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	JJ	102	BCR	C15-C16-C17	-3.47	116.36	123.47
19	A2	823	CLA	O2D-CGD-CBD	3.47	117.43	111.27
19	L1	207	CLA	CMB-C2B-C3B	3.47	131.16	124.68
19	A2	832	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
19	B2	801	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
19	B2	812	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
19	AA	832	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
23	F	305	BCR	C15-C14-C13	-3.46	122.38	127.31
23	L	205	BCR	C15-C16-C17	-3.46	116.39	123.47
19	AA	805	CLA	CMB-C2B-C3B	3.46	131.14	124.68
19	BB	801	CLA	O2D-CGD-CBD	3.46	117.41	111.27
19	B1	830	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	B2	816	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	KK	101	CLA	O2D-CGD-O1D	-3.44	117.10	123.84
19	AA	838	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
19	B2	831	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	B	816	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
19	K	101	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
19	F1	301	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
19	K1	103	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	A	840	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	A1	808	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
19	A	838	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
19	F	301	CLA	O2D-CGD-CBD	3.42	117.35	111.27
19	BB	855	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	A	822	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	K1	102	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
19	K1	102	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	B	806	CLA	C5-C3-C2	3.42	128.04	121.12
19	B	858	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
19	BB	807	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
19	A	814	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
19	BB	809	CLA	O2D-CGD-O1D	-3.41	117.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	835	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
20	A	803	CL0	C1D-ND-C4D	-3.41	103.91	106.33
19	BB	833	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
19	FF	302	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
28	B	856	DGD	O6D-C1D-O3G	-3.41	101.91	109.97
19	A1	831	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
23	B1	841	BCR	C15-C14-C13	-3.40	122.46	127.31
19	A	805	CLA	CMB-C2B-C3B	3.40	131.04	124.68
19	B2	807	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	A1	819	CLA	CMB-C2B-C3B	3.40	131.04	124.68
19	A	832	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
19	B1	834	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
20	AA	803	CL0	CMC-C2C-C1C	3.39	130.21	125.04
19	LL	201	CLA	C6-C5-C3	3.39	122.35	113.45
23	FF	303	BCR	C35-C13-C14	-3.39	118.17	122.92
19	BB	856	CLA	CHB-C4A-NA	3.39	129.20	124.51
19	K1	105	CLA	CBD-CHA-C1A	3.39	132.49	128.50
19	A2	806	CLA	CAA-C2A-C1A	-3.39	100.88	111.97
20	A1	802	CL0	O2D-CGD-O1D	-3.38	117.23	123.84
19	F1	301	CLA	CAA-C2A-C3A	-3.38	103.53	112.78
19	A1	822	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
19	B1	824	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
19	B	821	CLA	CMB-C2B-C3B	3.37	130.99	124.68
19	F	301	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	A	823	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
23	A	851	BCR	C2-C1-C6	3.37	115.67	110.48
19	L1	206	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
19	BB	806	CLA	C5-C3-C2	3.36	127.92	121.12
19	A2	838	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
19	B1	801	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
19	A1	812	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
19	B1	807	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
19	A	812	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
19	A2	820	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
19	BB	805	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
19	B	801	CLA	O2D-CGD-CBD	3.35	117.23	111.27
19	B	859	CLA	CHB-C4A-NA	3.35	129.15	124.51
19	B	820	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
19	A1	831	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
19	F1	302	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
19	BB	836	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
19	FF	301	CLA	CMB-C2B-C1B	-3.35	123.32	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	846	CLA	CMB-C2B-C3B	3.35	130.94	124.68
19	A	835	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
19	A2	802	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
19	B1	812	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	F	304	BCR	C24-C23-C22	-3.34	121.19	126.23
19	A1	805	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	FF	304	BCR	C24-C23-C22	-3.33	121.20	126.23
19	B1	836	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
19	B2	837	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
19	BB	845	CLA	CMB-C2B-C3B	3.33	130.91	124.68
19	A	820	CLA	CMB-C2B-C3B	3.33	130.90	124.68
19	A1	814	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
19	BB	810	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
19	K2	102	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
20	A	803	CL0	O2A-CGA-O1A	-3.32	115.20	123.59
19	B	810	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
23	I2	103	BCR	C15-C16-C17	-3.32	116.67	123.47
19	AA	820	CLA	CMB-C2B-C3B	3.32	130.89	124.68
19	B1	816	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	A2	815	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	L	203	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
19	B2	805	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
19	A2	829	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
19	B2	851	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
19	A1	852	CLA	C7-C6-C5	3.31	122.35	113.36
19	A2	805	CLA	CMB-C2B-C3B	3.31	130.87	124.68
19	B2	815	CLA	CMB-C2B-C3B	3.31	130.87	124.68
19	A1	827	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
19	AA	823	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
19	B1	806	CLA	C5-C3-C2	3.30	127.80	121.12
19	F1	305	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
19	AA	838	CLA	CMB-C2B-C3B	3.30	130.86	124.68
19	B	833	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
19	A2	820	CLA	CMB-C2B-C3B	3.30	130.85	124.68
23	F	303	BCR	C35-C13-C14	-3.30	118.31	122.92
19	A1	809	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
19	A2	813	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
19	AA	812	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
19	B	805	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	A1	813	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	BB	820	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
19	KK	102	CLA	CMB-C2B-C1B	-3.29	123.41	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	812	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	BB	826	CLA	C2D-C1D-ND	-3.29	107.68	110.10
26	B	841	ECH	C28-C27-C26	-3.29	115.62	118.65
19	B1	814	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
19	B	809	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
19	BB	801	CLA	CHB-C4A-NA	3.28	129.05	124.51
19	LL	202	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
19	BB	836	CLA	CHB-C4A-NA	3.28	129.05	124.51
19	AA	828	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	AA	806	CLA	CBA-CAA-C2A	3.28	123.53	113.86
19	A2	814	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	B	807	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	B1	850	CLA	CHB-C4A-NA	3.27	129.04	124.51
19	KK	101	CLA	CMB-C2B-C3B	3.27	130.80	124.68
19	A2	809	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
19	B	824	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
26	BB	840	ECH	C7-C8-C9	-3.27	121.29	126.23
19	B	814	CLA	CMB-C2B-C3B	3.27	130.79	124.68
19	F2	301	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
19	B	837	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
19	B1	805	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
19	A2	828	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
19	AA	811	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
19	B2	851	CLA	CHB-C4A-NA	3.26	129.02	124.51
23	F2	304	BCR	C24-C23-C22	-3.26	121.31	126.23
19	F	301	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
19	AA	832	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
19	B	811	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
23	L1	208	BCR	C15-C16-C17	-3.25	116.81	123.47
19	A	806	CLA	CBA-CAA-C2A	3.25	123.47	113.86
19	B1	833	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
20	A1	802	CL0	CMD-C2D-C3D	-3.25	120.14	127.61
19	BB	855	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
23	A1	851	BCR	C2-C1-C6	3.24	115.47	110.48
19	BB	824	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
19	B2	820	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
19	B1	820	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
19	B2	806	CLA	C5-C3-C2	3.23	127.66	121.12
19	L	202	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	AA	814	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	A2	840	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	BB	805	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	812	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	AA	835	CLA	CMB-C2B-C3B	3.23	130.71	124.68
19	A2	810	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
19	B2	846	CLA	CMB-C2B-C3B	3.22	130.71	124.68
19	B	834	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
19	F2	301	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
19	B2	805	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
19	A1	818	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
23	B2	842	BCR	C15-C14-C13	-3.22	122.71	127.31
19	K	101	CLA	CMB-C2B-C3B	3.22	130.71	124.68
19	A1	837	CLA	CMB-C2B-C3B	3.22	130.70	124.68
19	B1	803	CLA	CMB-C2B-C3B	3.21	130.69	124.68
19	L	204	CLA	CMB-C2B-C3B	3.21	130.69	124.68
19	B2	801	CLA	O2D-CGD-CBD	3.21	116.97	111.27
19	B1	811	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
19	A2	827	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
19	B1	845	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	K1	106	BCR	C24-C23-C22	-3.20	121.40	126.23
19	B	859	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
19	B1	832	CLA	CHB-C4A-NA	3.20	128.94	124.51
19	B	801	CLA	CHB-C4A-NA	3.20	128.94	124.51
26	B1	840	ECH	C12-C13-C14	-3.20	114.03	118.94
19	F2	301	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
19	B1	850	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
19	F1	301	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
20	A2	803	CL0	C9-C8-C10	3.19	122.86	111.29
23	A1	853	BCR	C15-C16-C17	-3.19	116.93	123.47
19	L1	206	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
19	B1	804	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
19	A2	808	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
19	A1	822	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
19	B2	809	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
23	A2	853	BCR	C15-C16-C17	-3.19	116.94	123.47
19	B2	811	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
19	A	841	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
23	A2	851	BCR	C2-C1-C6	3.19	115.39	110.48
19	L1	205	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
19	B	859	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
19	BB	829	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
26	B2	841	ECH	C12-C13-C14	-3.18	114.06	118.94
19	B1	809	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
19	AA	830	CLA	CMB-C2B-C1B	-3.18	123.58	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	819	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
23	J2	104	BCR	C24-C23-C22	-3.18	121.43	126.23
19	B1	820	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	BB	856	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
19	B2	826	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
19	A2	830	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	AA	841	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	LL	201	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	L2	205	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
19	BB	826	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
19	B1	836	CLA	CHB-C4A-NA	3.17	128.90	124.51
23	A	850	BCR	C15-C16-C17	-3.17	116.98	123.47
19	B1	826	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
19	A	830	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	I1	102	LMG	O6-C1-O1	-3.17	102.47	109.97
19	B1	815	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
23	M	101	BCR	C15-C16-C17	-3.17	116.99	123.47
19	BB	811	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
23	J1	104	BCR	C2-C1-C6	3.17	115.35	110.48
20	AA	803	CL0	CMD-C2D-C3D	-3.16	120.33	127.61
19	BB	832	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
19	A	838	CLA	CMB-C2B-C3B	3.16	130.60	124.68
23	A1	849	BCR	C2-C1-C6	3.16	115.35	110.48
23	B2	842	BCR	C30-C25-C26	-3.16	118.16	122.61
19	LL	201	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
19	B2	810	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
19	K	101	CLA	CAA-C2A-C3A	-3.16	104.13	112.78
19	B1	805	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
26	B	841	ECH	C12-C13-C14	-3.16	114.10	118.94
23	K	103	BCR	C15-C16-C17	-3.16	117.01	123.47
19	BB	834	CLA	CMB-C2B-C3B	3.15	130.58	124.68
19	B	834	CLA	O2A-CGA-O1A	-3.15	115.63	123.59
19	B2	833	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
20	A2	803	CL0	C1D-ND-C4D	-3.15	104.10	106.33
19	B2	828	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
19	F	301	CLA	CHB-C4A-NA	3.15	128.87	124.51
19	B2	837	CLA	CHB-C4A-NA	3.15	128.87	124.51
23	AA	850	BCR	C2-C1-C6	3.15	115.33	110.48
19	A1	837	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
19	A1	811	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
19	FF	302	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
19	B1	812	CLA	CMB-C2B-C1B	-3.14	123.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	818	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	A	828	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	A1	832	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
19	AA	811	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
23	AA	852	BCR	C2-C1-C6	3.14	115.31	110.48
19	A1	810	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
23	A2	849	BCR	C2-C1-C6	3.14	115.31	110.48
19	B	826	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
19	B1	819	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	B2	804	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	B	823	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	A	819	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	BB	814	CLA	CMB-C2B-C3B	3.13	130.54	124.68
19	B	805	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
19	A	806	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
20	A2	803	CL0	CMD-C2D-C3D	-3.13	120.41	127.61
19	A2	819	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	BB	813	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
19	A1	807	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	A2	838	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
19	BB	813	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	BB	823	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	B1	809	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	AA	829	CLA	CMB-C2B-C3B	3.13	130.53	124.68
19	A2	835	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	A	809	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
19	BB	809	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	LL	202	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	BB	833	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
23	II	104	BCR	C15-C16-C17	-3.12	117.07	123.47
20	A	803	CL0	C3D-C4D-ND	3.12	115.29	110.24
19	F2	302	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
19	A2	806	CLA	CBA-CAA-C2A	3.12	123.08	113.86
23	AA	851	BCR	C15-C16-C17	-3.12	117.08	123.47
19	A2	841	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	AA	806	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	KK	101	CLA	CAA-C2A-C3A	-3.12	104.24	112.78
19	K2	102	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	B1	818	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	L1	205	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
19	BB	801	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	A	810	CLA	CBA-CAA-C2A	3.12	123.06	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	809	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
19	B2	809	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
19	BB	833	CLA	O2A-CGA-O1A	-3.11	115.73	123.59
19	AA	841	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
19	A	823	CLA	CMB-C2B-C3B	3.11	130.49	124.68
23	A	854	BCR	C24-C23-C22	-3.11	121.54	126.23
20	A1	802	CL0	C1D-ND-C4D	-3.11	104.13	106.33
19	F1	301	CLA	CHB-C4A-NA	3.11	128.81	124.51
19	L	202	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
19	A	810	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
19	X2	101	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
19	A2	805	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
19	B1	849	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
19	B1	850	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
19	L	202	CLA	C6-C5-C3	3.10	121.58	113.45
19	AA	805	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
19	B2	824	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
23	F	305	BCR	C11-C10-C9	-3.09	122.90	127.31
19	A	839	CLA	CMB-C2B-C3B	3.09	130.46	124.68
23	J1	104	BCR	C24-C23-C22	-3.09	121.56	126.23
19	AA	813	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
19	B2	814	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
19	A2	810	CLA	O2D-CGD-CBD	3.09	116.76	111.27
19	X	101	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
19	BB	835	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
19	B2	812	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
19	B	825	CLA	CMB-C2B-C3B	3.09	130.46	124.68
19	A1	828	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	A	803	CL0	O2A-C1-C2	3.09	116.75	108.64
19	A	841	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
19	B	817	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
19	A1	804	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
19	A2	822	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
19	A1	819	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
19	J1	101	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
20	A	803	CL0	CMC-C2C-C1C	3.08	129.73	125.04
19	A	808	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
19	XX	101	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	A	829	CLA	CMB-C2B-C3B	3.08	130.44	124.68
19	AA	823	CLA	CMB-C2B-C3B	3.08	130.44	124.68
19	B2	850	CLA	CMB-C2B-C3B	3.08	130.44	124.68
19	B1	814	CLA	O2D-CGD-O1D	-3.08	117.82	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	831	CLA	CMB-C2B-C3B	3.08	130.44	124.68
19	B	834	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
19	A	839	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	AA	845	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	AA	819	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
19	X1	101	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
19	BB	814	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
19	AA	804	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
19	B	830	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	B1	810	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
19	AA	824	CLA	CMB-C2B-C3B	3.07	130.42	124.68
19	A	815	CLA	CHB-C4A-NA	3.06	128.75	124.51
19	AA	853	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	BB	852	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
19	B2	822	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
19	A1	814	CLA	CHB-C4A-NA	3.06	128.75	124.51
19	AA	821	CLA	CHB-C4A-NA	3.06	128.75	124.51
19	B	804	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	B2	851	CLA	CBA-CAA-C2A	3.06	122.89	113.86
19	A1	825	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
19	A1	839	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
19	AA	808	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
23	A	849	BCR	C2-C1-C6	3.06	115.19	110.48
19	B2	801	CLA	CHB-C4A-NA	3.06	128.74	124.51
19	B2	820	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
19	B	818	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
19	A2	815	CLA	CHB-C4A-NA	3.05	128.74	124.51
19	AA	839	CLA	CMB-C2B-C3B	3.05	130.39	124.68
19	BB	804	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
23	F2	305	BCR	C11-C10-C9	-3.05	122.96	127.31
19	B2	834	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
19	A1	840	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
19	A	844	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	B	814	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	B2	825	CLA	CMB-C2B-C3B	3.05	130.38	124.68
19	A1	844	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	A2	815	CLA	CMB-C2B-C3B	3.04	130.38	124.68
19	B1	833	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
19	B	828	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	AA	810	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
19	A1	816	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
23	F1	306	BCR	C11-C10-C9	-3.03	122.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	859	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
19	A1	808	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	B2	817	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	F1	302	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
19	B2	833	CLA	CHB-C4A-NA	3.03	128.70	124.51
19	A1	842	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
19	AA	809	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	A	805	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
20	A2	803	CL0	O2A-CGA-CBA	3.03	121.41	111.91
19	AA	815	CLA	CHB-C4A-NA	3.03	128.70	124.51
19	A2	844	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	BB	825	CLA	CMB-C2B-C3B	3.03	130.34	124.68
19	A1	807	CLA	O2A-CGA-O1A	-3.03	115.96	123.59
19	A2	801	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	AA	801	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	B1	833	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
19	L2	204	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
19	A1	840	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
20	A	803	CL0	O2D-CGD-O1D	-3.02	117.93	123.84
19	B	834	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
19	F2	301	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	B	837	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	B	802	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
19	A2	809	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	A	811	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
19	A	801	CLA	CHB-C4A-NA	3.02	128.68	124.51
19	A	833	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	BB	819	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
19	B1	824	CLA	CMB-C2B-C3B	3.01	130.32	124.68
23	J	104	BCR	C24-C23-C22	-3.01	121.68	126.23
19	BB	856	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
19	A	832	CLA	O2D-CGD-CBD	3.01	116.62	111.27
19	A	821	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	B	858	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	B1	804	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	BB	852	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	BB	828	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
20	AA	803	CL0	C1D-ND-C4D	-3.01	104.20	106.33
19	AA	814	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	B	813	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
23	B1	843	BCR	C33-C5-C6	-3.01	121.15	124.53
19	B1	829	CLA	O2D-CGD-O1D	-3.01	117.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	834	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	B1	813	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
19	A	852	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	A2	821	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	B2	807	CLA	CHB-C4A-NA	3.00	128.66	124.51
19	A	831	CLA	CMB-C2B-C3B	3.00	130.29	124.68
19	JJ	101	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
19	BB	855	CLA	CMB-C2B-C3B	3.00	130.29	124.68
19	A2	824	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	AA	821	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	I2	103	BCR	C24-C23-C22	-3.00	121.70	126.23
19	AA	810	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	L2	204	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	A1	821	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	J1	104	BCR	C1-C6-C5	-3.00	118.39	122.61
19	B2	852	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	B2	820	CLA	CAC-C3C-C2C	-3.00	122.40	127.53
19	B2	804	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	B	817	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
19	B2	834	CLA	O2A-CGA-O1A	-3.00	116.03	123.59
19	A	842	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	BB	828	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
19	B2	831	CLA	CMB-C2B-C3B	2.99	130.28	124.68
19	B1	817	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	A2	833	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	A2	817	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	B2	813	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
23	KK	103	BCR	C15-C16-C17	-2.99	117.34	123.47
19	A	821	CLA	CHB-C4A-NA	2.99	128.65	124.51
19	B2	806	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	AA	839	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	B	818	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	A1	814	CLA	CMB-C2B-C3B	2.99	130.27	124.68
19	A	824	CLA	CMB-C2B-C3B	2.99	130.27	124.68
19	BB	832	CLA	CMB-C2B-C3B	2.99	130.27	124.68
19	BB	820	CLA	CAC-C3C-C2C	-2.99	122.42	127.53
19	A2	840	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
20	AA	803	CL0	CMB-C2B-C3B	2.99	130.27	124.68
19	A2	823	CLA	CMB-C2B-C3B	2.99	130.26	124.68
23	B2	844	BCR	C33-C5-C6	-2.99	121.17	124.53
19	A2	811	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
19	F	302	CLA	CMB-C2B-C1B	-2.99	123.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	823	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
23	F2	304	BCR	C2-C1-C6	2.98	115.07	110.48
19	LL	203	CLA	C2D-C1D-ND	-2.98	107.91	110.10
19	B	833	CLA	CHB-C4A-NA	2.98	128.64	124.51
19	A	826	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	B2	823	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	J2	101	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	A	808	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	A1	801	CLA	CHB-C4A-NA	2.98	128.63	124.51
23	B	848	BCR	C1-C6-C5	-2.98	118.42	122.61
19	B1	825	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	A1	809	CLA	CAA-C2A-C1A	-2.98	102.22	111.97
19	AA	809	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
19	B	801	CLA	C4-C3-C5	2.98	120.28	115.27
23	J	102	BCR	C15-C14-C13	-2.98	123.06	127.31
19	A1	838	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	B	833	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	BB	843	BCR	C33-C5-C6	-2.98	121.19	124.53
23	M2	102	BCR	C35-C13-C14	-2.98	118.75	122.92
19	A2	830	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
19	BB	814	CLA	CHB-C4A-NA	2.97	128.62	124.51
19	B1	801	CLA	O2D-CGD-CBD	2.97	116.55	111.27
19	AA	842	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
23	B	844	BCR	C33-C5-C6	-2.97	121.19	124.53
23	K2	105	BCR	C24-C23-C22	-2.97	121.74	126.23
19	J	101	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
19	A1	830	CLA	CMB-C2B-C3B	2.97	130.23	124.68
19	BB	856	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
19	B	801	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
19	B1	801	CLA	CHB-C4A-NA	2.97	128.61	124.51
19	K2	104	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	B	835	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	FF	304	BCR	C2-C1-C6	2.96	115.05	110.48
19	A1	806	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	A2	823	CLA	CHB-C4A-NA	2.96	128.61	124.51
19	A2	810	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	A2	839	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	B2	839	BCR	C15-C14-C13	-2.96	123.08	127.31
19	A2	830	CLA	CMB-C2B-C3B	2.96	130.22	124.68
19	B2	802	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	A1	809	CLA	O2D-CGD-CBD	2.96	116.53	111.27
23	FF	306	BCR	C11-C10-C9	-2.96	123.08	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	816	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	K1	102	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
19	B1	850	CLA	CBA-CAA-C2A	2.96	122.60	113.86
19	A	813	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
19	B1	802	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	B1	806	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	A2	841	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	B	828	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	B	827	CLA	CHB-C4A-NA	2.95	128.60	124.51
19	A1	824	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	B2	821	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	AA	811	CLA	CMB-C2B-C3B	2.95	130.20	124.68
19	B2	835	CLA	CMB-C2B-C3B	2.95	130.20	124.68
19	B1	830	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	BB	817	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	B	816	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
19	B	829	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	B2	851	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
19	A2	832	CLA	O2D-CGD-CBD	2.95	116.50	111.27
19	A2	807	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	A2	822	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	B	803	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
19	AA	820	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
19	B	859	CLA	CBA-CAA-C2A	2.94	122.55	113.86
23	F1	304	BCR	C2-C1-C6	2.94	115.01	110.48
19	A	842	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	B1	801	CLA	CMB-C2B-C3B	2.94	130.18	124.68
19	K2	102	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
19	B2	806	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	B1	817	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
19	A1	823	CLA	CMB-C2B-C3B	2.94	130.17	124.68
19	K1	105	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
19	AA	842	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
19	A	835	CLA	CMB-C2B-C3B	2.93	130.17	124.68
19	A2	842	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
19	BB	830	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
23	B1	838	BCR	C15-C14-C13	-2.93	123.12	127.31
19	B1	807	CLA	CHB-C4A-NA	2.93	128.57	124.51
19	A1	829	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	B1	806	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
19	A1	820	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	A1	821	CLA	CMB-C2B-C1B	-2.93	123.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	808	CLA	CMB-C2B-C3B	2.93	130.15	124.68
19	A	820	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
19	A	832	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
23	M1	101	BCR	C35-C13-C14	-2.92	118.83	122.92
19	BB	802	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
23	F1	306	BCR	C24-C23-C22	-2.92	121.82	126.23
19	A	808	CLA	C1-O2A-CGA	2.92	124.11	116.44
19	K1	103	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	BB	831	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	A2	829	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	FF	305	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	AA	806	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
19	A2	806	CLA	CHB-C4A-NA	2.92	128.55	124.51
19	B1	828	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	A2	836	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
19	BB	818	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	BB	827	CLA	CHB-C4A-NA	2.92	128.55	124.51
23	FF	306	BCR	C33-C5-C6	-2.92	121.25	124.53
19	BB	810	CLA	CMB-C2B-C3B	2.92	130.13	124.68
19	BB	856	CLA	CBA-CAA-C2A	2.91	122.47	113.86
23	J2	104	BCR	C1-C6-C5	-2.91	118.51	122.61
25	B2	847	LMG	O6-C1-O1	-2.91	103.08	109.97
19	B	810	CLA	CMB-C2B-C3B	2.91	130.13	124.68
19	A	806	CLA	CAA-C2A-C1A	-2.91	102.43	111.97
19	B2	830	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	B	831	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
23	AA	855	BCR	C24-C23-C22	-2.91	121.84	126.23
19	A	804	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	AA	819	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	BB	807	CLA	CHB-C4A-NA	2.91	128.53	124.51
19	B	806	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
19	B2	813	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	A1	850	BCR	C33-C5-C6	-2.91	121.26	124.53
19	A1	826	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
25	I1	102	LMG	O6-C5-C4	2.90	114.97	109.69
19	A2	832	CLA	CMB-C2B-C3B	2.90	130.11	124.68
19	B1	811	CLA	CMB-C2B-C3B	2.90	130.11	124.68
19	B	831	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	B	814	CLA	CHB-C4A-NA	2.90	128.52	124.51
23	F2	303	BCR	C35-C13-C14	-2.90	118.86	122.92
19	L	203	CLA	CMB-C2B-C3B	2.90	130.10	124.68
19	A2	825	CLA	CMB-C2B-C1B	-2.90	124.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	852	BCR	C28-C27-C26	-2.90	108.90	114.08
19	JJ	103	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	A	825	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	A	851	BCR	C28-C27-C26	-2.90	108.91	114.08
19	AA	816	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	B2	801	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	A	837	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	B1	806	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	AA	826	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
19	A	842	CLA	C4-C3-C5	2.89	120.14	115.27
19	A	827	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	K1	102	CLA	CMB-C2B-C3B	2.89	130.09	124.68
23	KK	103	BCR	C35-C13-C14	-2.89	118.87	122.92
19	B1	815	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	A1	810	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	A1	827	CLA	CMB-C2B-C3B	2.89	130.08	124.68
19	A1	820	CLA	CHB-C4A-NA	2.89	128.50	124.51
19	B1	834	CLA	CMB-C2B-C3B	2.89	130.08	124.68
19	A1	815	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	B1	823	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	AA	803	CL0	CHC-C1C-C2C	-2.88	118.75	126.72
19	KK	102	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	B2	833	CLA	C5-C3-C2	2.88	126.95	121.12
19	B2	802	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
23	L1	208	BCR	C24-C23-C22	-2.88	121.88	126.23
19	BB	856	CLA	CAA-CBA-CGA	2.88	121.67	113.25
19	AA	817	CLA	CHB-C4A-NA	2.88	128.49	124.51
19	B2	821	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
20	A1	802	CL0	C9-C8-C7	2.88	121.71	111.29
19	B1	802	CLA	CHB-C4A-NA	2.88	128.49	124.51
19	A1	803	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	B2	817	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
19	A1	838	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
19	BB	816	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
19	B1	827	CLA	CHB-C4A-NA	2.88	128.49	124.51
19	B2	850	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
19	B	859	CLA	CMB-C2B-C3B	2.87	130.06	124.68
19	AA	831	CLA	CMB-C2B-C3B	2.87	130.06	124.68
19	BB	832	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
19	K	102	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	B2	814	CLA	CHB-C4A-NA	2.87	128.48	124.51
19	A	817	CLA	CHB-C4A-NA	2.87	128.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	810	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	B2	816	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	AA	825	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	B1	842	BCR	C15-C16-C17	-2.87	117.60	123.47
19	B	824	CLA	CMB-C2B-C3B	2.87	130.04	124.68
19	A2	838	CLA	CMB-C2B-C3B	2.87	130.04	124.68
19	B1	821	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
19	A2	802	CLA	CMB-C2B-C3B	2.87	130.04	124.68
19	BB	832	CLA	CHB-C4A-NA	2.86	128.47	124.51
19	A2	812	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	B2	814	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
19	BB	826	CLA	CMB-C2B-C3B	2.86	130.04	124.68
26	B2	841	ECH	C37-C22-C21	2.86	126.93	122.92
19	A	810	CLA	CMB-C2B-C3B	2.86	130.03	124.68
19	BB	808	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	A	844	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
19	A2	825	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	BB	824	CLA	CMB-C2B-C3B	2.86	130.03	124.68
19	A2	828	CLA	CMB-C2B-C3B	2.86	130.03	124.68
19	A1	835	CLA	CHB-C4A-NA	2.86	128.47	124.51
19	B	807	CLA	CHB-C4A-NA	2.86	128.46	124.51
19	F2	302	CLA	O2D-CGD-CBD	2.86	116.34	111.27
19	B1	848	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	B1	829	CLA	CMB-C2B-C1B	-2.86	124.08	128.46
19	B	819	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
23	B2	839	BCR	C35-C13-C14	-2.85	118.92	122.92
23	A	851	BCR	C3-C4-C5	-2.85	108.98	114.08
19	B1	824	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
19	B	821	CLA	C5-C3-C2	2.85	126.89	121.12
19	B	820	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
19	A2	824	CLA	CMB-C2B-C3B	2.85	130.02	124.68
19	A2	842	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	AA	855	BCR	C33-C5-C6	-2.85	121.33	124.53
19	A2	828	CLA	CHB-C4A-NA	2.85	128.46	124.51
19	A1	811	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	A2	826	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
19	A2	834	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
19	AA	827	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	I2	101	BCR	C33-C5-C6	-2.85	121.33	124.53
19	B	836	CLA	CMB-C2B-C3B	2.85	130.01	124.68
19	A2	820	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
19	A2	837	CLA	CMB-C2B-C3B	2.85	130.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A1	802	CL0	CMC-C2C-C1C	2.85	129.38	125.04
19	BB	820	CLA	O2D-CGD-CBD	2.85	116.33	111.27
23	F1	306	BCR	C33-C5-C6	-2.85	121.33	124.53
19	A1	831	CLA	O2D-CGD-CBD	2.85	116.33	111.27
19	A1	827	CLA	CHB-C4A-NA	2.85	128.45	124.51
19	B2	819	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	A	803	CL0	CHD-C1D-ND	-2.85	121.84	124.45
23	AA	851	BCR	C33-C5-C6	-2.85	121.33	124.53
19	A2	809	CLA	CMB-C2B-C3B	2.85	130.00	124.68
19	B2	834	CLA	CHB-C4A-NA	2.84	128.45	124.51
23	F	304	BCR	C2-C1-C6	2.84	114.86	110.48
19	A2	820	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	B2	850	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	A2	816	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	B2	807	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
19	A	836	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	BB	820	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
19	A1	823	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	B1	813	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
19	A1	839	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	B2	823	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	A	819	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	BB	840	ECH	C8-C7-C6	-2.84	119.22	127.20
20	A1	802	CL0	C3D-C4D-ND	2.84	114.83	110.24
19	BB	802	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	BB	833	CLA	O2D-CGD-CBD	2.84	116.31	111.27
19	A2	827	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	B	802	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
19	A	842	CLA	C5-C3-C2	-2.84	115.37	121.12
23	MM	101	BCR	C33-C5-C6	-2.84	121.34	124.53
23	K2	103	BCR	C33-C5-C6	-2.84	121.34	124.53
23	F	305	BCR	C33-C5-C6	-2.84	121.34	124.53
19	B	834	CLA	O2D-CGD-CBD	2.84	116.31	111.27
26	B	841	ECH	C37-C22-C21	2.84	126.90	122.92
19	LL	203	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
23	I1	101	BCR	C33-C5-C6	-2.84	121.34	124.53
23	A	850	BCR	C33-C5-C6	-2.84	121.34	124.53
19	A1	822	CLA	CMB-C2B-C3B	2.83	129.98	124.68
19	A	815	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
23	K	103	BCR	C33-C5-C6	-2.83	121.34	124.53
23	B1	839	BCR	C1-C6-C5	-2.83	118.62	122.61
19	B	832	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	821	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
19	A	821	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
23	JJ	104	BCR	C24-C23-C22	-2.83	121.96	126.23
19	K2	104	CLA	CHB-C4A-NA	2.83	128.43	124.51
19	AA	837	CLA	CMB-C2B-C3B	2.83	129.97	124.68
19	K	102	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
19	A2	839	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	B2	840	BCR	C1-C6-C5	-2.83	118.63	122.61
23	B1	838	BCR	C33-C5-C6	-2.83	121.35	124.53
23	A2	850	BCR	C33-C5-C6	-2.83	121.35	124.53
19	A	823	CLA	O2D-CGD-CBD	2.83	116.29	111.27
19	B	813	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
19	A1	827	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	B2	851	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	BB	840	ECH	C29-C30-C25	-2.83	106.13	110.48
19	A	811	CLA	CMB-C2B-C3B	2.83	129.97	124.68
23	K1	104	BCR	C33-C5-C6	-2.83	121.35	124.53
19	A1	801	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
19	B	817	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	B	841	ECH	C8-C7-C6	-2.83	119.27	127.20
19	LL	201	CLA	C4-C3-C2	-2.83	116.43	123.68
19	B1	832	CLA	C5-C3-C2	2.83	126.83	121.12
19	B1	818	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
23	A	854	BCR	C33-C5-C6	-2.82	121.36	124.53
23	II	101	BCR	C33-C5-C6	-2.82	121.36	124.53
19	A	820	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
19	B2	834	CLA	C3A-C2A-C1A	2.82	105.56	101.34
19	A2	828	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	A1	810	CLA	CMB-C2B-C3B	2.82	129.96	124.68
19	B2	818	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	A	824	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	FF	306	BCR	C35-C13-C14	-2.82	118.97	122.92
19	AA	830	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	BB	841	BCR	C15-C16-C17	-2.82	117.70	123.47
23	I	101	BCR	C33-C5-C6	-2.82	121.36	124.53
19	A2	836	CLA	CHB-C4A-NA	2.82	128.41	124.51
19	A1	834	CLA	C1-C2-C3	-2.82	121.17	126.04
19	A2	816	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	BB	806	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	BB	804	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
19	B	806	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	BB	817	CLA	CHB-C4A-NA	2.82	128.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	824	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	L	203	CLA	O2D-CGD-CBD	2.81	116.27	111.27
23	M	101	BCR	C33-C5-C6	-2.81	121.37	124.53
19	A1	841	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	B	840	BCR	C1-C6-C5	-2.81	118.65	122.61
19	B1	822	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	F1	301	CLA	O2D-CGD-CBD	2.81	116.26	111.27
19	L1	205	CLA	C4-C3-C2	-2.81	116.47	123.68
19	AA	828	CLA	CMB-C2B-C3B	2.81	129.94	124.68
19	B1	833	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	B1	850	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
19	A	835	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	B	827	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	LL	202	CLA	CHD-C1D-ND	-2.81	121.87	124.45
23	B2	839	BCR	C33-C5-C6	-2.81	121.37	124.53
19	B1	833	CLA	C3A-C2A-C1A	2.81	105.55	101.34
19	A	806	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	A1	809	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
19	B	804	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
19	B1	850	CLA	CMB-C2B-C3B	2.81	129.93	124.68
19	BB	823	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	B2	811	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	J1	102	BCR	C15-C14-C13	-2.81	123.31	127.31
19	AA	815	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
19	B1	821	CLA	CMB-C2B-C3B	2.81	129.93	124.68
19	A	823	CLA	CHB-C4A-NA	2.81	128.39	124.51
19	A2	818	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
19	BB	855	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
19	A2	811	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	B1	814	CLA	CMB-C2B-C3B	2.80	129.92	124.68
19	A2	835	CLA	C1-C2-C3	-2.80	121.19	126.04
19	B2	803	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	B	811	CLA	CMB-C2B-C3B	2.80	129.92	124.68
19	A2	804	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	A	811	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	A2	821	CLA	CHB-C4A-NA	2.80	128.39	124.51
19	A1	842	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	AA	824	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	BB	803	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	B2	827	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	L1	210	LMG	O6-C1-O1	-2.80	103.34	109.97
19	BB	808	CLA	CMB-C2B-C3B	2.80	129.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	859	CLA	CAA-CBA-CGA	2.80	121.43	113.25
19	A1	819	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	B1	849	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	L2	205	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	AA	828	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	B	842	BCR	C28-C27-C26	-2.80	109.08	114.08
23	BB	847	BCR	C1-C6-C5	-2.80	118.67	122.61
19	B	822	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	A	830	CLA	CMB-C2B-C3B	2.80	129.91	124.68
19	B	812	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	A1	853	BCR	C27-C26-C25	2.80	126.79	122.73
19	B	829	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	AA	840	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	A2	852	CLA	C6-C5-C3	2.80	120.79	113.45
19	B1	819	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	A	812	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	A2	853	BCR	C27-C26-C25	2.80	126.79	122.73
23	M2	102	BCR	C33-C5-C6	-2.80	121.39	124.53
23	A2	851	BCR	C28-C27-C26	-2.80	109.08	114.08
19	AA	833	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	A	840	CLA	CMB-C2B-C3B	2.79	129.91	124.68
20	A1	802	CL0	CMB-C2B-C3B	2.79	129.91	124.68
19	J2	103	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	A	828	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	AA	830	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	B	851	LMG	O6-C1-O1	-2.79	103.36	109.97
19	AA	836	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	A	817	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	A	840	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	BB	802	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	B2	833	CLA	C2A-C1A-CHA	2.79	128.74	123.86
19	BB	819	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	B1	838	BCR	C35-C13-C14	-2.79	119.02	122.92
23	II	104	BCR	C24-C23-C22	-2.79	122.02	126.23
19	B2	810	CLA	CMB-C2B-C3B	2.79	129.89	124.68
19	A	834	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
23	A1	847	BCR	C23-C22-C21	-2.79	118.61	124.81
19	B2	851	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
23	A	853	BCR	C27-C26-C25	2.79	126.78	122.73
23	AA	854	BCR	C27-C26-C25	2.79	126.78	122.73
19	BB	801	CLA	C4-C3-C2	-2.79	116.53	123.68
20	A2	803	CL0	CHC-C1C-C2C	-2.79	119.02	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	MM	101	BCR	C15-C16-C17	-2.79	117.77	123.47
19	A2	819	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
19	JJ	101	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
19	XX	101	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
19	B2	829	CLA	CMB-C2B-C3B	2.78	129.88	124.68
19	B	815	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	B	860	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	A	836	CLA	CHB-C4A-NA	2.78	128.36	124.51
19	BB	821	CLA	C5-C3-C2	2.78	126.75	121.12
19	AA	806	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	A2	847	BCR	C23-C22-C21	-2.78	118.62	124.81
19	BB	816	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	A	803	CL0	CHC-C1C-C2C	-2.78	119.03	126.72
23	B	842	BCR	C15-C16-C17	-2.78	117.78	123.47
19	AA	809	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	B1	841	BCR	C30-C25-C26	-2.78	118.70	122.61
19	A2	842	CLA	C5-C3-C2	-2.78	115.50	121.12
19	AA	823	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	F2	303	BCR	C33-C5-C6	-2.78	121.41	124.53
19	F1	302	CLA	CHB-C4A-NA	2.77	128.35	124.51
19	AA	817	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	L2	204	CLA	C4-C3-C2	-2.77	116.56	123.68
19	BB	856	CLA	CMB-C2B-C3B	2.77	129.87	124.68
23	B1	841	BCR	C15-C16-C17	-2.77	117.80	123.47
19	J2	101	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	B	805	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	L	206	BCR	C33-C5-C6	-2.77	121.42	124.53
19	B1	849	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	AA	803	CL0	C3D-C4D-ND	2.77	114.72	110.24
19	AA	812	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	JJ	104	BCR	C33-C5-C6	-2.77	121.42	124.53
19	A1	817	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
23	F2	305	BCR	C33-C5-C6	-2.77	121.42	124.53
19	AA	843	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	B2	805	CLA	CHB-C4A-NA	2.77	128.34	124.51
19	A1	833	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
19	B1	827	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	A	818	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	A	848	BCR	C33-C5-C6	-2.77	121.42	124.53
23	BB	847	BCR	C33-C5-C6	-2.77	121.42	124.53
23	KK	103	BCR	C33-C5-C6	-2.77	121.42	124.53
19	A	809	CLA	CHB-C4A-NA	2.76	128.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J1	103	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
19	B2	810	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
19	BB	807	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	AA	849	BCR	C33-C5-C6	-2.76	121.42	124.53
19	KK	102	CLA	CMB-C2B-C3B	2.76	129.85	124.68
19	A	816	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	B1	814	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	J2	102	BCR	C15-C14-C13	-2.76	123.37	127.31
19	BB	856	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
19	J1	101	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	B1	840	ECH	C8-C7-C6	-2.76	119.45	127.20
19	A2	840	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	A	830	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	BB	821	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	A2	807	CLA	CHB-C4A-NA	2.76	128.33	124.51
19	A2	824	CLA	CHB-C4A-NA	2.76	128.33	124.51
19	A1	818	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	B	819	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	F1	305	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	AA	806	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	B	858	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
26	B2	841	ECH	C8-C7-C6	-2.76	119.46	127.20
19	B1	807	CLA	O2A-CGA-O1A	-2.76	116.64	123.59
19	AA	845	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
19	A1	805	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
19	F2	302	CLA	CHB-C4A-NA	2.75	128.32	124.51
19	B2	806	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	B	820	CLA	CAC-C3C-C2C	-2.75	122.82	127.53
23	AA	848	BCR	C23-C22-C21	-2.75	118.69	124.81
19	AA	818	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
19	B2	824	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	AA	829	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	FF	303	BCR	C33-C5-C6	-2.75	121.44	124.53
19	A1	807	CLA	C1-O2A-CGA	2.75	123.66	116.44
20	A1	802	CL0	CHC-C1C-C2C	-2.75	119.11	126.72
19	B	823	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
19	A	816	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A2	810	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
19	A1	841	CLA	C5-C3-C2	-2.75	115.55	121.12
19	BB	811	CLA	CMB-C2B-C3B	2.75	129.82	124.68
19	A2	820	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
19	BB	805	CLA	CMB-C2B-C3B	2.75	129.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A1	851	BCR	C28-C27-C26	-2.75	109.17	114.08
19	A	812	CLA	CMB-C2B-C3B	2.75	129.82	124.68
19	A2	842	CLA	C4-C3-C5	2.75	119.89	115.27
19	A	811	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A	828	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A1	805	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
19	A1	836	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	A1	828	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	A2	842	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A	806	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	J	101	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	AA	828	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	A2	801	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	A1	815	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
21	A	843	PQN	C15-C13-C12	-2.74	115.57	121.12
19	A	842	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	B2	816	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	AA	806	CLA	CMB-C2B-C3B	2.74	129.81	124.68
23	F	303	BCR	C33-C5-C6	-2.74	121.45	124.53
19	B	836	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	A1	822	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	A1	841	CLA	C4-C3-C5	2.74	119.88	115.27
19	A1	812	CLA	CMB-C2B-C3B	2.74	129.80	124.68
19	B	806	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	A2	835	CLA	CMB-C2B-C3B	2.74	129.80	124.68
23	F1	303	BCR	C33-C5-C6	-2.74	121.45	124.53
19	B	824	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
19	AA	836	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
19	K1	105	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
19	B	815	CLA	C5-C3-C2	2.73	126.65	121.12
20	A1	802	CL0	CHD-C4C-C3C	-2.73	120.82	124.84
19	B1	805	CLA	CHB-C4A-NA	2.73	128.29	124.51
19	A1	819	CLA	O2A-CGA-O1A	-2.73	116.69	123.59
19	B2	826	CLA	CMB-C2B-C3B	2.73	129.79	124.68
19	A2	829	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	BB	827	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	BB	835	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	A	809	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
19	A1	841	CLA	CHB-C4A-NA	2.73	128.29	124.51
19	AA	826	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	B	805	CLA	CMB-C2B-C3B	2.73	129.78	124.68
23	F1	304	BCR	C38-C26-C25	-2.73	121.47	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	833	CLA	C5-C3-C2	2.73	126.63	121.12
19	BB	836	CLA	CBC-CAC-C3C	2.73	119.94	112.43
19	A2	811	CLA	CMB-C2B-C3B	2.72	129.78	124.68
20	A2	803	CL0	C3D-C4D-ND	2.72	114.64	110.24
19	BB	812	CLA	CMB-C2B-C3B	2.72	129.77	124.68
23	BB	839	BCR	C1-C6-C5	-2.72	118.78	122.61
19	A2	818	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	BB	824	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	F1	305	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	BB	832	CLA	CED-O2D-CGD	2.72	122.09	115.94
19	L	202	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	B	854	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	B1	850	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
19	B1	808	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
19	X	101	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	X	101	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	A	847	BCR	C23-C22-C21	-2.72	118.76	124.81
19	B	834	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	A1	824	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
19	AA	822	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
19	BB	831	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	A2	817	CLA	CHB-C4A-NA	2.71	128.27	124.51
19	B2	806	CLA	CHB-C4A-NA	2.71	128.27	124.51
20	A2	803	CL0	O2A-CGA-O1A	-2.71	116.74	123.59
19	B2	830	CLA	C5-C3-C2	2.71	126.61	121.12
19	A2	816	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
23	M1	101	BCR	C33-C5-C6	-2.71	121.48	124.53
19	A2	806	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	BB	841	BCR	C28-C27-C26	-2.71	109.23	114.08
19	B2	805	CLA	CMB-C2B-C3B	2.71	129.75	124.68
23	L2	207	BCR	C15-C16-C17	-2.71	117.92	123.47
26	BB	840	ECH	C37-C22-C21	2.71	126.72	122.92
19	AA	811	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	B	859	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
19	BB	833	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	F	302	CLA	O2D-CGD-CBD	2.71	116.09	111.27
19	B	832	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	BB	805	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	B	848	BCR	C33-C5-C6	-2.71	121.49	124.53
19	B1	848	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	B2	817	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	FF	305	CLA	O2D-CGD-O1D	-2.71	118.54	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	806	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	AA	816	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
19	F	301	CLA	C2A-C1A-CHA	2.71	128.59	123.86
20	A	803	CL0	CAC-C3C-C4C	2.71	128.32	124.81
23	F	305	BCR	C24-C23-C22	-2.71	122.14	126.23
19	B1	803	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
23	A1	851	BCR	C3-C4-C5	-2.71	109.24	114.08
19	A	834	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
19	B1	817	CLA	CHB-C4A-NA	2.71	128.25	124.51
26	B1	840	ECH	C40-C30-C25	2.71	114.69	110.30
19	B1	825	CLA	O2D-CGD-CBD	2.71	116.08	111.27
19	FF	301	CLA	O2D-CGD-CBD	2.71	116.08	111.27
23	I1	101	BCR	C8-C7-C6	-2.71	119.60	127.20
19	AA	810	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
19	A2	835	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
19	B2	849	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
19	AA	816	CLA	CHB-C4A-NA	2.70	128.25	124.51
20	A	803	CL0	CAA-C2A-C1A	2.70	120.83	111.97
19	A	820	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	B1	805	CLA	CMB-C2B-C3B	2.70	129.73	124.68
19	L1	205	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	A2	837	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	B	816	CLA	CMB-C2B-C3B	2.70	129.73	124.68
19	B1	850	CLA	CAA-CBA-CGA	2.70	121.15	113.25
19	A1	815	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	K1	106	BCR	C38-C26-C25	-2.70	121.50	124.53
19	A	829	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	A	807	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	A1	817	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	A1	816	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	K1	103	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	F	305	BCR	C35-C13-C14	-2.70	119.14	122.92
19	X2	101	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	B1	822	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
19	B2	802	CLA	CHB-C4A-NA	2.70	128.24	124.51
19	LL	202	CLA	O2D-CGD-CBD	2.69	116.05	111.27
19	B1	806	CLA	CMB-C2B-C3B	2.69	129.72	124.68
19	B2	807	CLA	CMB-C2B-C3B	2.69	129.72	124.68
19	B2	819	CLA	CMB-C2B-C3B	2.69	129.72	124.68
23	F2	303	BCR	C2-C1-C6	2.69	114.63	110.48
19	K	101	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	F1	306	BCR	C35-C13-C14	-2.69	119.15	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	F2	305	BCR	C35-C13-C14	-2.69	119.15	122.92
19	BB	801	CLA	C5-C3-C2	2.69	126.56	121.12
19	A	829	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	B	823	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	F	302	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	A2	802	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	II	101	BCR	C8-C7-C6	-2.69	119.65	127.20
19	A1	836	CLA	CMB-C2B-C3B	2.69	129.71	124.68
19	A2	806	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
19	AA	812	CLA	CMB-C2B-C3B	2.69	129.71	124.68
23	I	102	BCR	C2-C1-C6	2.69	114.62	110.48
19	XX	101	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	A2	844	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
19	B2	804	CLA	C1-C2-C3	-2.69	121.40	126.04
19	B2	822	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
19	A1	833	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
23	BB	841	BCR	C30-C25-C26	-2.68	118.83	122.61
19	AA	842	CLA	C4-C3-C5	2.68	119.79	115.27
19	B	810	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	B1	808	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
19	A2	813	CLA	CMB-C2B-C3B	2.68	129.70	124.68
19	A	828	CLA	CMB-C2B-C3B	2.68	129.70	124.68
19	AA	810	CLA	CBA-CAA-C2A	2.68	121.79	113.86
19	B1	819	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	B1	843	BCR	C27-C26-C25	2.68	126.63	122.73
19	A1	830	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
20	AA	803	CL0	C9-C8-C7	2.68	121.01	111.29
19	F	301	CLA	CMB-C2B-C3B	2.68	129.70	124.68
19	LL	202	CLA	CMB-C2B-C3B	2.68	129.70	124.68
19	X1	101	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	L2	204	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	A2	841	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	B1	830	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
19	B2	821	CLA	CMB-C2B-C3B	2.68	129.69	124.68
19	B2	851	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
19	BB	821	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	A1	835	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
19	AA	804	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	AA	842	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	B1	810	CLA	CMB-C2B-C3B	2.68	129.69	124.68
19	A	810	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
19	AA	823	CLA	O2D-CGD-CBD	2.68	116.02	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	816	CLA	CHB-C4A-NA	2.68	128.21	124.51
23	L1	209	BCR	C33-C5-C6	-2.68	121.52	124.53
19	B2	804	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	B2	809	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	AA	832	CLA	CMB-C2B-C3B	2.68	129.68	124.68
19	A2	815	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	L2	207	BCR	C33-C5-C6	-2.67	121.53	124.53
19	BB	823	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	A	814	CLA	CMB-C2B-C3B	2.67	129.68	124.68
19	A	825	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
19	A1	801	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	MM	101	BCR	C27-C26-C25	2.67	126.61	122.73
23	L1	209	BCR	C15-C16-C17	-2.67	118.00	123.47
19	A2	809	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	A1	806	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	L	203	CLA	CHD-C1D-ND	-2.67	122.00	124.45
23	F1	303	BCR	C35-C13-C14	-2.67	119.18	122.92
19	AA	845	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	BB	804	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	AA	811	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
19	B2	815	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	BB	817	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
19	A	804	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
19	A2	834	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
19	BB	833	CLA	C3A-C2A-C1A	2.67	105.33	101.34
23	J	104	BCR	C1-C6-C5	-2.67	118.86	122.61
19	A	841	CLA	CMB-C2B-C3B	2.67	129.67	124.68
19	B1	813	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	B	804	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	I2	101	BCR	C8-C7-C6	-2.67	119.72	127.20
19	A	810	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
19	BB	806	CLA	CHB-C4A-NA	2.66	128.20	124.51
19	B1	820	CLA	CMB-C2B-C3B	2.66	129.66	124.68
19	B2	828	CLA	CMB-C2B-C3B	2.66	129.66	124.68
19	BB	806	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
19	AA	835	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
19	A1	840	CLA	CHB-C4A-NA	2.66	128.20	124.51
19	BB	811	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
19	KK	101	CLA	O2D-CGD-CBD	2.66	116.00	111.27
23	A2	851	BCR	C3-C4-C5	-2.66	109.33	114.08
19	A2	808	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	I1	101	BCR	C38-C26-C25	-2.66	121.54	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	FF	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
19	K1	102	CLA	O2D-CGD-CBD	2.66	115.99	111.27
23	B2	843	BCR	C15-C16-C17	-2.66	118.03	123.47
19	F1	301	CLA	C2A-C1A-CHA	2.66	128.51	123.86
19	K2	102	CLA	CMB-C2B-C3B	2.66	129.65	124.68
19	B2	808	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
19	BB	815	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
19	B	858	CLA	CMB-C2B-C3B	2.66	129.65	124.68
19	A	816	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
23	BB	841	BCR	C35-C13-C14	-2.66	119.20	122.92
19	BB	833	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
19	L1	206	CLA	CMB-C2B-C3B	2.66	129.65	124.68
23	A2	848	BCR	C15-C16-C17	-2.66	118.03	123.47
23	II	104	BCR	C33-C5-C6	-2.65	121.55	124.53
19	A1	838	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	B1	828	CLA	CHD-C1D-ND	-2.65	122.02	124.45
19	X1	101	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
19	AA	841	CLA	CMB-C2B-C3B	2.65	129.64	124.68
19	A2	808	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	B1	812	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	B1	826	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	B1	836	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
19	A	813	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
19	B2	820	CLA	CMB-C2B-C3B	2.65	129.63	124.68
23	K1	106	BCR	C33-C5-C6	-2.65	121.56	124.53
19	B1	809	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	B1	802	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
19	B2	851	CLA	CAA-CBA-CGA	2.65	120.99	113.25
19	A1	808	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	B2	812	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	A1	823	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
19	BB	815	CLA	C5-C3-C2	2.64	126.47	121.12
26	B	841	ECH	C40-C30-C25	2.64	114.59	110.30
19	A2	807	CLA	CHD-C1D-ND	-2.64	122.02	124.45
19	K1	102	CLA	CHB-C4A-NA	2.64	128.17	124.51
19	A2	806	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
19	B	818	CLA	CHD-C1D-ND	-2.64	122.03	124.45
19	A	822	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	L	202	CLA	CMB-C2B-C3B	2.64	129.62	124.68
26	BB	840	ECH	C40-C30-C25	2.64	114.58	110.30
19	B2	820	CLA	CBC-CAC-C3C	2.64	119.71	112.43
19	AA	843	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	825	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
19	A	811	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
19	B	807	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	AA	826	CLA	CHD-C1D-ND	-2.64	122.03	124.45
19	A1	844	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
23	A1	848	BCR	C33-C5-C6	-2.64	121.57	124.53
19	A2	811	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A2	825	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	BB	836	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
19	AA	806	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
19	AA	808	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	B	810	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
19	AA	843	CLA	CHD-C4C-C3C	2.64	128.71	124.84
19	A2	839	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	LL	203	CLA	CAC-C3C-C4C	2.64	128.23	124.81
19	BB	825	CLA	O2D-CGD-CBD	2.63	115.95	111.27
22	A2	846	LHG	O4-P-O5	2.63	125.26	112.24
19	B1	807	CLA	CMB-C2B-C3B	2.63	129.61	124.68
19	BB	829	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
19	A1	809	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
22	A1	846	LHG	O4-P-O5	2.63	125.26	112.24
19	A2	841	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	A2	848	BCR	C33-C5-C6	-2.63	121.57	124.53
20	A1	802	CL0	CHD-C1D-ND	-2.63	122.03	124.45
23	B1	841	BCR	C28-C27-C26	-2.63	109.38	114.08
19	B	803	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	II	105	LMG	O6-C1-O1	-2.63	103.74	109.97
19	AA	813	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	A1	853	BCR	C15-C14-C13	-2.63	123.56	127.31
20	A1	802	CL0	O2A-C1-C2	2.63	115.55	108.64
19	AA	809	CLA	CMB-C2B-C3B	2.63	129.60	124.68
19	B1	835	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	A	846	LHG	O4-P-O5	2.63	125.24	112.24
19	L1	205	CLA	CMB-C2B-C3B	2.63	129.60	124.68
19	X2	101	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	K2	105	BCR	C33-C5-C6	-2.63	121.58	124.53
19	A2	807	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	B	854	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	B1	835	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	BB	832	CLA	C5-C3-C2	2.63	126.43	121.12
19	B	820	CLA	CBC-CAC-C3C	2.63	119.67	112.43
19	BB	852	CLA	CHB-C4A-NA	2.63	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	838	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
19	B	830	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
19	B	807	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
19	B	808	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
19	B	806	CLA	CMB-C2B-C3B	2.62	129.59	124.68
23	A2	853	BCR	C33-C5-C6	-2.62	121.58	124.53
19	B2	832	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	J	103	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
19	KK	101	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	A1	803	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
19	AA	807	CLA	CHD-C1D-ND	-2.62	122.05	124.45
19	A1	825	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	LL	201	CLA	CHB-C4A-NA	2.62	128.13	124.51
19	A2	813	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	A2	817	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	A2	832	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	X1	103	LHG	O4-P-O5	2.62	125.19	112.24
19	A	822	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	B1	833	CLA	C2A-C1A-CHA	2.62	128.44	123.86
19	F1	302	CLA	O2D-CGD-CBD	2.62	115.92	111.27
19	L1	206	CLA	O2D-CGD-CBD	2.62	115.92	111.27
19	AA	820	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	AA	853	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
19	B	823	CLA	CMB-C2B-C3B	2.62	129.57	124.68
19	A	801	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	BB	810	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	B1	824	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
19	A	806	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
19	A1	811	CLA	CMB-C2B-C3B	2.62	129.57	124.68
19	FF	301	CLA	CMB-C2B-C3B	2.62	129.57	124.68
19	K2	104	CLA	CMB-C2B-C3B	2.61	129.57	124.68
19	B	821	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	AA	854	BCR	C33-C5-C6	-2.61	121.59	124.53
23	F	303	BCR	C2-C1-C6	2.61	114.50	110.48
19	A1	825	CLA	CMB-C2B-C3B	2.61	129.57	124.68
19	A1	812	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	LL	203	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	A2	827	CLA	CMB-C2B-C3B	2.61	129.57	124.68
19	BB	809	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	A1	842	CLA	CHD-C4C-C3C	2.61	128.68	124.84
19	A2	825	CLA	CHD-C1D-ND	-2.61	122.05	124.45
19	AA	810	CLA	CHB-C4A-NA	2.61	128.12	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	803	CL0	CHD-C4C-C3C	-2.61	121.00	124.84
19	BB	845	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	M	101	BCR	C27-C26-C25	2.61	126.52	122.73
19	A	807	CLA	CHD-C1D-ND	-2.61	122.06	124.45
19	BB	819	CLA	CMB-C2B-C3B	2.61	129.56	124.68
19	B1	845	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	B	831	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	BB	810	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	BB	823	CLA	CMB-C2B-C3B	2.61	129.56	124.68
23	FF	306	BCR	C24-C23-C22	-2.61	122.29	126.23
19	B1	829	CLA	CMB-C2B-C3B	2.61	129.56	124.68
19	B	859	CLA	CHD-C1D-ND	-2.61	122.06	124.45
28	B	856	DGD	O5D-C6D-C5D	-2.61	104.22	109.05
19	B2	830	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
19	A	806	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
19	A1	806	CLA	CMB-C2B-C3B	2.61	129.55	124.68
19	B	834	CLA	C3A-C2A-C1A	2.61	105.24	101.34
19	B2	837	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
23	A	853	BCR	C33-C5-C6	-2.60	121.60	124.53
19	B2	811	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	LL	202	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	A	820	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	B	811	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	AA	814	CLA	CMB-C2B-C3B	2.60	129.55	124.68
19	A2	835	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
19	A	810	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	I	101	BCR	C8-C7-C6	-2.60	119.89	127.20
23	L1	209	BCR	C11-C10-C9	-2.60	123.60	127.31
19	A1	834	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	B1	811	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	B2	846	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	B2	834	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
19	A1	840	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	L2	208	LHG	O4-P-O5	2.60	125.09	112.24
22	B	853	LHG	O4-P-O5	2.60	125.09	112.24
19	AA	804	CLA	C1-C2-C3	-2.60	121.55	126.04
23	K	103	BCR	C24-C23-C22	-2.60	122.31	126.23
19	BB	832	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
19	A	826	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	B1	846	LMG	O6-C1-O1	-2.60	103.82	109.97
19	A	844	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	A2	807	CLA	CMB-C2B-C3B	2.60	129.54	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	828	CLA	CMB-C2B-C3B	2.60	129.54	124.68
19	AA	829	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	AA	835	CLA	C1-C2-C3	-2.60	121.55	126.04
19	A1	810	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	B	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	FF	304	BCR	C15-C16-C17	-2.60	118.16	123.47
23	J2	102	BCR	C1-C6-C5	-2.60	118.96	122.61
19	B2	810	CLA	C4-C3-C5	2.60	119.64	115.27
19	A1	813	CLA	CMB-C2B-C3B	2.60	129.53	124.68
19	BB	801	CLA	CMB-C2B-C3B	2.60	129.53	124.68
22	X2	103	LHG	O4-P-O5	2.60	125.07	112.24
19	BB	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	B1	823	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	AA	847	LHG	O4-P-O5	2.59	125.07	112.24
23	LL	204	BCR	C33-C5-C6	-2.59	121.61	124.53
19	F	301	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
20	AA	803	CL0	CMA-C3A-C4A	-2.59	104.81	111.77
19	BB	826	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
19	AA	834	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	A1	829	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	A	817	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	K1	105	CLA	CMB-C2B-C3B	2.59	129.52	124.68
19	B1	850	CLA	C6-C5-C3	2.59	120.25	113.45
19	AA	807	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	AA	834	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	AA	822	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	B	822	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
19	B1	815	CLA	C5-C3-C2	2.59	126.35	121.12
19	A2	822	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	B	844	BCR	C27-C26-C25	2.59	126.49	122.73
19	BB	830	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	A1	820	CLA	CMB-C2B-C1B	-2.58	124.49	128.46
19	A2	810	CLA	CBA-CAA-C2A	2.58	121.49	113.86
19	AA	842	CLA	C6-C5-C3	2.58	120.23	113.45
19	A1	805	CLA	O2D-CGD-CBD	2.58	115.86	111.27
19	AA	842	CLA	C5-C3-C2	-2.58	115.89	121.12
19	A1	842	CLA	CMB-C2B-C3B	2.58	129.51	124.68
19	F1	301	CLA	CMB-C2B-C3B	2.58	129.51	124.68
19	A	815	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	AA	846	LHG	O4-P-O5	2.58	125.02	112.24
19	BB	828	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	B	843	BCR	C15-C16-C17	-2.58	118.18	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J1	102	BCR	C1-C6-C5	-2.58	118.97	122.61
23	FF	303	BCR	C2-C1-C6	2.58	114.46	110.48
23	I	102	BCR	C33-C5-C6	-2.58	121.63	124.53
19	F2	301	CLA	C2A-C1A-CHA	2.58	128.37	123.86
23	L	205	BCR	C33-C5-C6	-2.58	121.63	124.53
22	B1	847	LHG	O4-P-O5	2.58	125.00	112.24
19	B2	851	CLA	C6-C5-C3	2.58	120.22	113.45
19	B2	829	CLA	CHD-C1D-ND	-2.58	122.08	124.45
19	A1	828	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	A	845	LHG	O4-P-O5	2.58	124.98	112.24
23	II	102	BCR	C2-C1-C6	2.58	114.45	110.48
19	AA	819	CLA	CMB-C2B-C3B	2.58	129.50	124.68
19	B	809	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	A1	845	LHG	O4-P-O5	2.58	124.98	112.24
19	BB	807	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
19	L	202	CLA	C4-C3-C2	-2.58	117.07	123.68
19	B1	816	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	LL	205	LHG	O4-P-O5	2.58	124.98	112.24
22	L	207	LHG	O4-P-O5	2.58	124.97	112.24
19	AA	807	CLA	CHB-C4A-NA	2.58	128.07	124.51
20	AA	803	CL0	C9-C8-C10	2.58	120.62	111.29
19	AA	831	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
19	A1	803	CLA	CHB-C4A-NA	2.58	128.07	124.51
19	A	826	CLA	CMB-C2B-C3B	2.57	129.49	124.68
23	I1	101	BCR	C24-C23-C22	-2.57	122.35	126.23
19	B2	852	CLA	CHD-C4C-C3C	2.57	128.62	124.84
19	A	835	CLA	C1-C2-C3	-2.57	121.59	126.04
23	K	103	BCR	C38-C26-C25	-2.57	121.64	124.53
19	B1	804	CLA	CMB-C2B-C3B	2.57	129.49	124.68
19	BB	835	CLA	CMB-C2B-C3B	2.57	129.49	124.68
23	KK	103	BCR	C24-C23-C22	-2.57	122.35	126.23
19	BB	830	CLA	CMB-C2B-C3B	2.57	129.49	124.68
19	B2	803	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	A	838	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
19	A1	807	CLA	CMB-C2B-C3B	2.57	129.49	124.68
22	XX	102	LHG	O4-P-O5	2.57	124.95	112.24
19	B	833	CLA	CED-O2D-CGD	2.57	121.75	115.94
19	B	802	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	AA	817	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
19	BB	822	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
19	B	846	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	B2	828	CLA	O2D-CGD-O1D	-2.57	118.82	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	I2	103	BCR	C33-C5-C6	-2.57	121.64	124.53
23	B	842	BCR	C30-C25-C26	-2.57	119.00	122.61
23	L1	208	BCR	C2-C1-C6	2.57	114.43	110.48
19	B1	804	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	B1	820	CLA	O2D-CGD-CBD	2.57	115.83	111.27
23	AA	854	BCR	C15-C14-C13	-2.57	123.65	127.31
23	KK	103	BCR	C38-C26-C25	-2.57	121.65	124.53
23	B2	842	BCR	C28-C27-C26	-2.57	109.50	114.08
19	B2	815	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
19	A1	839	CLA	CMB-C2B-C3B	2.56	129.48	124.68
23	I2	103	BCR	C7-C8-C9	-2.56	122.36	126.23
22	A2	845	LHG	O4-P-O5	2.56	124.92	112.24
22	X	102	LHG	O4-P-O5	2.56	124.92	112.24
19	B	820	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	B	841	ECH	C21-C20-C19	-2.56	115.22	123.22
19	B	833	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
19	B	831	CLA	CMB-C2B-C3B	2.56	129.47	124.68
23	A	853	BCR	C15-C14-C13	-2.56	123.65	127.31
19	A1	810	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
19	AA	815	CLA	CMB-C2B-C3B	2.56	129.47	124.68
19	B2	834	CLA	C2A-C1A-CHA	2.56	128.34	123.86
19	A1	818	CLA	CMB-C2B-C3B	2.56	129.47	124.68
19	A1	812	CLA	CHD-C1D-ND	-2.56	122.10	124.45
23	A2	851	BCR	C24-C23-C22	-2.56	122.36	126.23
23	II	102	BCR	C7-C8-C9	-2.56	122.37	126.23
19	A1	806	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
19	AA	835	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
23	A2	853	BCR	C15-C14-C13	-2.56	123.66	127.31
19	A2	814	CLA	CMB-C2B-C3B	2.56	129.46	124.68
19	B	830	CLA	CHD-C1D-ND	-2.56	122.10	124.45
19	AA	826	CLA	CMB-C2B-C3B	2.56	129.46	124.68
23	FF	303	BCR	C8-C7-C6	-2.56	120.02	127.20
19	A1	834	CLA	CMB-C2B-C3B	2.56	129.46	124.68
23	BB	838	BCR	C33-C5-C6	-2.56	121.66	124.53
23	B	848	BCR	C27-C26-C25	2.56	126.44	122.73
19	B2	835	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
19	B1	849	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
22	BB	851	LHG	O4-P-O5	2.55	124.86	112.24
26	BB	840	ECH	C21-C20-C19	-2.55	115.25	123.22
23	B2	844	BCR	C27-C26-C25	2.55	126.44	122.73
19	AA	801	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
23	L1	208	BCR	C33-C5-C6	-2.55	121.66	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	FF	302	CLA	O2D-CGD-CBD	2.55	115.80	111.27
23	F	305	BCR	C7-C8-C9	-2.55	122.38	126.23
19	A1	814	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
19	BB	813	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	K1	106	BCR	C28-C27-C26	-2.55	109.53	114.08
19	A2	831	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
19	A1	821	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	B2	804	CLA	CMB-C2B-C3B	2.55	129.45	124.68
19	B2	815	CLA	C5-C3-C2	2.55	126.28	121.12
23	B	840	BCR	C28-C27-C26	-2.55	109.53	114.08
19	L1	206	CLA	C1-O2A-CGA	2.55	123.13	116.44
19	BB	836	CLA	O2D-CGD-CBD	2.55	115.80	111.27
19	A	832	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	M	101	BCR	C15-C14-C13	-2.55	123.67	127.31
22	X1	102	LHG	O4-P-O5	2.55	124.83	112.24
19	F2	301	CLA	CMB-C2B-C3B	2.55	129.44	124.68
23	B	842	BCR	C35-C13-C14	-2.55	119.36	122.92
19	A2	826	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	K2	102	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	BB	809	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	A2	830	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	X2	102	LHG	O4-P-O5	2.54	124.82	112.24
23	I2	102	BCR	C2-C1-C6	2.54	114.40	110.48
23	J	104	BCR	C15-C16-C17	-2.54	118.26	123.47
19	B1	833	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
23	L	205	BCR	C24-C23-C22	-2.54	122.39	126.23
19	A1	809	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	BB	840	ECH	C35-C13-C14	2.54	126.48	122.92
19	A2	814	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
19	A2	844	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	B2	836	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	II	102	BCR	C33-C5-C6	-2.54	121.67	124.53
19	AA	804	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
23	I2	101	BCR	C38-C26-C25	-2.54	121.67	124.53
19	A	831	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	L	206	BCR	C27-C26-C25	2.54	126.42	122.73
23	B	839	BCR	C33-C5-C6	-2.54	121.68	124.53
19	B1	836	CLA	O2D-CGD-CBD	2.54	115.78	111.27
19	BB	835	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	B2	836	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	BB	847	BCR	C27-C26-C25	2.54	126.42	122.73
19	A	819	CLA	CMB-C2B-C3B	2.54	129.43	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	844	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	B1	831	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	B2	833	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
19	J1	101	CLA	CMB-C2B-C3B	2.54	129.43	124.68
19	A1	852	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	BB	804	CLA	C1-C2-C3	-2.54	121.66	126.04
19	B	836	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	A	852	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	B1	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	B1	815	CLA	O2D-CGD-CBD	2.54	115.77	111.27
23	J1	104	BCR	C15-C16-C17	-2.53	118.28	123.47
19	A2	811	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
19	A	824	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B1	804	CLA	C1-C2-C3	-2.53	121.66	126.04
19	B2	837	CLA	O2D-CGD-CBD	2.53	115.77	111.27
19	B2	809	CLA	CMB-C2B-C3B	2.53	129.42	124.68
19	B2	802	CLA	CHD-C1D-ND	-2.53	122.13	124.45
19	B2	820	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
23	I	102	BCR	C7-C8-C9	-2.53	122.41	126.23
19	XX	101	CLA	CMB-C2B-C3B	2.53	129.41	124.68
23	L1	201	BCR	C33-C5-C6	-2.53	121.69	124.53
19	K2	102	CLA	O2D-CGD-CBD	2.53	115.76	111.27
20	A2	803	CL0	CHD-C1D-ND	-2.53	122.13	124.45
19	B	825	CLA	O2D-CGD-CBD	2.53	115.76	111.27
19	B1	809	CLA	CMB-C2B-C3B	2.53	129.41	124.68
19	AA	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B2	822	CLA	CMB-C2B-C3B	2.53	129.41	124.68
23	F1	303	BCR	C2-C1-C6	2.53	114.37	110.48
19	BB	828	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B1	847	LHG	P-O3-C3	-2.53	106.86	121.68
21	A2	843	PQN	C15-C13-C12	-2.53	116.00	121.12
22	BB	850	LHG	O4-P-O5	2.53	124.73	112.24
26	B2	841	ECH	C40-C30-C25	2.52	114.39	110.30
19	B2	823	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	A2	804	CLA	CMB-C2B-C1B	-2.52	124.58	128.46
19	B1	832	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
26	B2	841	ECH	C29-C30-C25	-2.52	106.59	110.48
21	A1	843	PQN	C15-C13-C12	-2.52	116.01	121.12
19	A	821	CLA	CMB-C2B-C3B	2.52	129.40	124.68
19	BB	820	CLA	CMB-C2B-C3B	2.52	129.40	124.68
19	AA	810	CLA	O2D-CGD-CBD	2.52	115.75	111.27
23	LL	204	BCR	C27-C26-C25	2.52	126.39	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	859	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
19	A2	813	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	L1	201	BCR	C2-C1-C6	2.52	114.36	110.48
19	A1	829	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	B	860	CLA	CHD-C4C-C3C	2.52	128.54	124.84
19	A	801	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
22	B	852	LHG	O4-P-O5	2.52	124.69	112.24
19	LL	201	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	FF	304	BCR	C38-C26-C25	-2.52	121.70	124.53
26	B1	840	ECH	C29-C30-C25	-2.52	106.61	110.48
19	A2	823	CLA	C5-C3-C2	2.52	126.21	121.12
19	BB	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	BB	822	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
19	B2	812	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	B1	802	CLA	CHD-C1D-ND	-2.52	122.14	124.45
23	A	847	BCR	C33-C5-C6	-2.52	121.70	124.53
23	BB	839	BCR	C28-C27-C26	-2.52	109.58	114.08
23	L	206	BCR	C11-C10-C9	-2.52	123.72	127.31
19	X	101	CLA	CMB-C2B-C3B	2.52	129.38	124.68
19	B	835	CLA	CED-O2D-CGD	2.52	121.63	115.94
19	A	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	AA	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	BB	832	CLA	C2A-C1A-CHA	2.51	128.26	123.86
19	BB	809	CLA	O2D-CGD-CBD	2.51	115.74	111.27
26	B1	840	ECH	C37-C22-C21	2.51	126.44	122.92
19	B1	850	CLA	C4-C3-C5	2.51	119.50	115.27
19	B2	831	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	AA	838	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	B	833	CLA	C2A-C1A-CHA	2.51	128.25	123.86
23	A1	848	BCR	C15-C16-C17	-2.51	118.33	123.47
19	AA	815	CLA	CHD-C1D-ND	-2.51	122.14	124.45
23	A2	847	BCR	C33-C5-C6	-2.51	121.71	124.53
23	BB	839	BCR	C8-C7-C6	-2.51	120.15	127.20
19	K	102	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	AA	808	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	AA	852	BCR	C1-C6-C5	-2.51	119.08	122.61
19	A1	834	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
19	B	820	CLA	O2D-CGD-CBD	2.51	115.73	111.27
19	AA	832	CLA	O2D-CGD-CBD	2.51	115.72	111.27
19	AA	815	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
19	A1	809	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
19	A	807	CLA	CHB-C4A-NA	2.51	127.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B2	840	BCR	C28-C27-C26	-2.51	109.60	114.08
19	AA	810	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
23	JJ	104	BCR	C15-C16-C17	-2.51	118.34	123.47
19	AA	824	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	I2	105	LMG	O6-C1-O1	-2.51	104.04	109.97
25	M	102	LMG	C7-O1-C1	2.51	118.63	113.74
23	AA	855	BCR	C28-C27-C26	-2.51	109.60	114.08
19	B	809	CLA	O2D-CGD-CBD	2.50	115.72	111.27
23	F1	304	BCR	C15-C16-C17	-2.50	118.34	123.47
19	A1	837	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A1	801	CLA	CMB-C2B-C3B	2.50	129.36	124.68
19	A	824	CLA	CHD-C1D-ND	-2.50	122.15	124.45
23	A	850	BCR	C8-C7-C6	-2.50	120.17	127.20
19	A1	831	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A	825	CLA	CHD-C1D-ND	-2.50	122.15	124.45
23	F2	304	BCR	C33-C5-C6	-2.50	121.72	124.53
19	A2	836	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	BB	838	BCR	C15-C16-C17	-2.50	118.35	123.47
19	L2	206	CLA	C2D-C1D-ND	-2.50	108.26	110.10
19	A2	804	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	B2	808	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
19	B	801	CLA	CMB-C2B-C3B	2.50	129.35	124.68
19	A	838	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	BB	840	ECH	C8-C9-C10	2.50	122.78	118.94
19	B1	830	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	F	303	BCR	C8-C7-C6	-2.50	120.19	127.20
19	J2	101	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	B1	839	BCR	C33-C5-C6	-2.50	121.72	124.53
23	MM	101	BCR	C35-C13-C14	-2.50	119.42	122.92
19	AA	820	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	FF	304	BCR	C27-C26-C25	2.50	126.36	122.73
19	B	825	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	L1	211	LHG	O4-P-O5	2.50	124.58	112.24
19	B2	849	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	AA	813	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	F2	304	BCR	C27-C26-C25	2.50	126.36	122.73
23	AA	854	BCR	C2-C1-C6	2.50	114.32	110.48
23	J	104	BCR	C27-C26-C25	2.50	126.35	122.73
19	B1	832	CLA	CED-O2D-CGD	2.50	121.58	115.94
19	A	822	CLA	CHD-C1D-ND	-2.50	122.16	124.45
19	A	829	CLA	C5-C3-C2	2.50	126.17	121.12
19	B2	818	CLA	CMB-C2B-C3B	2.49	129.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	821	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	BB	856	CLA	CHD-C1D-ND	-2.49	122.16	124.45
23	F1	304	BCR	C27-C26-C25	2.49	126.35	122.73
19	B1	820	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	AA	838	CLA	O2D-CGD-CBD	2.49	115.70	111.27
19	B1	826	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B2	822	CLA	C5-C3-C2	2.49	126.16	121.12
19	BB	829	CLA	CMB-C2B-C3B	2.49	129.34	124.68
19	B1	812	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	K2	103	BCR	C27-C26-C25	2.49	126.35	122.73
19	AA	825	CLA	CHD-C1D-ND	-2.49	122.16	124.45
23	L	205	BCR	C2-C1-C6	2.49	114.32	110.48
23	A	853	BCR	C2-C1-C6	2.49	114.32	110.48
19	B1	826	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	AA	821	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	J	102	BCR	C1-C6-C5	-2.49	119.11	122.61
19	BB	802	CLA	CHD-C1D-ND	-2.49	122.17	124.45
23	F	303	BCR	C27-C26-C25	2.49	126.35	122.73
19	B1	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B2	852	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	A	835	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
19	K	101	CLA	O2D-CGD-CBD	2.49	115.69	111.27
23	I2	103	BCR	C2-C1-C6	2.49	114.31	110.48
26	B2	841	ECH	C21-C20-C19	-2.49	115.45	123.22
23	AA	851	BCR	C8-C7-C6	-2.49	120.21	127.20
19	A1	831	CLA	CMB-C2B-C3B	2.49	129.33	124.68
19	BB	834	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	A2	826	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
19	BB	856	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
19	B	816	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
19	A2	819	CLA	CMB-C2B-C3B	2.49	129.33	124.68
23	K1	104	BCR	C27-C26-C25	2.49	126.34	122.73
23	J2	104	BCR	C27-C26-C25	2.49	126.34	122.73
19	AA	840	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	B	822	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	BB	829	CLA	CHD-C1D-ND	-2.49	122.17	124.45
19	X1	101	CLA	CMB-C2B-C3B	2.48	129.33	124.68
19	A	804	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	L2	204	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	X2	101	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	A1	811	CLA	CBA-CAA-C2A	2.48	121.19	113.86
19	B2	822	CLA	C1B-CHB-C4A	-2.48	125.20	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	828	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
19	AA	810	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	A2	813	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
19	A	807	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
19	B	834	CLA	C2A-C1A-CHA	2.48	128.20	123.86
19	BB	802	CLA	CMB-C2B-C3B	2.48	129.32	124.68
23	I2	102	BCR	C15-C16-C17	-2.48	118.39	123.47
19	A	836	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
19	A2	802	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	B1	834	CLA	CHD-C1D-ND	-2.48	122.17	124.45
19	A2	826	CLA	CHD-C1D-ND	-2.48	122.17	124.45
19	A	842	CLA	CMB-C2B-C3B	2.48	129.32	124.68
23	K2	105	BCR	C28-C27-C26	-2.48	109.65	114.08
23	I	101	BCR	C15-C16-C17	-2.48	118.40	123.47
19	B	819	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	B2	851	CLA	CHD-C1D-ND	-2.48	122.18	124.45
19	A1	841	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
19	B1	803	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	A1	822	CLA	C5-C3-C2	2.48	126.13	121.12
26	B1	840	ECH	C21-C20-C19	-2.48	115.49	123.22
19	A	808	CLA	CMB-C2B-C3B	2.48	129.31	124.68
19	A2	826	CLA	CMB-C2B-C3B	2.48	129.31	124.68
23	I	101	BCR	C24-C23-C22	-2.48	122.50	126.23
19	A2	821	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
19	A1	805	CLA	CHD-C1D-ND	-2.47	122.18	124.45
23	A2	853	BCR	C2-C1-C6	2.47	114.29	110.48
19	L	204	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
19	B1	829	CLA	C5-C3-C2	2.47	126.12	121.12
19	B	833	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
19	B	809	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	812	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	FF	301	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
23	MM	101	BCR	C15-C14-C13	-2.47	123.78	127.31
23	F1	303	BCR	C11-C10-C9	-2.47	123.78	127.31
23	BB	843	BCR	C27-C26-C25	2.47	126.32	122.73
23	F	304	BCR	C38-C26-C25	-2.47	121.75	124.53
19	B2	811	CLA	CHD-C1D-ND	-2.47	122.19	124.45
23	L1	201	BCR	C15-C16-C17	-2.47	118.42	123.47
19	A2	852	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
19	A1	816	CLA	CMB-C2B-C3B	2.47	129.29	124.68
23	A2	847	BCR	C2-C1-C6	2.47	114.28	110.48
19	A2	820	CLA	CBA-CAA-C2A	2.47	121.14	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	II	104	BCR	C2-C1-C6	2.47	114.28	110.48
19	B	813	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	B	817	CLA	CMB-C2B-C3B	2.47	129.29	124.68
19	K1	105	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
19	AA	820	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	A	842	CLA	C6-C5-C3	2.46	119.92	113.45
22	A	846	LHG	P-O3-C3	-2.46	107.23	121.68
23	AA	848	BCR	C15-C16-C17	-2.46	118.43	123.47
23	A1	847	BCR	C2-C1-C6	2.46	114.27	110.48
19	A	813	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	A	844	CLA	CMB-C2B-C3B	2.46	129.29	124.68
19	A2	810	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	BB	856	CLA	C6-C5-C3	2.46	119.91	113.45
19	B2	820	CLA	O2D-CGD-CBD	2.46	115.64	111.27
19	B1	805	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
19	B2	819	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	BB	814	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
19	FF	301	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	F	303	BCR	C11-C10-C9	-2.46	123.80	127.31
19	BB	820	CLA	CBC-CAC-C3C	2.46	119.21	112.43
19	L	204	CLA	CAC-C3C-C4C	2.46	128.00	124.81
25	M	102	LMG	O1-C7-C8	-2.46	104.97	110.90
23	B	843	BCR	C33-C5-C6	-2.46	121.77	124.53
23	I2	101	BCR	C24-C23-C22	-2.46	122.52	126.23
22	AA	847	LHG	P-O3-C3	-2.46	107.27	121.68
19	A2	830	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	A1	812	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	FF	303	BCR	C27-C26-C25	2.46	126.30	122.73
19	JJ	101	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	B1	823	CLA	CMB-C2B-C3B	2.46	129.28	124.68
19	AA	813	CLA	CMB-C2B-C3B	2.46	129.28	124.68
23	F	304	BCR	C15-C16-C17	-2.46	118.44	123.47
23	M	101	BCR	C24-C23-C22	-2.46	122.52	126.23
19	B2	813	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	J	101	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	KK	101	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	I2	101	BCR	C15-C16-C17	-2.46	118.44	123.47
23	II	104	BCR	C27-C26-C25	2.46	126.30	122.73
22	A1	845	LHG	P-O6-C4	-2.45	107.29	121.68
19	B	819	CLA	CMB-C2B-C3B	2.45	129.27	124.68
23	F1	304	BCR	C33-C5-C6	-2.45	121.77	124.53
19	B2	829	CLA	O2D-CGD-O1D	-2.45	119.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	820	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	B	836	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	B	835	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	B1	807	CLA	C11-C12-C13	-2.45	107.99	115.92
19	BB	816	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	BB	852	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	A1	819	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	F1	303	BCR	C27-C26-C25	2.45	126.29	122.73
23	A1	847	BCR	C33-C5-C6	-2.45	121.78	124.53
19	B2	802	CLA	CMB-C2B-C3B	2.45	129.26	124.68
19	A1	829	CLA	CAC-C3C-C4C	2.45	127.99	124.81
19	B2	826	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A1	853	BCR	C33-C5-C6	-2.45	121.78	124.53
23	A1	847	BCR	C15-C16-C17	-2.45	118.46	123.47
23	A	847	BCR	C15-C16-C17	-2.45	118.46	123.47
19	A2	810	CLA	CMB-C2B-C3B	2.45	129.26	124.68
23	LL	204	BCR	C38-C26-C25	-2.45	121.78	124.53
19	BB	824	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	L1	201	BCR	C7-C8-C9	-2.45	122.53	126.23
25	B	851	LMG	O1-C7-C8	-2.45	104.99	110.90
19	A1	805	CLA	CMB-C2B-C3B	2.45	129.26	124.68
19	B1	818	CLA	CMB-C2B-C3B	2.45	129.26	124.68
23	I1	101	BCR	C15-C16-C17	-2.45	118.46	123.47
19	B	834	CLA	C4-C3-C5	2.45	119.39	115.27
19	B2	821	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A1	849	BCR	C33-C5-C6	-2.45	121.78	124.53
23	BB	839	BCR	C33-C5-C6	-2.45	121.78	124.53
19	A2	838	CLA	CHB-C4A-NA	2.45	127.89	124.51
19	A2	817	CLA	CMB-C2B-C3B	2.45	129.25	124.68
19	FF	305	CLA	CHD-C1D-ND	-2.45	122.21	124.45
19	A1	820	CLA	CMB-C2B-C3B	2.45	129.25	124.68
19	AA	830	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	J1	104	BCR	C38-C26-C25	-2.44	121.78	124.53
23	J2	102	BCR	C38-C26-C25	-2.44	121.78	124.53
23	F2	303	BCR	C27-C26-C25	2.44	126.28	122.73
19	B1	850	CLA	CHD-C1D-ND	-2.44	122.21	124.45
23	J1	104	BCR	C27-C26-C25	2.44	126.28	122.73
22	B2	848	LHG	O4-P-O5	2.44	124.32	112.24
19	B	820	CLA	CMB-C2B-C3B	2.44	129.25	124.68
19	A	815	CLA	CHD-C1D-ND	-2.44	122.21	124.45
19	B	829	CLA	CHD-C1D-ND	-2.44	122.21	124.45
19	JJ	101	CLA	CMB-C2B-C3B	2.44	129.25	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	839	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	M	102	LMG	C38-C37-C36	-2.44	102.04	114.42
23	F1	306	BCR	C7-C8-C9	-2.44	122.55	126.23
23	J2	104	BCR	C33-C5-C6	-2.44	121.79	124.53
23	L	205	BCR	C27-C26-C25	2.44	126.27	122.73
19	L2	205	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	B	814	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	J2	104	BCR	C38-C26-C25	-2.44	121.79	124.53
23	K2	105	BCR	C20-C21-C22	-2.44	123.83	127.31
23	JJ	102	BCR	C15-C14-C13	-2.44	123.83	127.31
23	M2	102	BCR	C24-C23-C22	-2.44	122.55	126.23
22	L	207	LHG	P-O3-C3	-2.44	107.40	121.68
23	B1	841	BCR	C35-C13-C14	-2.44	119.51	122.92
19	A1	841	CLA	C6-C5-C3	2.43	119.84	113.45
19	A	823	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	B	859	CLA	C6-C5-C3	2.43	119.84	113.45
23	F	304	BCR	C33-C5-C6	-2.43	121.80	124.53
19	BB	820	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	B2	813	CLA	CMB-C2B-C3B	2.43	129.23	124.68
22	A2	846	LHG	P-O3-C3	-2.43	107.41	121.68
19	B2	824	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	B	826	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	M1	101	BCR	C24-C23-C22	-2.43	122.56	126.23
19	B2	825	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	A	830	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	B1	831	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	LL	205	LHG	P-O3-C3	-2.43	107.42	121.68
19	J	101	CLA	CMB-C2B-C3B	2.43	129.23	124.68
19	BB	830	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
19	AA	831	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	BB	818	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
19	A	808	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	AA	823	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	A2	851	BCR	C1-C6-C5	-2.43	119.19	122.61
19	B	837	CLA	O2D-CGD-CBD	2.43	115.59	111.27
19	A2	815	CLA	CHD-C1D-ND	-2.43	122.22	124.45
19	AA	832	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	F2	305	BCR	C7-C8-C9	-2.43	122.56	126.23
19	B	804	CLA	C1-C2-C3	-2.43	121.84	126.04
19	B2	825	CLA	O2D-CGD-CBD	2.43	115.58	111.27
19	A	842	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
19	BB	826	CLA	O2D-CGD-CBD	2.43	115.58	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	813	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	A2	845	LHG	P-O6-C4	-2.43	107.45	121.68
19	BB	805	CLA	O2D-CGD-CBD	2.43	115.58	111.27
19	B2	805	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	F2	304	BCR	C15-C16-C17	-2.43	118.50	123.47
23	K2	105	BCR	C1-C6-C5	-2.43	119.20	122.61
19	AA	806	CLA	CHD-C1D-ND	-2.43	122.22	124.45
23	AA	848	BCR	C33-C5-C6	-2.42	121.81	124.53
19	B1	817	CLA	CMB-C2B-C3B	2.42	129.21	124.68
19	A1	832	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
19	L2	205	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
19	A2	806	CLA	CMB-C2B-C3B	2.42	129.21	124.68
23	J	102	BCR	C38-C26-C25	-2.42	121.81	124.53
23	J	104	BCR	C38-C26-C25	-2.42	121.81	124.53
23	L	205	BCR	C7-C8-C9	-2.42	122.57	126.23
19	A1	803	CLA	C1-C2-C3	-2.42	121.85	126.04
19	A1	825	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	A	833	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	A1	837	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
28	BB	854	DGD	C1D-C2D-C3D	-2.42	104.95	110.00
19	BB	813	CLA	CMB-C2B-C3B	2.42	129.21	124.68
23	A1	853	BCR	C2-C1-C6	2.42	114.21	110.48
19	B1	825	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	AA	848	BCR	C2-C1-C6	2.42	114.21	110.48
19	BB	834	CLA	CHD-C1D-ND	-2.42	122.23	124.45
19	B2	807	CLA	C11-C12-C13	-2.42	108.10	115.92
19	A1	817	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	L1	209	BCR	C38-C26-C25	-2.42	121.81	124.53
19	A1	820	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	JJ	102	BCR	C1-C6-C5	-2.42	119.21	122.61
23	A	854	BCR	C1-C6-C5	-2.42	119.21	122.61
19	A	810	CLA	O2D-CGD-CBD	2.42	115.56	111.27
19	A2	842	CLA	C6-C5-C3	2.42	119.79	113.45
19	F	301	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	A2	812	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	AA	833	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	II	101	BCR	C2-C1-C6	2.42	114.20	110.48
19	K1	103	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	B2	840	BCR	C33-C5-C6	-2.42	121.82	124.53
19	A1	801	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
19	A	838	CLA	O2D-CGD-CBD	2.41	115.56	111.27
19	B2	851	CLA	C4-C3-C5	2.41	119.33	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	835	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	KK	102	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	B2	840	BCR	C8-C7-C6	-2.41	120.42	127.20
19	K	101	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	BB	829	CLA	C5-C3-C2	2.41	126.00	121.12
19	A	830	CLA	CAC-C3C-C4C	2.41	127.94	124.81
19	BB	808	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	A2	812	CLA	CBA-CAA-C2A	2.41	120.98	113.86
23	K1	104	BCR	C38-C26-C25	-2.41	121.82	124.53
19	B1	814	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	A1	812	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	AA	818	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	A1	824	CLA	CHD-C1D-ND	-2.41	122.24	124.45
23	FF	306	BCR	C7-C8-C9	-2.41	122.59	126.23
23	I	101	BCR	C2-C1-C6	2.41	114.19	110.48
19	B1	829	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	A1	852	CLA	C6-C5-C3	2.41	119.77	113.45
23	BB	842	BCR	C33-C5-C6	-2.41	121.82	124.53
23	J1	102	BCR	C38-C26-C25	-2.41	121.82	124.53
19	B1	833	CLA	C4-C3-C5	2.41	119.32	115.27
19	BB	813	CLA	O2D-CGD-CBD	2.41	115.55	111.27
19	A2	842	CLA	CMB-C2B-C3B	2.41	129.18	124.68
23	F2	303	BCR	C11-C10-C9	-2.41	123.87	127.31
19	B2	821	CLA	C4-C3-C2	-2.41	117.50	123.68
19	AA	853	CLA	CHD-C1D-ND	-2.41	122.24	124.45
19	A2	807	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	BB	825	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	A	803	CL0	C9-C8-C7	2.41	120.01	111.29
23	MM	101	BCR	C11-C10-C9	-2.41	123.88	127.31
23	B1	842	BCR	C2-C1-C6	2.41	114.19	110.48
19	B2	851	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
23	F2	304	BCR	C38-C26-C25	-2.41	121.83	124.53
23	F1	306	BCR	C27-C26-C25	2.41	126.22	122.73
19	A	806	CLA	CHD-C1D-ND	-2.40	122.24	124.45
19	B	830	CLA	C5-C3-C2	2.40	125.98	121.12
19	AA	829	CLA	C5-C3-C2	2.40	125.98	121.12
25	II	105	LMG	O1-C1-C2	-2.40	104.55	108.30
19	BB	805	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	II	101	BCR	C38-C26-C25	-2.40	121.83	124.53
19	A2	812	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
22	B	853	LHG	P-O3-C3	-2.40	107.59	121.68
19	BB	817	CLA	CMB-C2B-C3B	2.40	129.17	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	829	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	K	102	CLA	CMB-C2B-C3B	2.40	129.17	124.68
23	B1	839	BCR	C8-C7-C6	-2.40	120.45	127.20
23	B	840	BCR	C8-C7-C6	-2.40	120.46	127.20
20	A1	802	CL0	C4-C3-C5	2.40	119.31	115.27
19	K1	102	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	K2	102	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	LL	202	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	B1	820	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	B	806	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
23	L2	207	BCR	C38-C26-C25	-2.40	121.83	124.53
19	B2	814	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	F1	303	BCR	C15-C16-C17	-2.40	118.56	123.47
19	A	809	CLA	CMB-C2B-C3B	2.40	129.16	124.68
19	AA	842	CLA	CMB-C2B-C3B	2.40	129.16	124.68
23	K	103	BCR	C2-C1-C6	2.40	114.17	110.48
19	B1	805	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
19	A2	808	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
23	A	847	BCR	C2-C1-C6	2.40	114.17	110.48
19	BB	812	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	B1	806	CLA	O2A-CGA-O1A	-2.40	117.55	123.59
23	I2	103	BCR	C27-C26-C25	2.40	126.21	122.73
19	A1	815	CLA	CMB-C2B-C3B	2.40	129.16	124.68
19	AA	818	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
23	I2	102	BCR	C7-C8-C9	-2.39	122.62	126.23
19	A	812	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	BB	847	BCR	C15-C14-C13	-2.39	123.89	127.31
21	A	843	PQN	C21-C22-C23	-2.39	108.18	115.92
19	B	803	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	A1	822	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
20	A1	802	CL0	CGD-CBD-CAD	-2.39	102.98	110.73
19	B1	850	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
19	A1	828	CLA	C4-C3-C5	2.39	119.29	115.27
19	BB	806	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	A2	823	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
20	A1	802	CL0	C4C-C3C-C2C	-2.39	103.41	106.90
19	B2	805	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
19	A1	826	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	A	813	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	A1	822	CLA	O2D-CGD-CBD	2.39	115.51	111.27
19	B	805	CLA	O2D-CGD-CBD	2.39	115.51	111.27
19	B1	832	CLA	C2A-C1A-CHA	2.39	128.04	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	813	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	B2	832	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	F2	305	BCR	C27-C26-C25	2.39	126.20	122.73
19	A1	819	CLA	CBA-CAA-C2A	2.39	120.91	113.86
23	A	849	BCR	C33-C5-C6	-2.39	121.85	124.53
19	BB	806	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
19	B1	810	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	A1	814	CLA	CHD-C1D-ND	-2.39	122.26	124.45
19	AA	826	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
19	B2	821	CLA	C5-C3-C2	2.38	125.94	121.12
19	A2	826	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
19	B2	806	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
19	A2	829	CLA	C5-C3-C2	2.38	125.94	121.12
19	B1	811	CLA	CHD-C1D-ND	-2.38	122.26	124.45
19	AA	837	CLA	CHB-C4A-NA	2.38	127.81	124.51
19	B2	817	CLA	CMB-C2B-C3B	2.38	129.13	124.68
23	J	102	BCR	C27-C26-C25	2.38	126.19	122.73
19	A2	816	CLA	C1-C2-C3	-2.38	122.90	126.75
19	B2	824	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	L1	207	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
19	FF	302	CLA	CMB-C2B-C3B	2.38	129.13	124.68
23	JJ	102	BCR	C2-C1-C6	2.38	114.14	110.48
19	A1	807	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	AA	844	PQN	C15-C13-C12	-2.38	116.31	121.12
19	BB	826	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	A2	810	CLA	CHD-C1D-ND	-2.38	122.27	124.45
19	B	805	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	FF	303	BCR	C11-C10-C9	-2.38	123.92	127.31
23	A1	850	BCR	C8-C7-C6	-2.38	120.53	127.20
19	A1	820	CLA	CBA-CAA-C2A	2.38	120.88	113.86
19	B	802	CLA	CMB-C2B-C3B	2.37	129.12	124.68
19	A1	817	CLA	CHD-C1D-ND	-2.37	122.27	124.45
19	A2	818	CLA	CHD-C1D-ND	-2.37	122.27	124.45
23	A2	853	BCR	C30-C25-C26	-2.37	119.27	122.61
19	AA	845	CLA	CMB-C2B-C3B	2.37	129.12	124.68
19	BB	824	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	A1	846	LHG	P-O3-C3	-2.37	107.76	121.68
19	A	821	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
19	B	829	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	B	860	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	K2	105	BCR	C15-C14-C13	-2.37	123.92	127.31
23	JJ	102	BCR	C38-C26-C25	-2.37	121.86	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	I2	105	LMG	O3-C3-C2	-2.37	104.87	110.35
19	BB	856	CLA	C2A-C1A-CHA	2.37	128.00	123.86
23	K1	106	BCR	C1-C6-C5	-2.37	119.28	122.61
19	A2	840	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	B2	810	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	K1	106	BCR	C15-C14-C13	-2.37	123.93	127.31
23	B1	842	BCR	C33-C5-C6	-2.37	121.87	124.53
23	L	206	BCR	C38-C26-C25	-2.37	121.87	124.53
19	B2	816	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	A1	801	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	A2	801	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	F1	301	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	X1	103	LHG	P-O3-C3	-2.37	107.79	121.68
19	L	203	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	L2	208	LHG	P-O3-C3	-2.37	107.80	121.68
19	A1	806	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	B2	823	CLA	CMB-C2B-C3B	2.37	129.10	124.68
19	K1	103	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
19	B2	826	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
23	F1	303	BCR	C8-C7-C6	-2.36	120.56	127.20
19	B	805	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
19	B2	831	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
23	A2	853	BCR	C35-C13-C14	-2.36	119.61	122.92
22	BB	851	LHG	P-O3-C3	-2.36	107.83	121.68
19	A	811	CLA	CAC-C3C-C4C	2.36	127.87	124.81
19	A	826	CLA	CHD-C1D-ND	-2.36	122.28	124.45
23	KK	103	BCR	C2-C1-C6	2.36	114.11	110.48
19	B	835	CLA	CHD-C1D-ND	-2.36	122.28	124.45
19	A2	801	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
25	L1	210	LMG	O1-C7-C8	-2.36	105.20	110.90
23	B	848	BCR	C15-C14-C13	-2.36	123.94	127.31
19	B2	833	CLA	O2D-CGD-CBD	2.36	115.46	111.27
23	A	847	BCR	C8-C7-C6	-2.36	120.58	127.20
19	B	825	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	BB	829	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	B2	843	BCR	C2-C1-C6	2.36	114.11	110.48
19	A1	813	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
19	B	860	CLA	CBC-CAC-C3C	2.36	118.93	112.43
19	B1	806	CLA	C4-C3-C2	-2.36	117.63	123.68
23	A1	851	BCR	C1-C6-C5	-2.36	119.30	122.61
19	F2	301	CLA	C1B-CHB-C4A	-2.36	125.45	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	F2	305	BCR	C24-C23-C22	-2.36	122.68	126.23
23	F2	303	BCR	C8-C7-C6	-2.36	120.59	127.20
19	B2	830	CLA	CMB-C2B-C3B	2.35	129.08	124.68
23	KK	103	BCR	C8-C7-C6	-2.35	120.59	127.20
23	K2	103	BCR	C38-C26-C25	-2.35	121.89	124.53
19	A1	809	CLA	CBA-CAA-C2A	2.35	120.81	113.86
23	A1	851	BCR	C24-C23-C22	-2.35	122.68	126.23
23	BB	838	BCR	C7-C8-C9	-2.35	122.68	126.23
19	A1	832	CLA	CHB-C4A-NA	2.35	127.77	124.51
19	B1	813	CLA	CMB-C2B-C3B	2.35	129.08	124.68
19	L1	206	CLA	CHD-C1D-ND	-2.35	122.29	124.45
23	L1	208	BCR	C7-C8-C9	-2.35	122.68	126.23
23	L1	209	BCR	C16-C15-C14	-2.35	118.66	123.47
19	BB	845	CLA	CAC-C3C-C4C	2.35	127.86	124.81
19	AA	837	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	A1	836	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	A	822	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	A2	801	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
19	A1	808	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	B2	827	CLA	CHD-C1D-ND	-2.35	122.29	124.45
23	A1	853	BCR	C30-C25-C26	-2.35	119.30	122.61
23	BB	843	BCR	C16-C15-C14	-2.35	118.66	123.47
23	K1	106	BCR	C15-C16-C17	-2.35	118.66	123.47
19	A	811	CLA	CHD-C1D-ND	-2.35	122.30	124.45
19	L1	205	CLA	C4-C3-C5	2.35	119.22	115.27
19	B1	819	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	AA	803	CL0	C4C-C3C-C2C	-2.35	103.47	106.90
19	A2	833	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
19	B2	835	CLA	CHD-C1D-ND	-2.35	122.30	124.45
19	AA	842	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	J2	101	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	BB	803	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	A2	834	CLA	CMB-C2B-C3B	2.35	129.07	124.68
19	A2	821	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
19	B	828	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B	827	CLA	O2A-CGA-O1A	-2.35	117.45	123.30
19	A2	814	CLA	CHB-C4A-NA	2.35	127.75	124.51
23	BB	842	BCR	C15-C16-C17	-2.34	118.67	123.47
19	AA	830	CLA	CAC-C3C-C4C	2.34	127.85	124.81
19	A	819	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	B	816	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A1	820	CLA	CAC-C3C-C4C	2.34	127.85	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	837	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
19	AA	807	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
19	B	830	CLA	CMB-C2B-C3B	2.34	129.06	124.68
23	II	102	BCR	C15-C16-C17	-2.34	118.68	123.47
19	B	804	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	AA	816	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	BB	812	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
23	B	848	BCR	C38-C26-C25	-2.34	121.90	124.53
23	B	844	BCR	C16-C15-C14	-2.34	118.68	123.47
19	A1	830	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	A2	825	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	B2	815	CLA	C4-C3-C2	-2.34	117.67	123.68
23	L1	208	BCR	C27-C26-C25	2.34	126.13	122.73
19	A	805	CLA	C5-C3-C2	2.34	125.85	121.12
19	B2	807	CLA	C1-O2A-CGA	2.34	122.58	116.44
19	A2	852	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	818	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	837	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	B	820	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	B	846	CLA	CAC-C3C-C4C	2.34	127.85	124.81
23	A2	850	BCR	C8-C7-C6	-2.34	120.63	127.20
19	BB	811	CLA	CHD-C1D-ND	-2.34	122.30	124.45
19	B1	834	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	JJ	103	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	B1	801	CLA	C5-C3-C2	2.34	125.85	121.12
19	B2	802	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	A2	831	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	BB	825	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	A2	829	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	845	LHG	P-O6-C4	-2.34	107.97	121.68
19	AA	801	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	A2	810	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	B2	843	BCR	C33-C5-C6	-2.34	121.90	124.53
19	B	804	CLA	CMB-C2B-C3B	2.34	129.05	124.68
19	B1	824	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
19	A1	839	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	A1	842	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	A	840	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	A2	816	CLA	CMB-C2B-C3B	2.34	129.05	124.68
20	AA	803	CL0	C1-O2A-CGA	-2.34	110.32	116.44
19	A1	815	CLA	C1-C2-C3	-2.34	122.97	126.75
19	B	811	CLA	CHD-C1D-ND	-2.34	122.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	811	CLA	CHD-C1D-ND	-2.34	122.31	124.45
19	A1	836	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	B	826	CLA	CMB-C2B-C3B	2.33	129.05	124.68
19	A2	842	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
23	A1	853	BCR	C35-C13-C14	-2.33	119.65	122.92
19	B1	822	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	B	816	CLA	CHD-C1D-ND	-2.33	122.31	124.45
19	B1	830	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
19	A2	836	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	JJ	104	BCR	C38-C26-C25	-2.33	121.91	124.53
23	B1	843	BCR	C24-C23-C22	-2.33	122.71	126.23
19	A1	818	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
19	A2	819	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
19	A2	818	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	FF	305	CLA	CHB-C4A-NA	2.33	127.74	124.51
23	M2	102	BCR	C7-C8-C9	-2.33	122.71	126.23
20	AA	803	CL0	C5-C3-C2	-2.33	116.40	121.12
19	A2	802	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	AA	839	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	BB	836	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	II	104	BCR	C7-C8-C9	-2.33	122.71	126.23
22	B	852	LHG	P-O6-C4	-2.33	108.02	121.68
23	B1	843	BCR	C16-C15-C14	-2.33	118.70	123.47
20	A1	802	CL0	C9-C8-C10	2.33	119.73	111.29
19	J	103	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	A1	833	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	B1	822	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	A	837	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	B2	801	CLA	CBA-CAA-C2A	2.33	120.74	113.86
19	B2	832	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
19	BB	804	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	B	841	ECH	C33-C5-C4	2.33	118.09	113.62
23	B1	842	BCR	C27-C26-C25	2.33	126.11	122.73
19	A2	806	CLA	CHD-C1D-ND	-2.33	122.31	124.45
19	AA	812	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	A1	811	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	B	806	CLA	C4-C3-C2	-2.33	117.71	123.68
19	B2	820	CLA	CHB-C4A-NA	2.33	127.73	124.51
23	A2	847	BCR	C8-C7-C6	-2.33	120.67	127.20
23	AA	852	BCR	C24-C23-C22	-2.33	122.72	126.23
23	BB	847	BCR	C35-C13-C14	-2.33	119.66	122.92
19	A	807	CLA	C1B-CHB-C4A	-2.33	125.51	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	849	BCR	C33-C5-C6	-2.33	121.92	124.53
19	J1	103	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
19	A1	835	CLA	O2D-CGD-CBD	2.33	115.40	111.27
23	JJ	102	BCR	C27-C26-C25	2.33	126.11	122.73
25	B	851	LMG	O1-C1-C2	-2.33	104.67	108.30
19	A	823	CLA	C5-C3-C2	2.33	125.82	121.12
19	AA	836	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
19	B1	802	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
19	A	801	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
19	BB	816	CLA	CHB-C4A-NA	2.32	127.73	124.51
19	BB	802	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	A	812	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	BB	854	DGD	O5D-C6D-C5D	-2.32	104.75	109.05
23	I2	103	BCR	C11-C10-C9	-2.32	124.00	127.31
19	B	824	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	BB	804	CLA	CHD-C1D-ND	-2.32	122.32	124.45
19	B2	816	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B2	828	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	FF	301	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	A2	821	CLA	CBA-CAA-C2A	2.32	120.71	113.86
19	JJ	103	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
19	AA	826	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B1	802	CLA	CMB-C2B-C3B	2.32	129.02	124.68
19	B	859	CLA	O2D-CGD-CBD	2.32	115.39	111.27
19	A2	809	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	BB	835	CLA	CHD-C1D-ND	-2.32	122.32	124.45
19	A2	834	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	AA	824	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	A	848	BCR	C38-C26-C25	-2.32	121.92	124.53
19	F2	301	CLA	O2D-CGD-CBD	2.32	115.39	111.27
23	B	844	BCR	C15-C16-C17	-2.32	118.73	123.47
19	A2	822	CLA	CMB-C2B-C3B	2.32	129.01	124.68
22	X2	103	LHG	P-O3-C3	-2.32	108.09	121.68
20	A1	802	CL0	CMA-C3A-C4A	-2.32	105.55	111.77
23	F1	304	BCR	C37-C22-C21	-2.32	119.68	122.92
19	AA	812	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	B2	805	CLA	O2D-CGD-CBD	2.32	115.38	111.27
19	L1	206	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	845	LHG	P-O3-C3	-2.32	108.10	121.68
19	A1	825	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	JJ	104	BCR	C27-C26-C25	2.32	126.09	122.73
19	A	852	CLA	CHD-C1D-ND	-2.32	122.33	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	804	CLA	CHD-C1D-ND	-2.32	122.33	124.45
19	B	837	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
23	J	102	BCR	C33-C5-C6	-2.31	121.93	124.53
19	BB	845	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
19	BB	827	CLA	CBA-CAA-C2A	2.31	120.69	113.86
23	B2	839	BCR	C15-C16-C17	-2.31	118.74	123.47
23	II	101	BCR	C15-C16-C17	-2.31	118.74	123.47
19	B2	830	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	AA	819	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	K1	105	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	B2	806	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	A1	849	BCR	C7-C8-C9	-2.31	122.74	126.23
19	B2	835	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	BB	808	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	B1	809	CLA	O2D-CGD-CBD	2.31	115.38	111.27
19	B2	809	CLA	O2D-CGD-CBD	2.31	115.38	111.27
19	A1	821	CLA	CMB-C2B-C3B	2.31	129.00	124.68
19	L1	207	CLA	C2D-C1D-ND	-2.31	108.40	110.10
19	K1	103	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	B	802	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	B2	809	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	II	101	BCR	C24-C23-C22	-2.31	122.75	126.23
23	K2	105	BCR	C15-C16-C17	-2.31	118.75	123.47
23	K1	104	BCR	C15-C16-C17	-2.31	118.75	123.47
23	B2	844	BCR	C16-C15-C14	-2.31	118.75	123.47
19	J1	103	CLA	CHB-C4A-NA	2.31	127.70	124.51
19	A	821	CLA	CBA-CAA-C2A	2.31	120.67	113.86
23	F2	303	BCR	C38-C26-C25	-2.31	121.94	124.53
23	B	843	BCR	C2-C1-C6	2.31	114.03	110.48
23	BB	842	BCR	C2-C1-C6	2.31	114.03	110.48
19	A2	838	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
19	F2	302	CLA	CMB-C2B-C3B	2.31	128.99	124.68
19	B1	831	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	A	854	BCR	C15-C16-C17	-2.31	118.75	123.47
23	AA	852	BCR	C15-C16-C17	-2.31	118.75	123.47
22	BB	850	LHG	P-O6-C4	-2.31	108.16	121.68
19	F1	305	CLA	CHB-C4A-NA	2.31	127.70	124.51
19	A	831	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	L2	207	BCR	C24-C23-C22	-2.31	122.75	126.23
19	A	836	CLA	O2D-CGD-CBD	2.31	115.36	111.27
19	A2	836	CLA	CMB-C2B-C3B	2.31	128.99	124.68
19	A	804	CLA	CMB-C2B-C3B	2.31	128.99	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AA	846	LHG	P-O6-C4	-2.31	108.16	121.68
19	B2	826	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	A	833	CLA	CHD-C1D-ND	-2.30	122.34	124.45
23	AA	849	BCR	C38-C26-C25	-2.30	121.94	124.53
19	A1	812	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	A2	845	LHG	P-O3-C3	-2.30	108.17	121.68
23	B	848	BCR	C35-C13-C14	-2.30	119.69	122.92
19	B	846	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
19	BB	804	CLA	CMB-C2B-C3B	2.30	128.99	124.68
19	A	809	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	B2	814	CLA	CMB-C2B-C3B	2.30	128.99	124.68
19	A2	838	CLA	O2D-CGD-CBD	2.30	115.36	111.27
23	F	304	BCR	C37-C22-C21	-2.30	119.70	122.92
19	AA	805	CLA	C5-C3-C2	2.30	125.78	121.12
19	AA	816	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	A2	851	BCR	C37-C22-C21	-2.30	119.70	122.92
19	BB	856	CLA	O2D-CGD-CBD	2.30	115.36	111.27
23	BB	838	BCR	C24-C23-C22	-2.30	122.76	126.23
19	A	826	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	A	815	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
23	A1	851	BCR	C15-C16-C17	-2.30	118.76	123.47
19	AA	831	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	AA	816	CLA	O2D-CGD-CBD	2.30	115.36	111.27
23	F1	304	BCR	C20-C21-C22	-2.30	124.03	127.31
23	F2	305	BCR	C20-C21-C22	-2.30	124.03	127.31
23	F2	303	BCR	C15-C16-C17	-2.30	118.76	123.47
19	A	829	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	BB	806	CLA	C4-C3-C2	-2.30	117.78	123.68
19	B2	806	CLA	C4-C3-C2	-2.30	117.78	123.68
19	B	824	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	B2	824	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	A2	849	BCR	C7-C8-C9	-2.30	122.76	126.23
19	B1	801	CLA	CBA-CAA-C2A	2.30	120.65	113.86
19	L1	207	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
19	AA	821	CLA	CBA-CAA-C2A	2.30	120.65	113.86
19	B	813	CLA	CMB-C2B-C3B	2.30	128.98	124.68
19	BB	815	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	A	825	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	AA	807	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	B	826	CLA	C6-C5-C3	2.30	119.48	113.45
19	B1	831	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	B2	821	CLA	O2A-CGA-O1A	-2.30	117.80	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	831	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	B2	852	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	F1	302	CLA	CMB-C2B-C3B	2.30	128.97	124.68
19	A1	809	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	AA	809	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	B1	840	ECH	C28-C27-C26	-2.30	116.53	118.65
23	A	849	BCR	C7-C8-C9	-2.30	122.77	126.23
19	A2	844	CLA	CMB-C2B-C3B	2.30	128.97	124.68
19	J2	103	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	B2	832	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	A2	802	CLA	CHD-C1D-ND	-2.29	122.34	124.45
19	A	818	CLA	CHD-C1D-ND	-2.29	122.34	124.45
19	AA	819	CLA	CHB-C4A-NA	2.29	127.69	124.51
19	B1	801	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
19	B2	827	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
19	A	822	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
23	B	844	BCR	C8-C7-C6	-2.29	120.76	127.20
23	II	101	BCR	C16-C15-C14	-2.29	118.78	123.47
19	A	828	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A	826	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	B2	827	CLA	O2A-CGA-O1A	-2.29	117.58	123.30
21	AA	844	PQN	C21-C22-C23	-2.29	108.51	115.92
19	AA	835	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	B1	809	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	B2	804	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A1	837	CLA	O2D-CGD-CBD	2.29	115.34	111.27
19	B1	801	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	BB	818	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	I1	102	LMG	O3-C3-C2	-2.29	105.05	110.35
19	B	834	CLA	C4-C3-C2	-2.29	117.80	123.68
19	L1	206	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	A1	843	PQN	C21-C22-C23	-2.29	108.52	115.92
19	L2	205	CLA	O2D-CGD-CBD	2.29	115.34	111.27
19	B	818	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	AA	836	CLA	O2D-CGD-CBD	2.29	115.33	111.27
23	FF	304	BCR	C33-C5-C6	-2.29	121.96	124.53
19	A	831	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A2	829	CLA	C4-C3-C2	-2.29	117.81	123.68
23	F	304	BCR	C20-C21-C22	-2.29	124.05	127.31
19	AA	809	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	B2	827	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	B2	829	CLA	C1B-CHB-C4A	-2.29	125.59	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	859	CLA	C2A-C1A-CHA	2.29	127.86	123.86
23	L1	209	BCR	C27-C26-C25	2.29	126.05	122.73
19	A2	831	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	J	103	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	B1	829	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	A1	827	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	B1	845	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	A	851	BCR	C1-C6-C5	-2.29	119.39	122.61
19	A	819	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
19	A2	852	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
19	A1	809	CLA	CMB-C2B-C3B	2.28	128.95	124.68
19	JJ	103	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	BB	805	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	B1	843	BCR	C8-C7-C6	-2.28	120.79	127.20
19	A1	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	A2	804	CLA	CMB-C2B-C3B	2.28	128.95	124.68
23	L1	208	BCR	C11-C10-C9	-2.28	124.05	127.31
19	A2	823	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	B1	838	BCR	C15-C16-C17	-2.28	118.80	123.47
19	A	812	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	B2	844	BCR	C8-C7-C6	-2.28	120.80	127.20
19	AA	834	CLA	CHB-C4A-NA	2.28	127.67	124.51
19	B	824	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
19	B2	833	CLA	CHA-C1A-NA	-2.28	121.18	126.40
23	I	102	BCR	C15-C16-C17	-2.28	118.80	123.47
23	B1	842	BCR	C38-C26-C25	-2.28	121.97	124.53
19	AA	818	CLA	CHD-C1D-ND	-2.28	122.36	124.45
19	BB	833	CLA	C2A-C1A-CHA	2.28	127.84	123.86
19	A1	817	CLA	CMB-C2B-C3B	2.28	128.94	124.68
19	B1	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	B1	803	CLA	C11-C12-C13	-2.28	108.55	115.92
19	A1	822	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
19	A1	830	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	A1	804	CLA	C5-C3-C2	2.28	125.73	121.12
19	BB	833	CLA	C4-C3-C5	2.28	119.10	115.27
19	B	829	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	B	814	CLA	C4-C3-C5	-2.28	111.44	115.27
23	F	304	BCR	C27-C26-C25	2.28	126.04	122.73
23	BB	842	BCR	C27-C26-C25	2.28	126.04	122.73
23	B2	839	BCR	C24-C23-C22	-2.28	122.79	126.23
19	A1	805	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	BB	836	CLA	CHD-C4C-C3C	2.28	128.19	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	848	BCR	C8-C7-C6	-2.28	120.81	127.20
19	A1	842	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	F	303	BCR	C15-C16-C17	-2.28	118.81	123.47
19	B	826	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	A	836	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	B1	827	CLA	O2A-CGA-O1A	-2.28	117.62	123.30
21	A2	843	PQN	C21-C22-C23	-2.28	108.56	115.92
19	B	826	CLA	C4-C3-C5	2.28	119.10	115.27
23	J	104	BCR	C3-C4-C5	-2.28	110.01	114.08
19	AA	804	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	X1	103	LHG	P-O6-C4	-2.28	108.33	121.68
23	BB	843	BCR	C15-C16-C17	-2.28	118.81	123.47
19	A	801	CLA	CMB-C2B-C3B	2.28	128.94	124.68
19	AA	836	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	BB	850	LHG	P-O3-C3	-2.28	108.34	121.68
23	K2	103	BCR	C15-C16-C17	-2.28	118.81	123.47
19	AA	816	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	B2	839	BCR	C7-C8-C9	-2.27	122.80	126.23
19	A2	833	CLA	CHD-C1D-ND	-2.27	122.36	124.45
23	JJ	102	BCR	C8-C7-C6	-2.27	120.82	127.20
19	B2	846	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
22	X2	103	LHG	P-O6-C4	-2.27	108.35	121.68
19	B2	849	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	A2	847	BCR	C15-C16-C17	-2.27	118.82	123.47
23	MM	101	BCR	C24-C23-C22	-2.27	122.80	126.23
19	B1	850	CLA	O2D-CGD-CBD	2.27	115.31	111.27
19	B	821	CLA	C4-C3-C2	-2.27	117.85	123.68
23	KK	103	BCR	C16-C15-C14	-2.27	118.82	123.47
19	BB	820	CLA	CHD-C4C-C3C	2.27	128.18	124.84
23	BB	847	BCR	C38-C26-C25	-2.27	121.98	124.53
23	B1	838	BCR	C7-C8-C9	-2.27	122.80	126.23
23	I1	101	BCR	C16-C15-C14	-2.27	118.82	123.47
19	B1	815	CLA	C4-C3-C2	-2.27	117.85	123.68
19	A1	833	CLA	CMB-C2B-C3B	2.27	128.93	124.68
19	A2	825	CLA	CMB-C2B-C3B	2.27	128.93	124.68
19	B1	835	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
19	A	835	CLA	CHD-C1D-ND	-2.27	122.37	124.45
19	B	860	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	L	203	CLA	C1-O2A-CGA	2.27	122.39	116.44
19	A2	828	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	A	824	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	A2	821	CLA	CMB-C2B-C3B	2.27	128.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A1	802	CL0	C1-C2-C3	2.27	129.97	126.04
23	BB	843	BCR	C8-C7-C6	-2.27	120.83	127.20
23	B2	843	BCR	C38-C26-C25	-2.27	121.98	124.53
19	AA	806	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
19	A	806	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	AA	855	BCR	C1-C6-C5	-2.27	119.42	122.61
19	A2	806	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	JJ	102	BCR	C33-C5-C6	-2.27	121.98	124.53
19	A1	841	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
19	B2	822	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	L2	206	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
19	BB	827	CLA	O2A-CGA-O1A	-2.27	117.65	123.30
23	A2	851	BCR	C8-C7-C6	-2.26	120.84	127.20
19	B2	826	CLA	O2D-CGD-CBD	2.26	115.29	111.27
19	A2	813	CLA	CHD-C1D-ND	-2.26	122.37	124.45
19	A1	816	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	B1	838	BCR	C24-C23-C22	-2.26	122.81	126.23
26	BB	840	ECH	C33-C5-C4	2.26	117.97	113.62
19	AA	801	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
19	L2	204	CLA	C4-C3-C5	2.26	119.08	115.27
23	J1	102	BCR	C27-C26-C25	2.26	126.01	122.73
19	A2	827	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	K	103	BCR	C8-C7-C6	-2.26	120.86	127.20
19	AA	810	CLA	CHD-C1D-ND	-2.26	122.38	124.45
19	AA	823	CLA	C5-C3-C2	2.26	125.69	121.12
19	B	815	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
19	AA	853	CLA	C7-C6-C5	2.26	119.49	113.36
19	B2	802	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
19	A1	824	CLA	CHB-C4A-NA	2.26	127.64	124.51
19	AA	829	CLA	C4-C3-C2	-2.26	117.89	123.68
19	BB	826	CLA	C6-C5-C3	2.26	119.38	113.45
23	I1	101	BCR	C27-C26-C25	2.26	126.01	122.73
19	B1	822	CLA	CMB-C2B-C3B	2.26	128.90	124.68
23	J	102	BCR	C35-C13-C14	-2.26	119.76	122.92
23	F	305	BCR	C27-C26-C25	2.26	126.01	122.73
19	A1	824	CLA	CMB-C2B-C3B	2.26	128.90	124.68
19	A2	813	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
19	B1	805	CLA	O2D-CGD-CBD	2.26	115.28	111.27
19	B	858	CLA	O2D-CGD-CBD	2.26	115.28	111.27
23	FF	303	BCR	C15-C16-C17	-2.26	118.85	123.47
19	J2	101	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
19	AA	828	CLA	C1B-CHB-C4A	-2.26	125.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	844	CLA	CMB-C2B-C3B	2.26	128.90	124.68
22	AA	846	LHG	P-O3-C3	-2.26	108.46	121.68
23	JJ	104	BCR	C8-C7-C6	-2.25	120.87	127.20
19	B1	848	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
19	A	809	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
23	BB	839	BCR	C15-C16-C17	-2.25	118.86	123.47
19	B1	824	CLA	CHD-C1D-ND	-2.25	122.38	124.45
19	A1	818	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	B1	846	LMG	O3-C3-C2	-2.25	105.14	110.35
23	B	840	BCR	C33-C5-C6	-2.25	122.00	124.53
19	AA	823	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
19	BB	824	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	B	843	BCR	C27-C26-C25	2.25	126.00	122.73
19	A2	821	CLA	CAC-C3C-C4C	2.25	127.73	124.81
19	B1	804	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	M	101	BCR	C8-C7-C6	-2.25	120.88	127.20
19	A1	828	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	J1	101	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	AA	855	BCR	C20-C21-C22	-2.25	124.10	127.31
23	B	839	BCR	C15-C16-C17	-2.25	118.86	123.47
23	LL	204	BCR	C15-C16-C17	-2.25	118.86	123.47
19	AA	843	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	I2	101	BCR	C27-C26-C25	2.25	126.00	122.73
19	B2	815	CLA	O2D-CGD-CBD	2.25	115.27	111.27
19	A2	809	CLA	CHD-C1D-ND	-2.25	122.39	124.45
19	A	810	CLA	CHD-C1D-ND	-2.25	122.39	124.45
19	FF	305	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	A2	834	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	AA	853	CLA	O2D-CGD-CBD	2.25	115.26	111.27
22	X	102	LHG	P-O3-C3	-2.25	108.50	121.68
25	B2	847	LMG	O3-C3-C2	-2.25	105.15	110.35
23	I2	101	BCR	C2-C1-C6	2.25	113.94	110.48
23	L2	207	BCR	C27-C26-C25	2.25	125.99	122.73
19	A	814	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
19	A2	833	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	AA	850	BCR	C7-C8-C9	-2.25	122.84	126.23
19	AA	820	CLA	CBA-CAA-C2A	2.25	120.49	113.86
19	B2	815	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	B	839	BCR	C7-C8-C9	-2.25	122.84	126.23
19	A	834	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	A	816	CLA	C1-C2-C3	-2.24	123.12	126.75
23	F1	304	BCR	C8-C7-C6	-2.24	120.90	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	834	CLA	C4-C3-C5	2.24	119.05	115.27
22	X2	102	LHG	P-O3-C3	-2.24	108.52	121.68
19	B	858	CLA	CHD-C1D-ND	-2.24	122.39	124.45
19	A	804	CLA	C1-C2-C3	-2.24	122.16	126.04
19	A1	811	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	BB	834	CLA	O2A-CGA-O1A	-2.24	117.71	123.30
19	LL	201	CLA	CHD-C1D-ND	-2.24	122.39	124.45
23	A2	851	BCR	C15-C16-C17	-2.24	118.88	123.47
19	A	804	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
19	A1	832	CLA	O2D-CGD-CBD	2.24	115.25	111.27
19	AA	829	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	BB	832	CLA	CHA-C1A-NA	-2.24	121.26	126.40
19	B2	818	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	AA	804	CLA	CMB-C2B-C3B	2.24	128.87	124.68
23	A1	848	BCR	C2-C1-C6	2.24	113.93	110.48
23	A2	848	BCR	C2-C1-C6	2.24	113.93	110.48
19	LL	203	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	B2	801	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	B1	827	CLA	CHD-C1D-ND	-2.24	122.39	124.45
19	A1	804	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	J1	101	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	AA	843	CLA	CBC-CAC-C3C	2.24	118.61	112.43
23	L	206	BCR	C15-C16-C17	-2.24	118.89	123.47
19	B2	830	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	B2	836	CLA	CHD-C1D-ND	-2.24	122.40	124.45
23	B2	840	BCR	C29-C30-C25	2.24	113.93	110.48
19	A1	840	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	BB	833	CLA	C4-C3-C2	-2.24	117.93	123.68
19	A2	817	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	A2	837	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	F2	304	BCR	C8-C7-C6	-2.24	120.92	127.20
25	B1	852	LMG	O3-C3-C2	-2.24	105.17	110.35
19	A	819	CLA	CHD-C1D-ND	-2.24	122.40	124.45
19	B2	830	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
19	A	801	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
19	B	835	CLA	O2A-CGA-O1A	-2.24	117.72	123.30
23	A2	848	BCR	C38-C26-C25	-2.24	122.02	124.53
23	AA	850	BCR	C33-C5-C6	-2.24	122.02	124.53
19	X2	101	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
25	B2	854	LMG	O3-C3-C2	-2.24	105.18	110.35
19	A	852	CLA	O2D-CGD-CBD	2.24	115.24	111.27
25	B2	854	LMG	C7-O1-C1	2.24	118.11	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	818	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
19	A2	819	CLA	CHD-C1D-ND	-2.24	122.40	124.45
23	FF	304	BCR	C37-C22-C21	-2.24	119.79	122.92
26	BB	840	ECH	C23-C24-C25	-2.23	120.92	127.20
19	A1	801	CLA	O1D-CGD-CBD	2.23	129.06	124.48
19	A2	835	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	A2	812	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
19	A	830	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	L2	208	LHG	O7-C7-C8	2.23	116.32	111.50
19	A1	839	CLA	CHD-C1D-ND	-2.23	122.40	124.45
19	AA	805	CLA	O2D-CGD-CBD	2.23	115.24	111.27
19	AA	811	CLA	C2D-C1D-ND	-2.23	108.46	110.10
23	J2	102	BCR	C33-C5-C6	-2.23	122.02	124.53
19	B1	806	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
19	J1	103	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
19	A2	812	CLA	CHD-C1D-ND	-2.23	122.40	124.45
23	J	102	BCR	C8-C7-C6	-2.23	120.93	127.20
19	B1	818	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	A1	818	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	B	808	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	AA	819	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
19	A	834	CLA	CMB-C2B-C3B	2.23	128.85	124.68
19	B1	825	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	B	810	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
23	L1	209	BCR	C8-C7-C6	-2.23	120.94	127.20
25	B	845	LMG	O3-C3-C2	-2.23	105.19	110.35
19	B1	816	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	A2	824	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	B1	826	CLA	O2D-CGD-CBD	2.23	115.23	111.27
19	B	836	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	A	851	BCR	C15-C16-C17	-2.23	118.91	123.47
19	B1	821	CLA	C5-C3-C2	2.23	125.63	121.12
19	A1	836	CLA	CHD-C1D-ND	-2.23	122.41	124.45
19	A	820	CLA	C1-C2-C3	-2.23	122.19	126.04
19	B2	808	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	M2	102	BCR	C15-C16-C17	-2.23	118.91	123.47
22	B	852	LHG	P-O3-C3	-2.23	108.61	121.68
19	A1	842	CLA	CBC-CAC-C3C	2.23	118.58	112.43
25	M	102	LMG	C1-C2-C3	-2.23	105.36	110.00
19	J	101	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	BB	821	CLA	CMB-C2B-C3B	2.23	128.85	124.68
19	A1	813	CLA	CHB-C4A-NA	2.23	127.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	FF	303	BCR	C38-C26-C25	-2.23	122.03	124.53
19	AA	801	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
23	K1	104	BCR	C2-C1-C6	2.23	113.91	110.48
23	B	840	BCR	C29-C30-C25	2.23	113.91	110.48
19	B1	808	CLA	CMB-C2B-C3B	2.23	128.84	124.68
19	A2	841	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	A	844	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	A	827	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	A	848	BCR	C15-C16-C17	-2.23	118.92	123.47
19	A	819	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	A	840	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	BB	830	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
23	MM	101	BCR	C8-C7-C6	-2.23	120.95	127.20
19	A	823	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
19	L2	204	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
19	B2	801	CLA	C5-C3-C2	2.22	125.61	121.12
23	J2	102	BCR	C27-C26-C25	2.22	125.96	122.73
26	B	841	ECH	C7-C6-C5	-2.22	116.08	121.46
19	B2	836	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
19	A1	804	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
23	M1	101	BCR	C15-C16-C17	-2.22	118.92	123.47
19	B	812	CLA	CMA-C3A-C2A	-2.22	110.91	116.10
23	BB	839	BCR	C29-C30-C25	2.22	113.90	110.48
19	A2	840	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	JJ	102	BCR	C11-C10-C9	-2.22	124.14	127.31
19	B1	804	CLA	CHD-C1D-ND	-2.22	122.41	124.45
19	B2	828	CLA	CHD-C1D-ND	-2.22	122.41	124.45
19	A	842	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	M2	102	BCR	C2-C1-C6	2.22	113.90	110.48
19	A1	834	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	A1	848	BCR	C38-C26-C25	-2.22	122.04	124.53
19	A1	829	CLA	CMB-C2B-C3B	2.22	128.83	124.68
19	BB	809	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
19	A1	823	CLA	CHD-C1D-ND	-2.22	122.42	124.45
23	J1	102	BCR	C35-C13-C14	-2.22	119.81	122.92
19	A	813	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
19	AA	837	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
19	A	814	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A2	811	CLA	C1-O2A-CGA	2.22	122.26	116.44
19	A1	823	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	I2	102	BCR	C8-C7-C6	-2.22	120.97	127.20
23	B2	843	BCR	C27-C26-C25	2.22	125.95	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	854	BCR	C20-C21-C22	-2.22	124.14	127.31
22	X1	102	LHG	P-O3-C3	-2.22	108.68	121.68
25	B1	852	LMG	C7-O1-C1	2.22	118.07	113.74
19	B2	819	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	A	816	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	A1	821	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	L1	205	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	AA	827	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	J1	102	BCR	C33-C5-C6	-2.22	122.04	124.53
23	AA	849	BCR	C2-C1-C6	2.22	113.89	110.48
19	B1	828	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	BB	835	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
20	A1	802	CL0	C5-C3-C2	-2.21	116.64	121.12
23	I1	101	BCR	C2-C1-C6	2.21	113.89	110.48
22	BB	851	LHG	O7-C7-C8	2.21	116.27	111.50
19	B1	810	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
23	A1	849	BCR	C38-C26-C25	-2.21	122.04	124.53
19	A2	818	CLA	CMB-C2B-C3B	2.21	128.82	124.68
19	F	302	CLA	CMB-C2B-C3B	2.21	128.82	124.68
23	FF	306	BCR	C35-C13-C12	2.21	121.56	118.08
19	AA	832	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	AA	827	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
23	A2	849	BCR	C15-C16-C17	-2.21	118.94	123.47
22	XX	102	LHG	P-O3-C3	-2.21	108.70	121.68
19	B1	813	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B1	818	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B	835	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	BB	810	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	JJ	101	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B1	850	CLA	C2A-C1A-CHA	2.21	127.73	123.86
25	M	102	LMG	O3-C3-C2	-2.21	105.23	110.35
23	I2	101	BCR	C16-C15-C14	-2.21	118.94	123.47
19	B	825	CLA	C2D-C1D-ND	-2.21	108.47	110.10
23	J2	104	BCR	C15-C16-C17	-2.21	118.94	123.47
26	BB	840	ECH	C7-C6-C5	-2.21	116.11	121.46
19	A	816	CLA	CMB-C2B-C3B	2.21	128.81	124.68
25	B1	844	LMG	C40-C39-C38	-2.21	103.20	114.42
19	A	839	CLA	CHD-C1D-ND	-2.21	122.42	124.45
19	A2	804	CLA	C1-C2-C3	-2.21	122.22	126.04
23	L2	207	BCR	C8-C7-C6	-2.21	121.00	127.20
19	A	829	CLA	C4-C3-C2	-2.21	118.01	123.68
19	B	816	CLA	O2A-CGA-O1A	-2.21	118.02	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	825	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
19	A	815	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
19	B	808	CLA	CHD-C1D-ND	-2.21	122.42	124.45
19	A1	844	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
19	J2	103	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	A	851	BCR	C24-C23-C22	-2.21	122.90	126.23
23	B	844	BCR	C24-C23-C22	-2.21	122.90	126.23
23	JJ	104	BCR	C2-C1-C6	2.21	113.88	110.48
19	AA	845	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
23	I2	103	BCR	C15-C14-C13	-2.21	124.16	127.31
23	FF	304	BCR	C20-C21-C22	-2.21	124.16	127.31
19	B	831	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
19	L	202	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
22	B2	848	LHG	P-O3-C3	-2.21	108.74	121.68
19	B2	822	CLA	C2D-C1D-ND	-2.21	108.48	110.10
19	B2	810	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
19	A2	811	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
26	B2	841	ECH	C8-C9-C10	2.21	122.33	118.94
19	B1	806	CLA	C1-C2-C3	2.21	129.86	126.04
19	A	827	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	A	835	CLA	CHB-C4A-NA	2.21	127.56	124.51
25	B2	845	LMG	O3-C3-C2	-2.21	105.25	110.35
25	BB	844	LMG	O3-C3-C2	-2.21	105.25	110.35
23	MM	101	BCR	C7-C8-C9	-2.21	122.90	126.23
19	A1	833	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	A	848	BCR	C2-C1-C6	2.20	113.88	110.48
23	JJ	102	BCR	C35-C13-C14	-2.20	119.83	122.92
19	B	813	CLA	O2D-CGD-CBD	2.20	115.19	111.27
22	B	853	LHG	P-O6-C4	-2.20	108.76	121.68
25	B1	844	LMG	O3-C3-C2	-2.20	105.25	110.35
19	B2	803	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
19	B1	828	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
25	B	845	LMG	C40-C39-C38	-2.20	103.24	114.42
22	A1	845	LHG	P-O3-C3	-2.20	108.76	121.68
19	AA	814	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	B2	850	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	A	805	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	A2	840	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	B	815	CLA	CBA-CAA-C2A	2.20	120.36	113.86
19	B2	852	CLA	C3C-C4C-NC	-2.20	108.10	110.57
19	AA	813	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
19	B	809	CLA	C1B-CHB-C4A	-2.20	125.76	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	808	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
19	B	802	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
25	L1	210	LMG	O3-C3-C2	-2.20	105.26	110.35
23	II	104	BCR	C15-C14-C13	-2.20	124.17	127.31
23	A1	847	BCR	C8-C7-C6	-2.20	121.02	127.20
19	A1	832	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	A2	830	CLA	CAC-C3C-C4C	2.20	127.66	124.81
19	A1	818	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	A	837	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	AA	812	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	F2	304	BCR	C20-C21-C22	-2.20	124.17	127.31
19	B2	812	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	BB	834	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	A	821	CLA	CAC-C3C-C4C	2.20	127.66	124.81
19	BB	836	CLA	CMB-C2B-C3B	2.20	128.79	124.68
19	A2	822	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	B1	826	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
19	F1	305	CLA	CHD-C1D-ND	-2.20	122.44	124.45
19	LL	201	CLA	C2D-C1D-ND	-2.20	108.48	110.10
23	A1	853	BCR	C7-C8-C9	-2.20	122.92	126.23
23	J2	102	BCR	C8-C7-C6	-2.20	121.03	127.20
19	B1	834	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
19	B	827	CLA	CBA-CAA-C2A	2.20	120.34	113.86
19	B	830	CLA	CHB-C4A-NA	2.20	127.55	124.51
19	B	826	CLA	O2D-CGD-CBD	2.20	115.17	111.27
19	B1	812	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
19	BB	831	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	B2	842	BCR	C35-C13-C14	-2.19	119.85	122.92
19	J1	101	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	B	822	CLA	CMB-C2B-C3B	2.19	128.78	124.68
19	B2	818	CLA	CHB-C4A-NA	2.19	127.55	124.51
25	B1	846	LMG	O1-C7-C8	-2.19	105.61	110.90
23	B	840	BCR	C15-C16-C17	-2.19	118.98	123.47
19	A1	841	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	BB	806	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
19	B1	845	CLA	CAC-C3C-C4C	2.19	127.65	124.81
19	A1	803	CLA	CMB-C2B-C3B	2.19	128.78	124.68
19	BB	812	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
19	B2	803	CLA	C11-C12-C13	-2.19	108.84	115.92
23	AA	849	BCR	C15-C16-C17	-2.19	118.99	123.47
19	A	817	CLA	CMB-C2B-C3B	2.19	128.78	124.68
19	L	204	CLA	C1-C2-C3	-2.19	122.25	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	K1	106	BCR	C35-C13-C14	-2.19	119.86	122.92
23	AA	848	BCR	C23-C24-C25	-2.19	123.32	126.28
19	B2	829	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	B	851	LMG	O3-C3-C2	-2.19	105.29	110.35
23	I	101	BCR	C16-C15-C14	-2.19	118.99	123.47
19	AA	833	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	B1	810	CLA	C5-C3-C2	2.19	125.55	121.12
19	A2	819	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
19	FF	301	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
19	B1	807	CLA	C16-C15-C13	-2.19	108.84	115.92
25	B1	852	LMG	C1-C2-C3	-2.19	105.44	110.00
26	B	841	ECH	C29-C30-C25	-2.19	107.11	110.48
19	A1	808	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	AA	832	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	A	841	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	A	853	BCR	C38-C26-C25	-2.19	122.07	124.53
19	B	830	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
19	AA	809	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
19	BB	801	CLA	C2A-C1A-CHA	2.19	127.68	123.86
19	A	809	CLA	C1-C2-C3	-2.19	123.21	126.75
19	B	833	CLA	CHA-C1A-NA	-2.19	121.39	126.40
19	B2	817	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
19	LL	202	CLA	C1-O2A-CGA	2.19	122.18	116.44
19	A2	827	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
23	AA	850	BCR	C15-C16-C17	-2.19	119.00	123.47
19	X1	101	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	B	806	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	XX	101	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	A2	804	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	A2	844	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
23	A	847	BCR	C15-C14-C13	-2.18	124.19	127.31
23	F	305	BCR	C20-C21-C22	-2.18	124.19	127.31
19	AA	841	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
25	II	105	LMG	O2-C2-C1	-2.18	104.74	110.05
23	A	854	BCR	C28-C27-C26	-2.18	110.18	114.08
26	B2	841	ECH	C23-C24-C25	-2.18	121.07	127.20
19	AA	834	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
23	L	205	BCR	C15-C14-C13	-2.18	124.19	127.31
19	A2	805	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	B	823	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
25	L1	210	LMG	C38-C37-C36	-2.18	103.34	114.42
19	B	803	CLA	CHD-C1D-ND	-2.18	122.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	845	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	L2	207	BCR	C11-C10-C9	-2.18	124.19	127.31
19	A1	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	AA	809	CLA	CAC-C3C-C4C	2.18	127.64	124.81
19	A2	819	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	BB	819	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	A1	817	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	BB	826	CLA	C16-C15-C13	-2.18	108.87	115.92
19	BB	815	CLA	CBA-CAA-C2A	2.18	120.30	113.86
19	BB	808	CLA	CHB-C4A-NA	2.18	127.53	124.51
28	B	856	DGD	C1D-C2D-C3D	-2.18	105.46	110.00
23	L	206	BCR	C8-C7-C6	-2.18	121.08	127.20
19	B2	835	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	J1	102	BCR	C8-C7-C6	-2.18	121.08	127.20
19	A1	815	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	A1	838	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	B	817	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
23	F	303	BCR	C38-C26-C25	-2.18	122.08	124.53
19	A	830	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
19	B2	810	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	J2	102	BCR	C35-C13-C14	-2.18	119.87	122.92
19	A2	836	CLA	O2D-CGD-CBD	2.18	115.14	111.27
23	A	848	BCR	C16-C15-C14	-2.18	119.01	123.47
19	BB	856	CLA	C4-C3-C5	2.18	118.93	115.27
19	A	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	B	805	CLA	C3A-C2A-C1A	2.18	104.60	101.34
19	B1	807	CLA	C1-O2A-CGA	2.18	122.16	116.44
19	A1	839	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
19	A	805	CLA	O2D-CGD-CBD	2.18	115.14	111.27
25	B2	854	LMG	C1-C2-C3	-2.18	105.46	110.00
19	B1	817	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
23	A	848	BCR	C8-C7-C6	-2.18	121.09	127.20
19	B2	836	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
19	B1	821	CLA	O2D-CGD-CBD	2.18	115.13	111.27
23	FF	303	BCR	C15-C14-C13	-2.17	124.21	127.31
26	B1	840	ECH	C8-C9-C10	2.17	122.28	118.94
19	X	101	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
23	M1	101	BCR	C27-C26-C25	2.17	125.89	122.73
23	B	843	BCR	C8-C7-C6	-2.17	121.10	127.20
23	AA	849	BCR	C8-C7-C6	-2.17	121.10	127.20
26	B2	841	ECH	C7-C6-C5	-2.17	116.20	121.46
19	B	846	CLA	CHD-C1D-ND	-2.17	122.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	803	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	BB	816	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	A2	814	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	B	837	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	AA	837	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	BB	831	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	B	832	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
25	II	105	LMG	O3-C3-C2	-2.17	105.33	110.35
23	B1	838	BCR	C27-C26-C25	2.17	125.88	122.73
19	B2	801	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	BB	826	CLA	C3A-C2A-C1A	2.17	104.59	101.34
19	B	860	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
19	L	203	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	A1	834	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	L1	210	LMG	O1-C1-C2	-2.17	104.92	108.30
19	B2	852	CLA	CBC-CAC-C3C	2.17	118.41	112.43
19	AA	835	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	AA	854	BCR	C38-C26-C25	-2.17	122.09	124.53
19	A	808	CLA	CED-O2D-CGD	2.17	120.84	115.94
19	B	826	CLA	C16-C15-C13	-2.17	108.91	115.92
19	A1	828	CLA	C4-C3-C2	-2.17	118.11	123.68
19	B1	816	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	A	834	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
19	A2	820	CLA	O2D-CGD-CBD	2.17	115.12	111.27
20	A2	803	CL0	CGD-CBD-CAD	-2.17	103.71	110.73
19	AA	825	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	B2	837	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	A2	814	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
19	AA	817	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
19	B1	832	CLA	CHA-C1A-NA	-2.17	121.44	126.40
25	B	851	LMG	O2-C2-C1	-2.17	104.78	110.05
19	KK	102	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
19	AA	816	CLA	C1-C2-C3	-2.17	123.25	126.75
19	A	809	CLA	CAC-C3C-C4C	2.17	127.62	124.81
26	B	841	ECH	C8-C9-C10	2.17	122.26	118.94
19	A1	824	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
19	B1	836	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
19	AA	817	CLA	CMB-C2B-C3B	2.17	128.73	124.68
26	B1	840	ECH	C7-C6-C5	-2.16	116.22	121.46
19	BB	823	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	L1	211	LHG	P-O6-C4	-2.16	108.99	121.68
23	B2	839	BCR	C27-C26-C25	2.16	125.87	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	I2	102	BCR	C33-C5-C6	-2.16	122.10	124.53
19	B1	810	CLA	C6-C5-C3	2.16	119.13	113.45
23	A1	847	BCR	C16-C15-C14	-2.16	119.05	123.47
22	A2	846	LHG	P-O6-C4	-2.16	109.00	121.68
26	B1	840	ECH	C33-C5-C4	2.16	117.77	113.62
19	BB	830	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
25	B	851	LMG	C38-C37-C36	-2.16	103.45	114.42
19	B2	815	CLA	CBA-CAA-C2A	2.16	120.24	113.86
23	AA	855	BCR	C15-C16-C17	-2.16	119.05	123.47
19	AA	842	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	BB	805	CLA	C3A-C2A-C1A	2.16	104.57	101.34
19	A2	805	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	B	842	BCR	C1-C6-C5	-2.16	119.57	122.61
23	AA	848	BCR	C38-C26-C25	-2.16	122.10	124.53
19	A	828	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	A2	848	BCR	C8-C7-C6	-2.16	121.14	127.20
19	A2	816	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	L	206	BCR	C16-C15-C14	-2.16	119.06	123.47
26	B2	841	ECH	C33-C5-C4	2.16	117.76	113.62
19	A	814	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
19	AA	815	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
19	BB	803	CLA	C11-C12-C13	-2.16	108.95	115.92
19	B1	808	CLA	CHB-C4A-NA	2.16	127.49	124.51
19	AA	805	CLA	CHB-C4A-NA	2.16	127.49	124.51
19	A1	842	CLA	C2D-C1D-ND	-2.16	108.52	110.10
19	A2	818	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
23	A1	850	BCR	C2-C1-C6	2.16	113.80	110.48
19	A	805	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	B	854	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	A2	833	CLA	CHB-C4A-NA	2.16	127.49	124.51
23	L	205	BCR	C8-C7-C6	-2.15	121.15	127.20
23	L1	201	BCR	C24-C23-C22	-2.15	122.98	126.23
19	A	842	CLA	O2A-C1-C2	-2.15	102.97	108.64
23	L1	208	BCR	C8-C7-C6	-2.15	121.15	127.20
19	B1	826	CLA	C3A-C2A-C1A	2.15	104.57	101.34
19	A1	835	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
19	B1	827	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
19	A1	810	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
19	B1	804	CLA	CBA-CAA-C2A	2.15	120.22	113.86
19	B2	837	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
23	A	847	BCR	C23-C24-C25	-2.15	123.37	126.28
19	B	813	CLA	C1B-CHB-C4A	-2.15	125.85	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	FF	302	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
22	L	207	LHG	P-O6-C4	-2.15	109.06	121.68
22	LL	205	LHG	P-O6-C4	-2.15	109.06	121.68
19	AA	826	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
28	B	856	DGD	O6E-C1E-O5D	-2.15	104.88	109.97
25	L1	210	LMG	O2-C2-C1	-2.15	104.82	110.05
19	AA	824	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
19	A2	805	CLA	O2D-CGD-CBD	2.15	115.09	111.27
19	A1	810	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	A1	811	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	A1	815	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	B	804	CLA	CBA-CAA-C2A	2.15	120.21	113.86
19	B2	807	CLA	C16-C15-C13	-2.15	108.97	115.92
23	A	847	BCR	C38-C26-C25	-2.15	122.11	124.53
19	AA	813	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	L1	205	CLA	C6-C5-C3	2.15	119.09	113.45
19	B2	804	CLA	CBA-CAA-C2A	2.15	120.21	113.86
19	B2	837	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
25	B1	844	LMG	O2-C2-C1	-2.15	104.83	110.05
23	A1	848	BCR	C8-C7-C6	-2.15	121.17	127.20
19	BB	856	CLA	O2A-CGA-CBA	2.15	118.65	111.91
23	LL	204	BCR	C11-C10-C9	-2.15	124.24	127.31
23	M1	101	BCR	C7-C8-C9	-2.15	122.99	126.23
19	B1	823	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	B	801	CLA	C6-C5-C3	2.15	119.09	113.45
23	A2	847	BCR	C21-C20-C19	-2.15	119.31	124.67
26	B	841	ECH	C23-C24-C25	-2.15	121.17	127.20
19	A1	810	CLA	C1-O2A-CGA	2.15	122.08	116.44
19	B1	821	CLA	C4-C3-C2	-2.15	118.17	123.68
19	B1	835	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	A2	815	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	J	103	CLA	CAC-C3C-C4C	2.15	127.59	124.81
19	AA	840	CLA	CMB-C2B-C1B	-2.15	125.17	128.46
23	K2	103	BCR	C8-C7-C6	-2.15	121.17	127.20
23	K2	103	BCR	C2-C1-C6	2.15	113.78	110.48
19	B1	815	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
19	B	815	CLA	C4-C3-C2	-2.15	118.17	123.68
19	J2	103	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	BB	825	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	A2	850	BCR	C2-C1-C6	2.15	113.78	110.48
19	B2	851	CLA	C2A-C1A-CHA	2.15	127.61	123.86
19	A	832	CLA	CMB-C2B-C3B	2.14	128.69	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	II	104	BCR	C8-C7-C6	-2.14	121.18	127.20
19	AA	833	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
19	K1	102	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
22	A1	846	LHG	P-O6-C4	-2.14	109.11	121.68
23	I	102	BCR	C24-C23-C22	-2.14	123.00	126.23
19	AA	824	CLA	CHD-C1D-ND	-2.14	122.48	124.45
23	B2	844	BCR	C15-C16-C17	-2.14	119.09	123.47
19	A	817	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
23	BB	838	BCR	C8-C7-C6	-2.14	121.19	127.20
19	AA	843	CLA	C3C-C4C-NC	-2.14	108.17	110.57
19	A1	814	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
19	F1	302	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
25	BB	844	LMG	O1-C1-C2	-2.14	104.96	108.30
19	BB	804	CLA	CBA-CAA-C2A	2.14	120.18	113.86
28	BB	854	DGD	O3E-C3E-C2E	-2.14	105.40	110.35
23	L	205	BCR	C11-C10-C9	-2.14	124.26	127.31
19	BB	817	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
23	B1	843	BCR	C15-C16-C17	-2.14	119.09	123.47
19	BB	828	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
19	B1	833	CLA	C4-C3-C2	-2.14	118.19	123.68
19	B2	804	CLA	CHD-C1D-ND	-2.14	122.49	124.45
19	J2	101	CLA	CHD-C1D-ND	-2.14	122.49	124.45
25	BB	844	LMG	O2-C2-C1	-2.14	104.85	110.05
23	AA	848	BCR	C21-C20-C19	-2.14	119.33	124.67
19	A	801	CLA	O1D-CGD-CBD	2.14	128.86	124.48
19	B	801	CLA	CBA-CAA-C2A	2.14	120.17	113.86
23	A2	849	BCR	C38-C26-C25	-2.14	122.13	124.53
23	M2	102	BCR	C27-C26-C25	2.14	125.83	122.73
23	AA	854	BCR	C11-C10-C9	-2.14	124.26	127.31
19	F2	302	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
23	A1	851	BCR	C8-C7-C6	-2.14	121.20	127.20
22	AA	847	LHG	P-O6-C4	-2.14	109.16	121.68
19	FF	301	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
19	B	828	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	FF	304	BCR	C8-C7-C6	-2.13	121.21	127.20
19	B2	813	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
19	B	837	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
26	B	841	ECH	C23-C22-C21	-2.13	115.67	118.94
23	A	849	BCR	C38-C26-C25	-2.13	122.13	124.53
19	B2	808	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
19	A2	831	CLA	C2D-C1D-ND	-2.13	108.53	110.10
25	I2	105	LMG	C1-C2-C3	-2.13	105.55	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B2	845	LMG	O2-C2-C1	-2.13	104.86	110.05
19	B	823	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	AA	850	BCR	C3-C4-C5	-2.13	110.27	114.08
19	BB	829	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	BB	841	BCR	C1-C6-C5	-2.13	119.61	122.61
19	B1	836	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
19	A	833	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
19	BB	855	CLA	CHB-C4A-NA	2.13	127.46	124.51
19	A2	801	CLA	CMB-C2B-C3B	2.13	128.67	124.68
19	K	101	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
23	I2	102	BCR	C37-C22-C21	-2.13	119.94	122.92
19	B1	813	CLA	O2D-CGD-CBD	2.13	115.05	111.27
19	BB	829	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	B	839	BCR	C35-C13-C14	-2.13	119.94	122.92
19	B1	829	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	BB	836	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	AA	850	BCR	C38-C26-C25	-2.13	122.14	124.53
19	A	820	CLA	C2D-C1D-ND	-2.13	108.53	110.10
19	B	812	CLA	O1D-CGD-CBD	2.13	128.84	124.48
22	A	846	LHG	P-O6-C4	-2.13	109.20	121.68
19	B2	830	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	BB	831	CLA	O2D-CGD-CBD	2.13	115.05	111.27
19	A1	819	CLA	C2D-C1D-ND	-2.13	108.54	110.10
19	A2	826	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
19	L	204	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	B1	815	CLA	CBA-CAA-C2A	2.13	120.14	113.86
19	B2	846	CLA	CAC-C3C-C4C	2.13	127.57	124.81
19	BB	819	CLA	CMA-C3A-C2A	-2.13	111.13	116.10
19	A1	822	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	A1	819	CLA	C1-C2-C3	-2.13	122.37	126.04
23	A	849	BCR	C16-C15-C14	-2.13	119.12	123.47
19	B	834	CLA	C1D-ND-C4D	-2.13	104.83	106.33
19	F1	305	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
19	B1	807	CLA	C2D-C1D-ND	-2.13	108.54	110.10
23	A1	849	BCR	C15-C16-C17	-2.13	119.12	123.47
19	A	821	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
23	K1	104	BCR	C8-C7-C6	-2.12	121.24	127.20
19	BB	833	CLA	C1D-ND-C4D	-2.12	104.83	106.33
23	A2	851	BCR	C16-C15-C14	-2.12	119.12	123.47
19	AA	805	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
19	AA	830	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
23	K1	106	BCR	C20-C21-C22	-2.12	124.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	842	BCR	C8-C7-C6	-2.12	121.24	127.20
19	B1	836	CLA	CMB-C2B-C3B	2.12	128.65	124.68
19	A1	813	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
19	A1	820	CLA	C6-C5-C3	2.12	119.02	113.45
19	B2	805	CLA	C3A-C2A-C1A	2.12	104.52	101.34
23	A2	847	BCR	C16-C15-C14	-2.12	119.12	123.47
23	B	844	BCR	C38-C26-C25	-2.12	122.14	124.53
19	A2	832	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	AA	848	BCR	C15-C14-C13	-2.12	124.28	127.31
23	B2	839	BCR	C38-C26-C25	-2.12	122.14	124.53
23	K2	105	BCR	C35-C13-C14	-2.12	119.95	122.92
19	K2	102	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
19	A	826	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
19	B2	807	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
19	AA	818	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
19	KK	101	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
28	B	856	DGD	O3E-C3E-C2E	-2.12	105.45	110.35
22	B	853	LHG	O7-C7-C8	2.12	116.07	111.50
19	AA	811	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
23	A	850	BCR	C27-C26-C25	2.12	125.81	122.73
19	AA	823	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	BB	838	BCR	C11-C10-C9	-2.12	124.28	127.31
21	B	838	PQN	C26-C25-C23	-2.12	109.07	115.92
25	BB	844	LMG	C40-C39-C38	-2.12	103.67	114.42
19	B	828	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
19	A2	824	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	A1	853	BCR	C8-C7-C6	-2.12	121.25	127.20
23	A1	847	BCR	C21-C20-C19	-2.12	119.38	124.67
19	BB	802	CLA	C4-C3-C5	2.12	118.83	115.27
25	B	845	LMG	O2-C2-C1	-2.12	104.90	110.05
19	B1	805	CLA	C3A-C2A-C1A	2.12	104.51	101.34
19	L2	204	CLA	C6-C5-C3	2.12	119.01	113.45
19	B2	816	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	A	834	CLA	CHD-C1D-ND	-2.12	122.51	124.45
20	A2	803	CL0	C9-C8-C7	2.12	118.96	111.29
23	I2	101	BCR	C16-C17-C18	-2.12	124.29	127.31
19	B1	849	CLA	CHB-C4A-NA	2.12	127.44	124.51
19	B2	852	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
19	A2	824	CLA	O2A-CGA-O1A	-2.12	118.03	123.30
19	AA	822	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
23	AA	854	BCR	C7-C8-C9	-2.12	123.04	126.23
23	L1	208	BCR	C37-C22-C21	-2.11	119.96	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	837	CLA	CHB-C4A-NA	2.11	127.44	124.51
19	B2	835	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
19	AA	808	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
25	B2	854	LMG	O2-C2-C1	-2.11	104.91	110.05
23	A	848	BCR	C27-C26-C25	2.11	125.80	122.73
19	A1	823	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
19	B1	845	CLA	CHD-C1D-ND	-2.11	122.51	124.45
19	A2	852	CLA	CHD-C1D-ND	-2.11	122.51	124.45
19	KK	102	CLA	CHD-C1D-ND	-2.11	122.51	124.45
19	BB	826	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	F	302	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
23	A2	853	BCR	C8-C7-C6	-2.11	121.28	127.20
19	B2	846	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	BB	815	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	A1	848	BCR	C27-C26-C25	2.11	125.79	122.73
19	BB	816	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	A1	829	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	J1	102	BCR	C2-C1-C6	2.11	113.73	110.48
19	B	836	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	AA	838	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	AA	839	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	B1	838	BCR	C38-C26-C25	-2.11	122.16	124.53
23	L1	208	BCR	C15-C14-C13	-2.11	124.30	127.31
19	A1	844	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	L	202	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	A	847	BCR	C21-C20-C19	-2.11	119.41	124.67
23	F	303	BCR	C15-C14-C13	-2.11	124.30	127.31
28	BB	854	DGD	C3G-C2G-C1G	-2.11	106.81	111.79
23	AA	849	BCR	C16-C15-C14	-2.11	119.16	123.47
19	B1	808	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
19	B2	825	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	B	859	CLA	C4-C3-C5	2.11	118.81	115.27
19	B	819	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
23	L1	209	BCR	C24-C23-C22	-2.11	123.05	126.23
19	B	858	CLA	CHB-C4A-NA	2.11	127.42	124.51
23	AA	849	BCR	C27-C26-C25	2.10	125.79	122.73
19	A2	812	CLA	CMB-C2B-C3B	2.10	128.62	124.68
19	K	102	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
23	B2	844	BCR	C38-C26-C25	-2.10	122.17	124.53
19	A	839	CLA	O2D-CGD-CBD	2.10	115.01	111.27
19	L	202	CLA	C2D-C1D-ND	-2.10	108.55	110.10
19	B1	850	CLA	O2A-CGA-CBA	2.10	118.51	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A2	803	CL0	O2A-C1-C2	2.10	114.16	108.64
19	B	812	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
23	B	839	BCR	C8-C7-C6	-2.10	121.30	127.20
19	B	831	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	A1	804	CLA	O2D-CGD-CBD	2.10	115.00	111.27
19	B1	815	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	A2	842	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	A2	805	CLA	C5-C3-C2	2.10	125.37	121.12
23	AA	852	BCR	C33-C5-C6	-2.10	122.17	124.53
19	BB	820	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
19	B1	810	CLA	CAC-C3C-C4C	2.10	127.53	124.81
19	AA	814	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
25	B1	852	LMG	O2-C2-C1	-2.10	104.94	110.05
19	BB	813	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	A	807	CLA	C1-C2-C3	-2.10	122.41	126.04
23	A2	849	BCR	C11-C10-C9	-2.10	124.31	127.31
19	B1	819	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	A2	837	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	B	818	CLA	CMB-C2B-C3B	2.10	128.60	124.68
23	F2	304	BCR	C37-C22-C21	-2.10	119.98	122.92
23	A	851	BCR	C8-C7-C6	-2.10	121.31	127.20
19	B2	814	CLA	C2D-C1D-ND	-2.10	108.56	110.10
23	B	839	BCR	C15-C14-C13	-2.10	124.32	127.31
19	A2	839	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	B2	828	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	LL	201	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	B1	833	CLA	C1D-ND-C4D	-2.10	104.84	106.33
19	AA	822	CLA	CMB-C2B-C3B	2.10	128.60	124.68
19	A	808	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	B1	825	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	A2	822	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	A2	839	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	AA	834	CLA	CMB-C2B-C3B	2.10	128.60	124.68
19	B1	829	CLA	CHB-C4A-NA	2.10	127.41	124.51
19	B	825	CLA	C1-O2A-CGA	2.10	121.94	116.44
19	BB	852	CLA	CMB-C2B-C3B	2.10	128.60	124.68
19	A	818	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
19	B	834	CLA	C6-C7-C8	-2.10	109.14	115.92
19	B1	814	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	A	825	CLA	CMB-C2B-C3B	2.10	128.60	124.68
22	L1	211	LHG	O7-C7-C8	2.10	116.02	111.50
19	B	817	CLA	O2D-CGD-CBD	2.10	114.99	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	834	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
19	B1	835	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	A	825	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
19	A2	852	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
19	A2	808	CLA	O1D-CGD-CBD	2.09	128.77	124.48
19	A1	831	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	BB	822	CLA	O2D-CGD-CBD	2.09	114.99	111.27
26	B1	840	ECH	C23-C24-C25	-2.09	121.33	127.20
28	BB	854	DGD	O6E-C5E-C4E	2.09	113.49	109.69
19	B2	833	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
23	A	849	BCR	C24-C23-C22	-2.09	123.07	126.23
19	B	835	CLA	O2D-CGD-CBD	2.09	114.98	111.27
19	BB	810	CLA	CAC-C3C-C4C	2.09	127.52	124.81
19	A2	808	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
23	M	101	BCR	C16-C15-C14	-2.09	119.19	123.47
22	B1	847	LHG	P-O6-C4	-2.09	109.42	121.68
19	A1	804	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	B	808	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	BB	803	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
23	AA	851	BCR	C27-C26-C25	2.09	125.77	122.73
19	B2	837	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	B1	802	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	B	822	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	AA	825	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	B	860	CLA	C3C-C4C-NC	-2.09	108.23	110.57
25	M	102	LMG	O2-C2-C1	-2.09	104.97	110.05
19	AA	820	CLA	C1-C2-C3	-2.09	122.43	126.04
23	A	853	BCR	C8-C7-C6	-2.09	121.33	127.20
20	A	803	CL0	C9-C8-C10	2.09	118.86	111.29
19	A	807	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	J1	103	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	B	827	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	BB	818	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
23	A	853	BCR	C7-C8-C9	-2.09	123.08	126.23
19	B	801	CLA	C5-C3-C2	2.09	125.34	121.12
19	A1	825	CLA	CHD-C1D-ND	-2.09	122.54	124.45
19	K	102	CLA	CHD-C1D-ND	-2.09	122.54	124.45
19	A1	825	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
22	BB	851	LHG	P-O6-C4	-2.09	109.45	121.68
19	B	859	CLA	O2A-CGA-CBA	2.08	118.45	111.91
23	II	101	BCR	C27-C26-C25	2.08	125.76	122.73
23	L	206	BCR	C24-C23-C22	-2.08	123.09	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M	101	BCR	C11-C10-C9	-2.08	124.34	127.31
19	A2	834	CLA	CAA-C2A-C3A	-2.08	111.23	116.10
19	B2	814	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	BB	821	CLA	C4-C3-C2	-2.08	118.33	123.68
23	AA	848	BCR	C16-C15-C14	-2.08	119.21	123.47
19	BB	827	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
19	B1	819	CLA	CMA-C3A-C2A	-2.08	111.24	116.10
19	A1	842	CLA	C3C-C4C-NC	-2.08	108.24	110.57
19	B1	802	CLA	C4-C3-C5	2.08	118.77	115.27
19	A1	834	CLA	C11-C10-C8	-2.08	109.19	115.92
19	B2	825	CLA	C1-O2A-CGA	2.08	121.91	116.44
19	BB	819	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
19	A	820	CLA	CBA-CAA-C2A	2.08	120.00	113.86
19	AA	831	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	B	839	BCR	C11-C10-C9	-2.08	124.34	127.31
19	A	838	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	AA	839	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
19	A	839	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
26	B	841	ECH	C35-C13-C14	2.08	125.83	122.92
19	B	808	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
19	A1	827	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	A1	830	CLA	C2D-C1D-ND	-2.08	108.57	110.10
19	A	811	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
19	A	816	CLA	CHD-C1D-ND	-2.08	122.55	124.45
19	K1	105	CLA	C2A-C1A-CHA	2.08	125.93	122.71
19	B1	827	CLA	CBA-CAA-C2A	2.08	119.99	113.86
19	A	839	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	B2	807	CLA	C2D-C1D-ND	-2.07	108.58	110.10
19	A	824	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
23	A	853	BCR	C11-C10-C9	-2.07	124.35	127.31
19	B1	836	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	B2	808	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	A	849	BCR	C15-C16-C17	-2.07	119.23	123.47
19	L2	205	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	BB	820	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	A2	848	BCR	C27-C26-C25	2.07	125.74	122.73
19	B1	807	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
19	LL	203	CLA	CHC-C1C-NC	2.07	127.35	124.20
19	B2	812	CLA	O1D-CGD-CBD	2.07	128.72	124.48
19	A2	812	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
19	AA	808	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	L1	201	BCR	C8-C7-C6	-2.07	121.38	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	FF	306	BCR	C27-C26-C25	2.07	125.74	122.73
25	B	845	LMG	O1-C7-C8	-2.07	105.90	110.90
19	B	815	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	B	825	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	I2	103	BCR	C8-C7-C6	-2.07	121.39	127.20
19	B2	823	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
23	AA	854	BCR	C8-C7-C6	-2.07	121.39	127.20
19	AA	841	CLA	O2D-CGD-CBD	2.07	114.94	111.27
19	B	820	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
20	AA	803	CL0	CHD-C1D-ND	-2.07	122.55	124.45
23	F	304	BCR	C8-C7-C6	-2.07	121.39	127.20
19	BB	821	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
23	AA	850	BCR	C24-C23-C22	-2.07	123.11	126.23
19	AA	825	CLA	CMB-C2B-C3B	2.07	128.55	124.68
23	A1	849	BCR	C11-C10-C9	-2.07	124.36	127.31
23	AA	850	BCR	C16-C15-C14	-2.07	119.24	123.47
23	FF	306	BCR	C20-C21-C22	-2.07	124.36	127.31
19	A	852	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	X2	103	LHG	O7-C7-C8	2.07	115.95	111.50
20	A	803	CL0	CGD-CBD-CAD	-2.07	104.05	110.73
19	A1	830	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
19	BB	833	CLA	C6-C7-C8	-2.06	109.25	115.92
25	B2	845	LMG	C40-C39-C38	-2.06	103.94	114.42
19	B	827	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	B	831	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	A	851	BCR	C38-C26-C25	-2.06	122.21	124.53
19	K1	105	CLA	CAC-C3C-C4C	2.06	127.49	124.81
23	B1	841	BCR	C36-C18-C19	2.06	121.33	118.08
23	J2	104	BCR	C2-C3-C4	2.06	115.99	111.38
19	A	809	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	A	832	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	B	826	CLA	C3A-C2A-C1A	2.06	104.43	101.34
19	F1	302	CLA	CAA-C2A-C3A	-2.06	109.11	114.26
19	B1	825	CLA	C2D-C1D-ND	-2.06	108.58	110.10
23	MM	101	BCR	C16-C15-C14	-2.06	119.25	123.47
19	B2	809	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
23	L2	207	BCR	C15-C14-C13	-2.06	124.37	127.31
19	A1	821	CLA	O2D-CGD-CBD	2.06	114.93	111.27
19	B2	826	CLA	C3A-C2A-C1A	2.06	104.43	101.34
19	A2	828	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	B	833	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
20	A	803	CL0	C4C-C3C-C2C	-2.06	103.89	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	828	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
25	B1	846	LMG	C1-C2-C3	-2.06	105.70	110.00
19	B1	821	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	A	832	CLA	C1-C2-C3	-2.06	122.48	126.04
19	B1	809	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
23	K	103	BCR	C27-C26-C25	2.06	125.72	122.73
19	AA	832	CLA	C1-C2-C3	-2.06	122.48	126.04
19	B	801	CLA	C2A-C1A-CHA	2.06	127.46	123.86
19	A	808	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
19	B2	821	CLA	CBA-CAA-C2A	2.06	119.94	113.86
23	A2	849	BCR	C16-C15-C14	-2.06	119.26	123.47
23	KK	103	BCR	C27-C26-C25	2.06	125.72	122.73
19	BB	818	CLA	CMB-C2B-C3B	2.06	128.52	124.68
23	M	101	BCR	C7-C8-C9	-2.05	123.13	126.23
19	L2	206	CLA	CHB-C4A-NA	2.05	127.35	124.51
19	A1	833	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	A2	816	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	B	851	LMG	C40-C39-C38	-2.05	104.00	114.42
19	A1	821	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	B1	816	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	B1	807	CLA	CHA-C4D-ND	2.05	136.79	132.50
23	M2	102	BCR	C38-C26-C25	-2.05	122.22	124.53
23	A1	850	BCR	C27-C26-C25	2.05	125.71	122.73
19	B	826	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	A1	830	CLA	CAC-C3C-C4C	2.05	127.47	124.81
19	B1	808	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	A2	822	CLA	O2D-CGD-CBD	2.05	114.91	111.27
19	B2	813	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	A	828	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	A2	835	CLA	C11-C10-C8	-2.05	109.29	115.92
19	A2	827	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	A2	831	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	B1	816	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	A2	811	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	II	102	BCR	C24-C23-C22	-2.05	123.14	126.23
23	A1	851	BCR	C37-C22-C21	-2.05	120.05	122.92
19	AA	810	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
19	AA	821	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
19	A1	808	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	B	841	ECH	C10-C11-C12	-2.05	116.83	123.22
19	A	814	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	J	101	CLA	CHD-C1D-ND	-2.05	122.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K2	104	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
23	A	849	BCR	C35-C13-C12	2.05	121.30	118.08
19	B	803	CLA	C11-C12-C13	-2.05	109.30	115.92
23	L1	209	BCR	C34-C9-C10	-2.05	120.06	122.92
19	L1	205	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	A2	830	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	B	839	BCR	C24-C23-C22	-2.05	123.14	126.23
19	L2	204	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	A2	833	CLA	O2D-CGD-CBD	2.05	114.90	111.27
19	B	815	CLA	O2D-CGD-CBD	2.05	114.90	111.27
23	A1	850	BCR	C24-C23-C22	-2.04	123.14	126.23
23	M	101	BCR	C38-C26-C25	-2.04	122.23	124.53
19	A1	821	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	A	854	BCR	C8-C7-C6	-2.04	121.46	127.20
23	B	848	BCR	C7-C8-C9	-2.04	123.15	126.23
19	BB	814	CLA	C4-C3-C5	-2.04	111.83	115.27
26	B2	841	ECH	C10-C11-C12	-2.04	116.84	123.22
19	AA	840	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
19	AA	853	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
19	B1	833	CLA	C6-C7-C8	-2.04	109.32	115.92
19	A2	834	CLA	CMA-C3A-C2A	-2.04	111.33	116.10
25	B2	845	LMG	C1-C2-C3	-2.04	105.74	110.00
19	A1	841	CLA	CMB-C2B-C3B	2.04	128.50	124.68
23	AA	854	BCR	C35-C13-C14	-2.04	120.06	122.92
19	A2	835	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	AA	828	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	JJ	101	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	B2	808	CLA	CMB-C2B-C3B	2.04	128.50	124.68
25	B1	844	LMG	O1-C1-C2	-2.04	105.12	108.30
23	A	849	BCR	C3-C4-C5	-2.04	110.43	114.08
23	A2	849	BCR	C8-C7-C6	-2.04	121.47	127.20
23	A2	850	BCR	C27-C26-C25	2.04	125.69	122.73
19	B2	813	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	M2	102	BCR	C35-C13-C12	2.04	121.29	118.08
19	B2	834	CLA	CBA-CAA-C2A	2.04	119.88	113.86
21	AA	844	PQN	C2M-C2-C3	-2.04	121.07	124.40
19	A2	833	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	J2	104	BCR	C8-C7-C6	-2.04	121.48	127.20
23	M1	101	BCR	C38-C26-C25	-2.04	122.24	124.53
19	A2	832	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
19	AA	805	CLA	C4-C3-C2	-2.04	118.45	123.68
22	L	207	LHG	O7-C7-C8	2.04	115.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	822	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	K2	104	CLA	CHA-C1A-NA	-2.04	121.73	126.40
25	II	105	LMG	C38-C37-C36	-2.04	104.09	114.42
19	BB	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	BB	828	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	BB	814	CLA	C2D-C1D-ND	-2.04	108.60	110.10
26	B1	840	ECH	C10-C11-C12	-2.04	116.87	123.22
19	B2	851	CLA	O2D-CGD-CBD	2.03	114.88	111.27
19	A1	826	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
19	A1	833	CLA	CAA-C2A-C3A	-2.03	111.35	116.10
19	BB	825	CLA	C2D-C1D-ND	-2.03	108.61	110.10
23	K1	106	BCR	C8-C7-C6	-2.03	121.49	127.20
23	A2	850	BCR	C24-C23-C22	-2.03	123.16	126.23
23	J	102	BCR	C11-C10-C9	-2.03	124.41	127.31
19	B2	807	CLA	CHA-C4D-ND	2.03	136.75	132.50
26	B	841	ECH	C39-C30-C25	-2.03	107.00	110.30
19	A1	829	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
19	F1	301	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	AA	855	BCR	C29-C30-C25	2.03	113.61	110.48
19	BB	806	CLA	C1-C2-C3	2.03	129.56	126.04
19	BB	818	CLA	C2D-C1D-ND	-2.03	108.61	110.10
23	B2	842	BCR	C24-C23-C22	-2.03	123.17	126.23
22	LL	205	LHG	O7-C7-C8	2.03	115.88	111.50
19	AA	830	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
19	B	804	CLA	O2D-CGD-CBD	2.03	114.88	111.27
19	B	814	CLA	O2D-CGD-CBD	2.03	114.88	111.27
23	AA	854	BCR	C36-C18-C17	-2.03	120.08	122.92
19	B2	850	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	AA	840	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	A	847	BCR	C16-C15-C14	-2.03	119.32	123.47
23	B1	842	BCR	C8-C7-C6	-2.03	121.50	127.20
19	AA	821	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
23	BB	843	BCR	C24-C23-C22	-2.03	123.17	126.23
23	J2	104	BCR	C16-C15-C14	-2.03	119.32	123.47
19	B1	812	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	B2	827	CLA	CBA-CAA-C2A	2.03	119.85	113.86
19	B1	832	CLA	CAA-C2A-C1A	2.03	118.62	111.97
23	A1	849	BCR	C16-C15-C14	-2.03	119.32	123.47
23	J2	104	BCR	C35-C13-C14	-2.03	120.08	122.92
25	B2	845	LMG	C42-C41-C40	-2.03	104.14	114.42
25	M	102	LMG	O6-C1-O1	-2.03	105.18	109.97
19	BB	809	CLA	O2A-CGA-O1A	-2.03	118.25	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	829	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	F	305	BCR	C35-C13-C12	2.03	121.27	118.08
19	F2	301	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	A1	837	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	A	823	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	B1	832	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
19	A1	852	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
20	A2	803	CL0	CHD-C4C-C3C	-2.02	121.86	124.84
19	B	834	CLA	C1-O2A-CGA	2.02	121.75	116.44
19	AA	839	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
19	AA	853	CLA	CHB-C4A-NA	2.02	127.31	124.51
19	A2	807	CLA	C1-C2-C3	-2.02	122.54	126.04
23	J	104	BCR	C16-C15-C14	-2.02	119.33	123.47
23	K2	105	BCR	C8-C7-C6	-2.02	121.52	127.20
19	B1	833	CLA	C1-O2A-CGA	2.02	121.75	116.44
19	BB	815	CLA	C4-C3-C2	-2.02	118.49	123.68
19	BB	802	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	L1	205	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	A	808	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	JJ	104	BCR	C16-C15-C14	-2.02	119.33	123.47
19	B2	834	CLA	C1-O2A-CGA	2.02	121.75	116.44
19	JJ	103	CLA	CAC-C3C-C4C	2.02	127.43	124.81
19	B1	849	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	A1	801	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
19	B1	822	CLA	O2D-CGD-CBD	2.02	114.86	111.27
23	A	853	BCR	C36-C18-C17	-2.02	120.09	122.92
19	A2	809	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	B2	801	CLA	C4-C3-C2	-2.02	118.50	123.68
19	AA	814	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	AA	853	CLA	CMB-C2B-C3B	2.02	128.45	124.68
19	A1	838	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	A1	826	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	B1	838	BCR	C8-C7-C6	-2.02	121.54	127.20
23	B1	838	BCR	C11-C10-C9	-2.02	124.43	127.31
23	A	854	BCR	C15-C14-C13	-2.02	124.43	127.31
23	BB	838	BCR	C20-C21-C22	-2.02	124.43	127.31
19	B	809	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
19	B1	834	CLA	CED-O2D-CGD	2.02	120.50	115.94
23	A	847	BCR	C35-C13-C14	-2.02	120.10	122.92
19	L	204	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
23	KK	103	BCR	C35-C13-C12	2.02	121.25	118.08
23	B2	843	BCR	C8-C7-C6	-2.02	121.54	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	855	BCR	C8-C7-C6	-2.02	121.54	127.20
19	A	836	CLA	CMB-C2B-C3B	2.01	128.45	124.68
19	A2	819	CLA	C4-C3-C2	-2.01	118.51	123.68
23	A2	851	BCR	C33-C5-C6	-2.01	122.27	124.53
19	A	840	CLA	CHD-C1D-ND	-2.01	122.60	124.45
19	AA	845	CLA	CHD-C1D-ND	-2.01	122.60	124.45
19	J2	103	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
19	B2	851	CLA	O2A-CGA-CBA	2.01	118.23	111.91
19	F	301	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
19	AA	811	CLA	CAC-C3C-C4C	2.01	127.42	124.81
19	BB	814	CLA	O2D-CGD-CBD	2.01	114.84	111.27
19	B	806	CLA	C1-O2A-CGA	2.01	121.72	116.44
23	B2	839	BCR	C8-C7-C6	-2.01	121.55	127.20
25	I2	105	LMG	O2-C2-C1	-2.01	105.16	110.05
19	B1	803	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	AA	827	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	AA	851	BCR	C2-C1-C6	2.01	113.58	110.48
23	AA	854	BCR	C30-C25-C26	-2.01	119.78	122.61
19	A	834	CLA	CMA-C3A-C2A	-2.01	111.40	116.10
19	BB	804	CLA	O2D-CGD-CBD	2.01	114.84	111.27
23	AA	852	BCR	C8-C7-C6	-2.01	121.55	127.20
19	L	204	CLA	C5-C3-C2	2.01	125.19	121.12
19	A1	820	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	B2	839	BCR	C11-C10-C9	-2.01	124.44	127.31
23	A1	849	BCR	C8-C7-C6	-2.01	121.56	127.20
19	BB	829	CLA	CBC-CAC-C3C	2.01	117.97	112.43
19	B	810	CLA	CAC-C3C-C4C	2.01	127.42	124.81
19	A1	807	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	I	102	BCR	C38-C26-C25	-2.01	122.27	124.53
19	B2	831	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	JJ	103	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	A	804	CLA	C4-C3-C5	2.01	118.65	115.27
19	AA	842	CLA	O2A-C1-C2	-2.01	103.36	108.64
19	A	806	CLA	CAA-C2A-C3A	2.01	118.27	112.78
19	B	802	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
19	A	842	CLA	C1-O2A-CGA	2.01	121.71	116.44
23	AA	850	BCR	C35-C13-C12	2.01	121.24	118.08
19	BB	814	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	B	843	BCR	C38-C26-C25	-2.01	122.28	124.53
19	B	819	CLA	CMA-C3A-C2A	-2.00	111.42	116.10
19	A1	806	CLA	C1-C2-C3	-2.00	122.58	126.04
23	A	848	BCR	C24-C23-C22	-2.00	123.21	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	819	CLA	CHD-C1D-ND	-2.00	122.61	124.45
19	A	832	CLA	C3A-C2A-C1A	2.00	104.34	101.34
19	A1	832	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	AA	821	CLA	CAC-C3C-C4C	2.00	127.41	124.81
19	B	830	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
19	AA	801	CLA	CMB-C2B-C3B	2.00	128.43	124.68
19	B2	823	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	B2	834	CLA	C3B-C4B-NB	-2.00	106.62	109.21
23	J	102	BCR	C2-C3-C4	2.00	115.85	111.38
19	BB	833	CLA	CHA-C4D-ND	2.00	136.68	132.50
25	II	105	LMG	O7-C10-O9	-2.00	118.87	123.70
19	J2	103	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (385) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A1	801	CLA	ND
19	A1	803	CLA	ND
19	A1	804	CLA	ND
19	A1	806	CLA	ND
19	A1	807	CLA	ND
19	A1	808	CLA	ND
19	A1	809	CLA	ND
19	A1	810	CLA	ND
19	A1	811	CLA	ND
19	A1	812	CLA	ND
19	A1	813	CLA	ND
19	A1	814	CLA	ND
19	A1	815	CLA	ND
19	A1	816	CLA	ND
19	A1	817	CLA	ND
19	A1	818	CLA	ND
19	A1	820	CLA	ND
19	A1	821	CLA	ND
19	A1	822	CLA	ND
19	A1	823	CLA	ND
19	A1	824	CLA	ND
19	A1	825	CLA	ND
19	A1	826	CLA	ND
19	A1	827	CLA	ND
19	A1	828	CLA	ND
19	A1	829	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A1	830	CLA	ND
19	A1	831	CLA	ND
19	A1	832	CLA	ND
19	A1	833	CLA	ND
19	A1	834	CLA	ND
19	A1	835	CLA	ND
19	A1	836	CLA	ND
19	A1	837	CLA	ND
19	A1	838	CLA	ND
19	A1	839	CLA	ND
19	A1	840	CLA	ND
19	A1	841	CLA	ND
19	A1	842	CLA	ND
19	A1	844	CLA	ND
19	A1	852	CLA	ND
19	B1	801	CLA	ND
19	B1	802	CLA	ND
19	B1	803	CLA	ND
19	B1	804	CLA	ND
19	B1	805	CLA	ND
19	B1	806	CLA	ND
19	B1	807	CLA	ND
19	B1	808	CLA	ND
19	B1	809	CLA	ND
19	B1	810	CLA	ND
19	B1	811	CLA	ND
19	B1	812	CLA	ND
19	B1	813	CLA	ND
19	B1	814	CLA	ND
19	B1	815	CLA	ND
19	B1	816	CLA	ND
19	B1	817	CLA	ND
19	B1	818	CLA	ND
19	B1	819	CLA	ND
19	B1	820	CLA	ND
19	B1	821	CLA	ND
19	B1	822	CLA	ND
19	B1	823	CLA	ND
19	B1	824	CLA	ND
19	B1	825	CLA	ND
19	B1	826	CLA	ND
19	B1	827	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B1	828	CLA	ND
19	B1	829	CLA	ND
19	B1	830	CLA	ND
19	B1	831	CLA	ND
19	B1	832	CLA	ND
19	B1	833	CLA	ND
19	B1	834	CLA	ND
19	B1	835	CLA	ND
19	B1	836	CLA	ND
19	B1	845	CLA	ND
19	B1	848	CLA	ND
19	B1	849	CLA	ND
19	B1	850	CLA	ND
19	F1	301	CLA	ND
19	F1	302	CLA	ND
19	F1	305	CLA	ND
19	J1	101	CLA	ND
19	J1	103	CLA	ND
19	K1	102	CLA	ND
19	K1	103	CLA	ND
19	K1	105	CLA	ND
19	L1	205	CLA	ND
19	L1	206	CLA	ND
19	L1	207	CLA	ND
19	X1	101	CLA	ND
19	A2	801	CLA	ND
19	A2	802	CLA	ND
19	A2	804	CLA	ND
19	A2	805	CLA	ND
19	A2	806	CLA	ND
19	A2	807	CLA	ND
19	A2	808	CLA	ND
19	A2	809	CLA	ND
19	A2	810	CLA	ND
19	A2	811	CLA	ND
19	A2	812	CLA	ND
19	A2	813	CLA	ND
19	A2	814	CLA	ND
19	A2	815	CLA	ND
19	A2	816	CLA	ND
19	A2	817	CLA	ND
19	A2	818	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A2	819	CLA	ND
19	A2	820	CLA	ND
19	A2	821	CLA	ND
19	A2	822	CLA	ND
19	A2	823	CLA	ND
19	A2	824	CLA	ND
19	A2	825	CLA	ND
19	A2	826	CLA	ND
19	A2	827	CLA	ND
19	A2	828	CLA	ND
19	A2	829	CLA	ND
19	A2	830	CLA	ND
19	A2	831	CLA	ND
19	A2	832	CLA	ND
19	A2	833	CLA	ND
19	A2	834	CLA	ND
19	A2	835	CLA	ND
19	A2	837	CLA	ND
19	A2	838	CLA	ND
19	A2	839	CLA	ND
19	A2	840	CLA	ND
19	A2	841	CLA	ND
19	A2	842	CLA	ND
19	A2	844	CLA	ND
19	A2	852	CLA	ND
19	B2	801	CLA	ND
19	B2	802	CLA	ND
19	B2	803	CLA	ND
19	B2	804	CLA	ND
19	B2	805	CLA	ND
19	B2	806	CLA	ND
19	B2	807	CLA	ND
19	B2	808	CLA	ND
19	B2	809	CLA	ND
19	B2	810	CLA	ND
19	B2	811	CLA	ND
19	B2	812	CLA	ND
19	B2	813	CLA	ND
19	B2	814	CLA	ND
19	B2	815	CLA	ND
19	B2	816	CLA	ND
19	B2	817	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B2	818	CLA	ND
19	B2	819	CLA	ND
19	B2	820	CLA	ND
19	B2	821	CLA	ND
19	B2	822	CLA	ND
19	B2	823	CLA	ND
19	B2	824	CLA	ND
19	B2	825	CLA	ND
19	B2	826	CLA	ND
19	B2	827	CLA	ND
19	B2	828	CLA	ND
19	B2	829	CLA	ND
19	B2	830	CLA	ND
19	B2	831	CLA	ND
19	B2	832	CLA	ND
19	B2	834	CLA	ND
19	B2	835	CLA	ND
19	B2	836	CLA	ND
19	B2	837	CLA	ND
19	B2	846	CLA	ND
19	B2	849	CLA	ND
19	B2	850	CLA	ND
19	B2	851	CLA	ND
19	B2	852	CLA	ND
19	F2	301	CLA	ND
19	F2	302	CLA	ND
19	J2	101	CLA	ND
19	J2	103	CLA	ND
19	K2	102	CLA	ND
19	K2	104	CLA	ND
19	L2	204	CLA	ND
19	L2	205	CLA	ND
19	L2	206	CLA	ND
19	X2	101	CLA	ND
19	A	801	CLA	ND
19	A	804	CLA	ND
19	A	805	CLA	ND
19	A	806	CLA	ND
19	A	807	CLA	ND
19	A	808	CLA	ND
19	A	809	CLA	ND
19	A	810	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	811	CLA	ND
19	A	812	CLA	ND
19	A	813	CLA	ND
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND
19	A	817	CLA	ND
19	A	818	CLA	ND
19	A	819	CLA	ND
19	A	821	CLA	ND
19	A	822	CLA	ND
19	A	823	CLA	ND
19	A	824	CLA	ND
19	A	825	CLA	ND
19	A	826	CLA	ND
19	A	827	CLA	ND
19	A	828	CLA	ND
19	A	829	CLA	ND
19	A	830	CLA	ND
19	A	831	CLA	ND
19	A	832	CLA	ND
19	A	833	CLA	ND
19	A	834	CLA	ND
19	A	835	CLA	ND
19	A	836	CLA	ND
19	A	837	CLA	ND
19	A	838	CLA	ND
19	A	839	CLA	ND
19	A	840	CLA	ND
19	A	841	CLA	ND
19	A	842	CLA	ND
19	A	844	CLA	ND
19	A	852	CLA	ND
19	B	801	CLA	ND
19	B	802	CLA	ND
19	B	803	CLA	ND
19	B	804	CLA	ND
19	B	805	CLA	ND
19	B	806	CLA	ND
19	B	807	CLA	ND
19	B	808	CLA	ND
19	B	809	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	810	CLA	ND
19	B	811	CLA	ND
19	B	812	CLA	ND
19	B	813	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND
19	B	816	CLA	ND
19	B	817	CLA	ND
19	B	818	CLA	ND
19	B	819	CLA	ND
19	B	820	CLA	ND
19	B	821	CLA	ND
19	B	822	CLA	ND
19	B	823	CLA	ND
19	B	824	CLA	ND
19	B	825	CLA	ND
19	B	826	CLA	ND
19	B	827	CLA	ND
19	B	828	CLA	ND
19	B	829	CLA	ND
19	B	830	CLA	ND
19	B	831	CLA	ND
19	B	832	CLA	ND
19	B	834	CLA	ND
19	B	835	CLA	ND
19	B	836	CLA	ND
19	B	837	CLA	ND
19	B	846	CLA	ND
19	B	854	CLA	ND
19	B	858	CLA	ND
19	B	859	CLA	ND
19	B	860	CLA	ND
19	F	301	CLA	ND
19	F	302	CLA	ND
19	J	101	CLA	ND
19	K	101	CLA	ND
19	K	102	CLA	ND
19	L	202	CLA	ND
19	L	203	CLA	ND
19	L	204	CLA	ND
19	X	101	CLA	ND
19	AA	801	CLA	ND

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Mol	Chain	Res	Type	Atom
19	AA	804	CLA	ND
19	AA	805	CLA	ND
19	AA	806	CLA	ND
19	AA	807	CLA	ND
19	AA	808	CLA	ND
19	AA	809	CLA	ND
19	AA	810	CLA	ND
19	AA	811	CLA	ND
19	AA	812	CLA	ND
19	AA	813	CLA	ND
19	AA	814	CLA	ND
19	AA	815	CLA	ND
19	AA	816	CLA	ND
19	AA	817	CLA	ND
19	AA	818	CLA	ND
19	AA	819	CLA	ND
19	AA	820	CLA	ND
19	AA	821	CLA	ND
19	AA	823	CLA	ND
19	AA	824	CLA	ND
19	AA	825	CLA	ND
19	AA	826	CLA	ND
19	AA	827	CLA	ND
19	AA	828	CLA	ND
19	AA	829	CLA	ND
19	AA	830	CLA	ND
19	AA	831	CLA	ND
19	AA	832	CLA	ND
19	AA	833	CLA	ND
19	AA	834	CLA	ND
19	AA	835	CLA	ND
19	AA	836	CLA	ND
19	AA	837	CLA	ND
19	AA	838	CLA	ND
19	AA	839	CLA	ND
19	AA	840	CLA	ND
19	AA	841	CLA	ND
19	AA	842	CLA	ND
19	AA	843	CLA	ND
19	AA	845	CLA	ND
19	AA	853	CLA	ND
19	BB	801	CLA	ND

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Mol	Chain	Res	Type	Atom
19	BB	802	CLA	ND
19	BB	803	CLA	ND
19	BB	804	CLA	ND
19	BB	805	CLA	ND
19	BB	806	CLA	ND
19	BB	807	CLA	ND
19	BB	808	CLA	ND
19	BB	809	CLA	ND
19	BB	810	CLA	ND
19	BB	811	CLA	ND
19	BB	812	CLA	ND
19	BB	813	CLA	ND
19	BB	814	CLA	ND
19	BB	815	CLA	ND
19	BB	816	CLA	ND
19	BB	817	CLA	ND
19	BB	818	CLA	ND
19	BB	819	CLA	ND
19	BB	820	CLA	ND
19	BB	821	CLA	ND
19	BB	822	CLA	ND
19	BB	823	CLA	ND
19	BB	824	CLA	ND
19	BB	825	CLA	ND
19	BB	826	CLA	ND
19	BB	827	CLA	ND
19	BB	828	CLA	ND
19	BB	829	CLA	ND
19	BB	830	CLA	ND
19	BB	831	CLA	ND
19	BB	833	CLA	ND
19	BB	834	CLA	ND
19	BB	835	CLA	ND
19	BB	836	CLA	ND
19	BB	845	CLA	ND
19	BB	852	CLA	ND
19	BB	855	CLA	ND
19	BB	856	CLA	ND
19	FF	301	CLA	ND
19	FF	302	CLA	ND
19	FF	305	CLA	ND
19	JJ	101	CLA	ND

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Mol	Chain	Res	Type	Atom
19	JJ	103	CLA	ND
19	KK	101	CLA	ND
19	KK	102	CLA	ND
19	LL	201	CLA	ND
19	LL	202	CLA	ND
19	LL	203	CLA	ND
19	XX	101	CLA	ND
20	A1	802	CL0	NC
20	A1	802	CL0	ND
20	A1	802	CL0	NA
20	A1	802	CL0	C8
20	A2	803	CL0	NC
20	A2	803	CL0	ND
20	A2	803	CL0	NA
20	A2	803	CL0	C8
20	A	803	CL0	NC
20	A	803	CL0	ND
20	A	803	CL0	NA
20	A	803	CL0	C8
20	AA	803	CL0	NC
20	AA	803	CL0	ND
20	AA	803	CL0	NA
20	AA	803	CL0	C8

All (5830) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A1	803	CLA	CBD-CGD-O2D-CED
19	A1	804	CLA	C1A-C2A-CAA-CBA
19	A1	804	CLA	C3A-C2A-CAA-CBA
19	A1	804	CLA	CHA-CBD-CGD-O1D
19	A1	804	CLA	CHA-CBD-CGD-O2D
19	A1	805	CLA	C1A-C2A-CAA-CBA
19	A1	805	CLA	C3A-C2A-CAA-CBA
19	A1	806	CLA	C1A-C2A-CAA-CBA
19	A1	806	CLA	C3A-C2A-CAA-CBA
19	A1	806	CLA	CHA-CBD-CGD-O1D
19	A1	806	CLA	CHA-CBD-CGD-O2D
19	A1	806	CLA	CAD-CBD-CGD-O1D
19	A1	807	CLA	O1A-CGA-O2A-C1
19	A1	809	CLA	C3A-C2A-CAA-CBA
19	A1	809	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A1	809	CLA	C4-C3-C5-C6
19	A1	810	CLA	CBD-CGD-O2D-CED
19	A1	810	CLA	C2-C3-C5-C6
19	A1	810	CLA	C4-C3-C5-C6
19	A1	811	CLA	C1A-C2A-CAA-CBA
19	A1	811	CLA	C3A-C2A-CAA-CBA
19	A1	811	CLA	CBD-CGD-O2D-CED
19	A1	813	CLA	C1A-C2A-CAA-CBA
19	A1	814	CLA	CHA-CBD-CGD-O1D
19	A1	814	CLA	CHA-CBD-CGD-O2D
19	A1	815	CLA	C1A-C2A-CAA-CBA
19	A1	815	CLA	C3A-C2A-CAA-CBA
19	A1	815	CLA	CBD-CGD-O2D-CED
19	A1	819	CLA	C3A-C2A-CAA-CBA
19	A1	820	CLA	C1A-C2A-CAA-CBA
19	A1	820	CLA	C3A-C2A-CAA-CBA
19	A1	822	CLA	CBD-CGD-O2D-CED
19	A1	823	CLA	CHA-CBD-CGD-O1D
19	A1	823	CLA	CHA-CBD-CGD-O2D
19	A1	824	CLA	C1A-C2A-CAA-CBA
19	A1	825	CLA	C1A-C2A-CAA-CBA
19	A1	825	CLA	C3A-C2A-CAA-CBA
19	A1	825	CLA	CHA-CBD-CGD-O1D
19	A1	825	CLA	CHA-CBD-CGD-O2D
19	A1	827	CLA	C1A-C2A-CAA-CBA
19	A1	828	CLA	C1A-C2A-CAA-CBA
19	A1	828	CLA	C3A-C2A-CAA-CBA
19	A1	828	CLA	CHA-CBD-CGD-O1D
19	A1	828	CLA	CHA-CBD-CGD-O2D
19	A1	828	CLA	C11-C10-C8-C9
19	A1	833	CLA	CHA-CBD-CGD-O1D
19	A1	833	CLA	CHA-CBD-CGD-O2D
19	A1	833	CLA	CBD-CGD-O2D-CED
19	A1	836	CLA	CHA-CBD-CGD-O1D
19	A1	836	CLA	CHA-CBD-CGD-O2D
19	A1	840	CLA	CHA-CBD-CGD-O1D
19	A1	840	CLA	CHA-CBD-CGD-O2D
19	A1	841	CLA	C4-C3-C5-C6
19	A1	842	CLA	C2C-C3C-CAC-CBC
19	A1	842	CLA	C4C-C3C-CAC-CBC
19	A1	844	CLA	CBD-CGD-O2D-CED
19	A1	852	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A1	852	CLA	CHA-CBD-CGD-O1D
19	A1	852	CLA	CHA-CBD-CGD-O2D
19	A1	852	CLA	CAD-CBD-CGD-O1D
19	B1	802	CLA	CHA-CBD-CGD-O1D
19	B1	802	CLA	CHA-CBD-CGD-O2D
19	B1	803	CLA	CHA-CBD-CGD-O1D
19	B1	803	CLA	CHA-CBD-CGD-O2D
19	B1	804	CLA	CHA-CBD-CGD-O1D
19	B1	804	CLA	CHA-CBD-CGD-O2D
19	B1	806	CLA	CHA-CBD-CGD-O1D
19	B1	806	CLA	CHA-CBD-CGD-O2D
19	B1	807	CLA	C6-C7-C8-C9
19	B1	809	CLA	CHA-CBD-CGD-O1D
19	B1	809	CLA	CHA-CBD-CGD-O2D
19	B1	809	CLA	CAD-CBD-CGD-O1D
19	B1	810	CLA	CHA-CBD-CGD-O1D
19	B1	810	CLA	CHA-CBD-CGD-O2D
19	B1	811	CLA	CHA-CBD-CGD-O1D
19	B1	811	CLA	CHA-CBD-CGD-O2D
19	B1	812	CLA	CAD-CBD-CGD-O1D
19	B1	812	CLA	CAD-CBD-CGD-O2D
19	B1	813	CLA	C1A-C2A-CAA-CBA
19	B1	813	CLA	CHA-CBD-CGD-O1D
19	B1	813	CLA	CHA-CBD-CGD-O2D
19	B1	814	CLA	CHA-CBD-CGD-O1D
19	B1	814	CLA	CHA-CBD-CGD-O2D
19	B1	815	CLA	C3A-C2A-CAA-CBA
19	B1	815	CLA	C14-C13-C15-C16
19	B1	818	CLA	CHA-CBD-CGD-O1D
19	B1	818	CLA	CHA-CBD-CGD-O2D
19	B1	821	CLA	CHA-CBD-CGD-O1D
19	B1	821	CLA	CHA-CBD-CGD-O2D
19	B1	823	CLA	CHA-CBD-CGD-O1D
19	B1	823	CLA	CHA-CBD-CGD-O2D
19	B1	824	CLA	C1A-C2A-CAA-CBA
19	B1	824	CLA	C3A-C2A-CAA-CBA
19	B1	824	CLA	CHA-CBD-CGD-O1D
19	B1	824	CLA	CHA-CBD-CGD-O2D
19	B1	824	CLA	CBD-CGD-O2D-CED
19	B1	825	CLA	CHA-CBD-CGD-O1D
19	B1	825	CLA	CHA-CBD-CGD-O2D
19	B1	825	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B1	827	CLA	C3A-C2A-CAA-CBA
19	B1	827	CLA	CBD-CGD-O2D-CED
19	B1	830	CLA	CHA-CBD-CGD-O1D
19	B1	830	CLA	CHA-CBD-CGD-O2D
19	B1	831	CLA	C1A-C2A-CAA-CBA
19	B1	831	CLA	C3A-C2A-CAA-CBA
19	B1	832	CLA	CBD-CGD-O2D-CED
19	B1	833	CLA	C1A-C2A-CAA-CBA
19	B1	835	CLA	C6-C7-C8-C9
19	B1	848	CLA	CHA-CBD-CGD-O1D
19	B1	848	CLA	CBD-CGD-O2D-CED
19	F1	301	CLA	C1A-C2A-CAA-CBA
19	F1	302	CLA	C1A-C2A-CAA-CBA
19	F1	302	CLA	C3A-C2A-CAA-CBA
19	F1	302	CLA	CBD-CGD-O2D-CED
19	K1	103	CLA	C1A-C2A-CAA-CBA
19	K1	103	CLA	C3A-C2A-CAA-CBA
19	K1	103	CLA	CBA-CGA-O2A-C1
19	K1	105	CLA	CHA-CBD-CGD-O1D
19	K1	105	CLA	CHA-CBD-CGD-O2D
19	K1	105	CLA	CBD-CGD-O2D-CED
19	L1	207	CLA	CHA-CBD-CGD-O1D
19	L1	207	CLA	CHA-CBD-CGD-O2D
19	A2	802	CLA	C1A-C2A-CAA-CBA
19	A2	802	CLA	C3A-C2A-CAA-CBA
19	A2	802	CLA	CBA-CGA-O2A-C1
19	A2	802	CLA	CHA-CBD-CGD-O1D
19	A2	802	CLA	CHA-CBD-CGD-O2D
19	A2	802	CLA	CAD-CBD-CGD-O1D
19	A2	804	CLA	CBD-CGD-O2D-CED
19	A2	805	CLA	C1A-C2A-CAA-CBA
19	A2	805	CLA	C3A-C2A-CAA-CBA
19	A2	805	CLA	CHA-CBD-CGD-O1D
19	A2	805	CLA	CHA-CBD-CGD-O2D
19	A2	806	CLA	C1A-C2A-CAA-CBA
19	A2	806	CLA	CHA-CBD-CGD-O1D
19	A2	806	CLA	CHA-CBD-CGD-O2D
19	A2	806	CLA	CAD-CBD-CGD-O1D
19	A2	807	CLA	C1A-C2A-CAA-CBA
19	A2	807	CLA	C3A-C2A-CAA-CBA
19	A2	807	CLA	CHA-CBD-CGD-O1D
19	A2	807	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A2	807	CLA	CAD-CBD-CGD-O1D
19	A2	810	CLA	C2-C3-C5-C6
19	A2	810	CLA	C4-C3-C5-C6
19	A2	811	CLA	C3A-C2A-CAA-CBA
19	A2	811	CLA	C2-C3-C5-C6
19	A2	811	CLA	C4-C3-C5-C6
19	A2	812	CLA	C1A-C2A-CAA-CBA
19	A2	812	CLA	C3A-C2A-CAA-CBA
19	A2	812	CLA	CBD-CGD-O2D-CED
19	A2	814	CLA	C1A-C2A-CAA-CBA
19	A2	815	CLA	CHA-CBD-CGD-O1D
19	A2	815	CLA	CHA-CBD-CGD-O2D
19	A2	816	CLA	C1A-C2A-CAA-CBA
19	A2	816	CLA	C3A-C2A-CAA-CBA
19	A2	820	CLA	C3A-C2A-CAA-CBA
19	A2	821	CLA	C1A-C2A-CAA-CBA
19	A2	821	CLA	C3A-C2A-CAA-CBA
19	A2	823	CLA	CBD-CGD-O2D-CED
19	A2	824	CLA	CHA-CBD-CGD-O1D
19	A2	824	CLA	CHA-CBD-CGD-O2D
19	A2	825	CLA	CBD-CGD-O2D-CED
19	A2	826	CLA	C1A-C2A-CAA-CBA
19	A2	826	CLA	CHA-CBD-CGD-O1D
19	A2	826	CLA	CHA-CBD-CGD-O2D
19	A2	828	CLA	C1A-C2A-CAA-CBA
19	A2	828	CLA	CBD-CGD-O2D-CED
19	A2	829	CLA	C1A-C2A-CAA-CBA
19	A2	829	CLA	C3A-C2A-CAA-CBA
19	A2	829	CLA	C2A-CAA-CBA-CGA
19	A2	829	CLA	CHA-CBD-CGD-O1D
19	A2	829	CLA	CHA-CBD-CGD-O2D
19	A2	831	CLA	CHA-CBD-CGD-O1D
19	A2	831	CLA	CHA-CBD-CGD-O2D
19	A2	834	CLA	CHA-CBD-CGD-O1D
19	A2	834	CLA	CHA-CBD-CGD-O2D
19	A2	834	CLA	CBD-CGD-O2D-CED
19	A2	835	CLA	CBD-CGD-O2D-CED
19	A2	841	CLA	CHA-CBD-CGD-O1D
19	A2	841	CLA	CHA-CBD-CGD-O2D
19	A2	842	CLA	C4-C3-C5-C6
19	A2	844	CLA	CBD-CGD-O2D-CED
19	B2	802	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B2	802	CLA	CHA-CBD-CGD-O2D
19	B2	802	CLA	CAD-CBD-CGD-O1D
19	B2	803	CLA	CHA-CBD-CGD-O1D
19	B2	804	CLA	CHA-CBD-CGD-O1D
19	B2	804	CLA	CHA-CBD-CGD-O2D
19	B2	806	CLA	CHA-CBD-CGD-O1D
19	B2	806	CLA	CHA-CBD-CGD-O2D
19	B2	806	CLA	CBD-CGD-O2D-CED
19	B2	809	CLA	CHA-CBD-CGD-O1D
19	B2	809	CLA	CHA-CBD-CGD-O2D
19	B2	809	CLA	CAD-CBD-CGD-O1D
19	B2	810	CLA	CHA-CBD-CGD-O1D
19	B2	810	CLA	CHA-CBD-CGD-O2D
19	B2	810	CLA	CBD-CGD-O2D-CED
19	B2	811	CLA	CHA-CBD-CGD-O1D
19	B2	811	CLA	CHA-CBD-CGD-O2D
19	B2	811	CLA	CAD-CBD-CGD-O1D
19	B2	812	CLA	CAD-CBD-CGD-O1D
19	B2	812	CLA	CAD-CBD-CGD-O2D
19	B2	813	CLA	C1A-C2A-CAA-CBA
19	B2	814	CLA	CHA-CBD-CGD-O1D
19	B2	814	CLA	CHA-CBD-CGD-O2D
19	B2	815	CLA	C3A-C2A-CAA-CBA
19	B2	815	CLA	C14-C13-C15-C16
19	B2	816	CLA	CBD-CGD-O2D-CED
19	B2	818	CLA	CHA-CBD-CGD-O1D
19	B2	818	CLA	CHA-CBD-CGD-O2D
19	B2	820	CLA	C2C-C3C-CAC-CBC
19	B2	820	CLA	C4C-C3C-CAC-CBC
19	B2	821	CLA	C1A-C2A-CAA-CBA
19	B2	821	CLA	C3A-C2A-CAA-CBA
19	B2	823	CLA	CHA-CBD-CGD-O1D
19	B2	823	CLA	CHA-CBD-CGD-O2D
19	B2	823	CLA	C6-C7-C8-C9
19	B2	824	CLA	C1A-C2A-CAA-CBA
19	B2	824	CLA	C3A-C2A-CAA-CBA
19	B2	824	CLA	CHA-CBD-CGD-O1D
19	B2	824	CLA	CHA-CBD-CGD-O2D
19	B2	825	CLA	CHA-CBD-CGD-O1D
19	B2	825	CLA	CHA-CBD-CGD-O2D
19	B2	825	CLA	CAD-CBD-CGD-O1D
19	B2	826	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B2	826	CLA	C4-C3-C5-C6
19	B2	827	CLA	C3A-C2A-CAA-CBA
19	B2	831	CLA	CHA-CBD-CGD-O1D
19	B2	831	CLA	CHA-CBD-CGD-O2D
19	B2	831	CLA	CAD-CBD-CGD-O1D
19	B2	831	CLA	CAD-CBD-CGD-O2D
19	B2	832	CLA	C1A-C2A-CAA-CBA
19	B2	832	CLA	C3A-C2A-CAA-CBA
19	B2	833	CLA	CHA-CBD-CGD-O2D
19	B2	834	CLA	C1A-C2A-CAA-CBA
19	B2	849	CLA	CHA-CBD-CGD-O1D
19	B2	849	CLA	CHA-CBD-CGD-O2D
19	B2	849	CLA	CBD-CGD-O2D-CED
19	B2	849	CLA	C2-C3-C5-C6
19	B2	849	CLA	C4-C3-C5-C6
19	B2	851	CLA	CBD-CGD-O2D-CED
19	B2	852	CLA	C2C-C3C-CAC-CBC
19	B2	852	CLA	C4C-C3C-CAC-CBC
19	F2	301	CLA	C1A-C2A-CAA-CBA
19	F2	301	CLA	CHA-CBD-CGD-O1D
19	F2	301	CLA	CHA-CBD-CGD-O2D
19	F2	302	CLA	C1A-C2A-CAA-CBA
19	F2	302	CLA	C3A-C2A-CAA-CBA
19	F2	302	CLA	CBD-CGD-O2D-CED
19	K2	104	CLA	C3A-C2A-CAA-CBA
19	L2	206	CLA	CHA-CBD-CGD-O1D
19	L2	206	CLA	CHA-CBD-CGD-O2D
19	L2	206	CLA	CBD-CGD-O2D-CED
19	A	805	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	CAD-CBD-CGD-O1D
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	807	CLA	CHA-CBD-CGD-O1D
19	A	807	CLA	CHA-CBD-CGD-O2D
19	A	808	CLA	O1A-CGA-O2A-C1
19	A	811	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	C2-C3-C5-C6
19	A	811	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	O1D-CGD-O2D-CED
19	A	814	CLA	C1A-C2A-CAA-CBA
19	A	815	CLA	CHA-CBD-CGD-O1D
19	A	815	CLA	CHA-CBD-CGD-O2D
19	A	816	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C3A-C2A-CAA-CBA
19	A	816	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	CHA-CBD-CGD-O1D
19	A	822	CLA	CHA-CBD-CGD-O2D
19	A	823	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CHA-CBD-CGD-O1D
19	A	824	CLA	CHA-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O1D
19	A	826	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	CBD-CGD-O2D-CED
19	A	829	CLA	CHA-CBD-CGD-O1D
19	A	829	CLA	CHA-CBD-CGD-O2D
19	A	830	CLA	CBD-CGD-O2D-CED
19	A	831	CLA	CHA-CBD-CGD-O1D
19	A	831	CLA	CHA-CBD-CGD-O2D
19	A	834	CLA	CHA-CBD-CGD-O1D
19	A	834	CLA	CHA-CBD-CGD-O2D
19	A	835	CLA	CBD-CGD-O2D-CED
19	A	839	CLA	CHA-CBD-CGD-O1D
19	A	839	CLA	CHA-CBD-CGD-O2D
19	A	841	CLA	CHA-CBD-CGD-O1D
19	A	841	CLA	CHA-CBD-CGD-O2D
19	A	844	CLA	CAD-CBD-CGD-O1D
19	A	852	CLA	C2A-CAA-CBA-CGA
19	B	801	CLA	CBD-CGD-O2D-CED
19	B	802	CLA	C1A-C2A-CAA-CBA
19	B	803	CLA	CHA-CBD-CGD-O1D
19	B	803	CLA	CBD-CGD-O2D-CED
19	B	804	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	CHA-CBD-CGD-O2D
19	B	806	CLA	CHA-CBD-CGD-O1D
19	B	806	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	O1A-CGA-O2A-C1
19	B	809	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	CAD-CBD-CGD-O1D
19	B	810	CLA	CHA-CBD-CGD-O1D
19	B	810	CLA	CHA-CBD-CGD-O2D
19	B	810	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	CHA-CBD-CGD-O1D
19	B	811	CLA	CHA-CBD-CGD-O2D
19	B	811	CLA	CAD-CBD-CGD-O1D
19	B	812	CLA	CAD-CBD-CGD-O1D
19	B	812	CLA	CAD-CBD-CGD-O2D
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	815	CLA	C3A-C2A-CAA-CBA
19	B	815	CLA	CHA-CBD-CGD-O1D
19	B	815	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	C14-C13-C15-C16
19	B	816	CLA	C4-C3-C5-C6
19	B	818	CLA	CHA-CBD-CGD-O1D
19	B	818	CLA	CHA-CBD-CGD-O2D
19	B	820	CLA	C2C-C3C-CAC-CBC
19	B	820	CLA	C4C-C3C-CAC-CBC
19	B	820	CLA	CHA-CBD-CGD-O1D
19	B	820	CLA	CHA-CBD-CGD-O2D
19	B	823	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	823	CLA	C6-C7-C8-C9
19	B	824	CLA	CHA-CBD-CGD-O1D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	CHA-CBD-CGD-O1D
19	B	825	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O1D
19	B	826	CLA	C4-C3-C5-C6
19	B	827	CLA	C3A-C2A-CAA-CBA
19	B	827	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	831	CLA	CHA-CBD-CGD-O1D
19	B	831	CLA	CHA-CBD-CGD-O2D
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C4-C3-C5-C6
19	B	854	CLA	CHA-CBD-CGD-O1D
19	B	854	CLA	CHA-CBD-CGD-O2D
19	B	854	CLA	C2-C3-C5-C6
19	B	854	CLA	C4-C3-C5-C6
19	B	860	CLA	C2C-C3C-CAC-CBC
19	B	860	CLA	C4C-C3C-CAC-CBC
19	F	301	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C3A-C2A-CAA-CBA
19	F	302	CLA	CBD-CGD-O2D-CED
19	J	103	CLA	CHA-CBD-CGD-O1D
19	J	103	CLA	CHA-CBD-CGD-O2D
19	K	102	CLA	C1A-C2A-CAA-CBA
19	K	102	CLA	C3A-C2A-CAA-CBA
19	K	102	CLA	CBA-CGA-O2A-C1
19	K	102	CLA	O1A-CGA-O2A-C1
19	K	102	CLA	CHA-CBD-CGD-O1D
19	K	102	CLA	CHA-CBD-CGD-O2D
19	K	102	CLA	CAD-CBD-CGD-O1D
19	L	202	CLA	CHA-CBD-CGD-O1D
19	L	202	CLA	CHA-CBD-CGD-O2D
19	L	202	CLA	CAD-CBD-CGD-O1D
19	L	202	CLA	CAD-CBD-CGD-O2D
19	L	203	CLA	C1A-C2A-CAA-CBA
19	L	203	CLA	C3A-C2A-CAA-CBA
19	L	204	CLA	CHA-CBD-CGD-O1D
19	L	204	CLA	CHA-CBD-CGD-O2D
19	L	204	CLA	CBD-CGD-O2D-CED
19	AA	804	CLA	CBD-CGD-O2D-CED
19	AA	805	CLA	C3A-C2A-CAA-CBA
19	AA	805	CLA	CHA-CBD-CGD-O1D
19	AA	805	CLA	CHA-CBD-CGD-O2D
19	AA	806	CLA	C1A-C2A-CAA-CBA
19	AA	806	CLA	C3A-C2A-CAA-CBA
19	AA	806	CLA	CHA-CBD-CGD-O1D
19	AA	806	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	AA	807	CLA	C1A-C2A-CAA-CBA
19	AA	807	CLA	C3A-C2A-CAA-CBA
19	AA	807	CLA	CHA-CBD-CGD-O1D
19	AA	807	CLA	CHA-CBD-CGD-O2D
19	AA	807	CLA	CAD-CBD-CGD-O1D
19	AA	808	CLA	C1A-C2A-CAA-CBA
19	AA	811	CLA	CBD-CGD-O2D-CED
19	AA	811	CLA	C2-C3-C5-C6
19	AA	811	CLA	C4-C3-C5-C6
19	AA	812	CLA	C1A-C2A-CAA-CBA
19	AA	812	CLA	C3A-C2A-CAA-CBA
19	AA	812	CLA	CBD-CGD-O2D-CED
19	AA	814	CLA	C1A-C2A-CAA-CBA
19	AA	815	CLA	CHA-CBD-CGD-O1D
19	AA	815	CLA	CHA-CBD-CGD-O2D
19	AA	816	CLA	C1A-C2A-CAA-CBA
19	AA	816	CLA	C3A-C2A-CAA-CBA
19	AA	816	CLA	CBD-CGD-O2D-CED
19	AA	820	CLA	C3A-C2A-CAA-CBA
19	AA	821	CLA	C1A-C2A-CAA-CBA
19	AA	821	CLA	C3A-C2A-CAA-CBA
19	AA	824	CLA	C1A-C2A-CAA-CBA
19	AA	824	CLA	C3A-C2A-CAA-CBA
19	AA	824	CLA	CHA-CBD-CGD-O1D
19	AA	824	CLA	CHA-CBD-CGD-O2D
19	AA	824	CLA	CAD-CBD-CGD-O1D
19	AA	826	CLA	C1A-C2A-CAA-CBA
19	AA	826	CLA	C3A-C2A-CAA-CBA
19	AA	826	CLA	CHA-CBD-CGD-O1D
19	AA	826	CLA	CHA-CBD-CGD-O2D
19	AA	828	CLA	C1A-C2A-CAA-CBA
19	AA	828	CLA	CBD-CGD-O2D-CED
19	AA	829	CLA	C1A-C2A-CAA-CBA
19	AA	829	CLA	C3A-C2A-CAA-CBA
19	AA	829	CLA	CHA-CBD-CGD-O1D
19	AA	829	CLA	CHA-CBD-CGD-O2D
19	AA	830	CLA	CHA-CBD-CGD-O1D
19	AA	830	CLA	CHA-CBD-CGD-O2D
19	AA	830	CLA	CBD-CGD-O2D-CED
19	AA	831	CLA	CHA-CBD-CGD-O1D
19	AA	831	CLA	CHA-CBD-CGD-O2D
19	AA	834	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	AA	834	CLA	CHA-CBD-CGD-O2D
19	AA	835	CLA	CBD-CGD-O2D-CED
19	AA	839	CLA	CHA-CBD-CGD-O2D
19	AA	841	CLA	CHA-CBD-CGD-O1D
19	AA	841	CLA	CHA-CBD-CGD-O2D
19	AA	843	CLA	C2C-C3C-CAC-CBC
19	AA	843	CLA	C4C-C3C-CAC-CBC
19	AA	845	CLA	CBD-CGD-O2D-CED
19	AA	853	CLA	C1A-C2A-CAA-CBA
19	AA	853	CLA	C2A-CAA-CBA-CGA
19	BB	801	CLA	C1A-C2A-CAA-CBA
19	BB	802	CLA	CHA-CBD-CGD-O1D
19	BB	802	CLA	CHA-CBD-CGD-O2D
19	BB	802	CLA	CAD-CBD-CGD-O1D
19	BB	803	CLA	CHA-CBD-CGD-O1D
19	BB	803	CLA	CHA-CBD-CGD-O2D
19	BB	803	CLA	CBD-CGD-O2D-CED
19	BB	804	CLA	CHA-CBD-CGD-O1D
19	BB	804	CLA	CHA-CBD-CGD-O2D
19	BB	805	CLA	CHA-CBD-CGD-O2D
19	BB	806	CLA	CHA-CBD-CGD-O1D
19	BB	806	CLA	CHA-CBD-CGD-O2D
19	BB	806	CLA	CBD-CGD-O2D-CED
19	BB	809	CLA	CHA-CBD-CGD-O1D
19	BB	809	CLA	CHA-CBD-CGD-O2D
19	BB	809	CLA	CAD-CBD-CGD-O1D
19	BB	809	CLA	CAD-CBD-CGD-O2D
19	BB	810	CLA	CHA-CBD-CGD-O1D
19	BB	810	CLA	CHA-CBD-CGD-O2D
19	BB	810	CLA	CBD-CGD-O2D-CED
19	BB	811	CLA	CHA-CBD-CGD-O1D
19	BB	811	CLA	CHA-CBD-CGD-O2D
19	BB	811	CLA	CAD-CBD-CGD-O1D
19	BB	812	CLA	CHA-CBD-CGD-O1D
19	BB	812	CLA	CHA-CBD-CGD-O2D
19	BB	812	CLA	CAD-CBD-CGD-O1D
19	BB	813	CLA	C1A-C2A-CAA-CBA
19	BB	813	CLA	CHA-CBD-CGD-O1D
19	BB	813	CLA	CHA-CBD-CGD-O2D
19	BB	815	CLA	C1A-C2A-CAA-CBA
19	BB	815	CLA	C3A-C2A-CAA-CBA
19	BB	815	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	BB	815	CLA	CHA-CBD-CGD-O2D
19	BB	818	CLA	CHA-CBD-CGD-O1D
19	BB	818	CLA	CHA-CBD-CGD-O2D
19	BB	820	CLA	C2C-C3C-CAC-CBC
19	BB	820	CLA	C4C-C3C-CAC-CBC
19	BB	820	CLA	CAD-CBD-CGD-O2D
19	BB	821	CLA	CHA-CBD-CGD-O2D
19	BB	823	CLA	CHA-CBD-CGD-O1D
19	BB	823	CLA	CHA-CBD-CGD-O2D
19	BB	824	CLA	CHA-CBD-CGD-O1D
19	BB	824	CLA	CHA-CBD-CGD-O2D
19	BB	825	CLA	CHA-CBD-CGD-O1D
19	BB	825	CLA	CHA-CBD-CGD-O2D
19	BB	825	CLA	CAD-CBD-CGD-O1D
19	BB	826	CLA	CHA-CBD-CGD-O2D
19	BB	826	CLA	C2-C3-C5-C6
19	BB	826	CLA	C4-C3-C5-C6
19	BB	827	CLA	C3A-C2A-CAA-CBA
19	BB	830	CLA	CHA-CBD-CGD-O1D
19	BB	830	CLA	CHA-CBD-CGD-O2D
19	BB	832	CLA	CBD-CGD-O2D-CED
19	BB	833	CLA	C1A-C2A-CAA-CBA
19	BB	836	CLA	C2C-C3C-CAC-CBC
19	BB	836	CLA	C4C-C3C-CAC-CBC
19	BB	852	CLA	CBD-CGD-O2D-CED
19	BB	852	CLA	C4-C3-C5-C6
19	BB	855	CLA	CHA-CBD-CGD-O1D
19	BB	855	CLA	CHA-CBD-CGD-O2D
19	FF	301	CLA	CHA-CBD-CGD-O1D
19	FF	301	CLA	CHA-CBD-CGD-O2D
19	FF	302	CLA	C1A-C2A-CAA-CBA
19	FF	302	CLA	C3A-C2A-CAA-CBA
19	FF	302	CLA	CBD-CGD-O2D-CED
19	KK	102	CLA	C1A-C2A-CAA-CBA
19	KK	102	CLA	C3A-C2A-CAA-CBA
19	KK	102	CLA	CBA-CGA-O2A-C1
19	KK	102	CLA	CHA-CBD-CGD-O1D
19	KK	102	CLA	CHA-CBD-CGD-O2D
19	LL	203	CLA	C1A-C2A-CAA-CBA
19	LL	203	CLA	C3A-C2A-CAA-CBA
20	A1	802	CL0	C2-C1-O2A-CGA
20	A1	802	CL0	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A1	802	CL0	C4-C3-C5-C6
20	A2	803	CL0	C6-C7-C8-C9
20	A	803	CL0	C1A-C2A-CAA-CBA
20	A	803	CL0	C2-C1-O2A-CGA
20	AA	803	CL0	C2A-CAA-CBA-CGA
20	AA	803	CL0	C2-C1-O2A-CGA
21	A1	843	PQN	C12-C13-C15-C16
21	A1	843	PQN	C14-C13-C15-C16
21	A2	843	PQN	C14-C13-C15-C16
21	A	843	PQN	C14-C13-C15-C16
21	AA	844	PQN	C12-C13-C15-C16
21	AA	844	PQN	C14-C13-C15-C16
22	A1	846	LHG	O1-C1-C2-C3
22	B1	847	LHG	C3-O3-P-O5
22	L1	211	LHG	O9-C7-O7-C5
22	X1	102	LHG	O1-C1-C2-O2
22	X1	102	LHG	O1-C1-C2-C3
22	X1	102	LHG	C3-O3-P-O5
22	X1	102	LHG	C4-O6-P-O3
22	X1	102	LHG	C4-O6-P-O4
22	X1	102	LHG	C4-O6-P-O5
22	X1	103	LHG	C3-O3-P-O5
22	X1	103	LHG	O9-C7-O7-C5
22	X1	103	LHG	C8-C7-O7-C5
22	A2	845	LHG	C1-C2-C3-O3
22	A2	845	LHG	O2-C2-C3-O3
22	A2	846	LHG	O1-C1-C2-C3
22	L2	208	LHG	C1-C2-C3-O3
22	L2	208	LHG	O9-C7-O7-C5
22	X2	102	LHG	O1-C1-C2-O2
22	X2	102	LHG	O1-C1-C2-C3
22	X2	102	LHG	C3-O3-P-O5
22	X2	102	LHG	C4-O6-P-O3
22	X2	102	LHG	C4-O6-P-O4
22	X2	103	LHG	C3-O3-P-O5
22	X2	103	LHG	C3-O3-P-O6
22	X2	103	LHG	O9-C7-O7-C5
22	X2	103	LHG	C8-C7-O7-C5
22	A	845	LHG	C1-C2-C3-O3
22	A	845	LHG	O2-C2-C3-O3
22	A	846	LHG	O1-C1-C2-C3
22	B	853	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
22	B	853	LHG	C3-O3-P-O6
22	B	853	LHG	O9-C7-O7-C5
22	B	853	LHG	C8-C7-O7-C5
22	L	207	LHG	O9-C7-O7-C5
22	X	102	LHG	O1-C1-C2-O2
22	X	102	LHG	O1-C1-C2-C3
22	X	102	LHG	C3-O3-P-O5
22	AA	846	LHG	C1-C2-C3-O3
22	AA	846	LHG	O2-C2-C3-O3
22	AA	847	LHG	O1-C1-C2-C3
22	BB	851	LHG	C3-O3-P-O5
22	BB	851	LHG	C3-O3-P-O6
22	BB	851	LHG	O9-C7-O7-C5
22	BB	851	LHG	C8-C7-O7-C5
22	LL	205	LHG	O9-C7-O7-C5
22	XX	102	LHG	O1-C1-C2-O2
22	XX	102	LHG	O1-C1-C2-C3
22	XX	102	LHG	C4-O6-P-O3
22	XX	102	LHG	C4-O6-P-O4
22	XX	102	LHG	C4-O6-P-O5
23	A1	847	BCR	C11-C10-C9-C34
23	A1	847	BCR	C11-C12-C13-C35
23	A1	847	BCR	C36-C18-C19-C20
23	A1	848	BCR	C7-C8-C9-C10
23	A1	848	BCR	C11-C12-C13-C14
23	A1	848	BCR	C11-C12-C13-C35
23	A1	848	BCR	C16-C17-C18-C36
23	A1	848	BCR	C36-C18-C19-C20
23	A1	848	BCR	C37-C22-C23-C24
23	A1	849	BCR	C7-C8-C9-C34
23	A1	849	BCR	C11-C10-C9-C34
23	A1	849	BCR	C11-C12-C13-C14
23	A1	849	BCR	C11-C12-C13-C35
23	A1	849	BCR	C17-C18-C19-C20
23	A1	849	BCR	C20-C21-C22-C37
23	A1	849	BCR	C37-C22-C23-C24
23	A1	849	BCR	C23-C24-C25-C30
23	A1	850	BCR	C7-C8-C9-C34
23	A1	850	BCR	C11-C10-C9-C8
23	A1	850	BCR	C11-C10-C9-C34
23	A1	850	BCR	C10-C11-C12-C13
23	A1	850	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A1	850	BCR	C16-C17-C18-C19
23	A1	850	BCR	C16-C17-C18-C36
23	A1	850	BCR	C37-C22-C23-C24
23	A1	851	BCR	C7-C8-C9-C34
23	A1	851	BCR	C11-C10-C9-C8
23	A1	851	BCR	C11-C10-C9-C34
23	A1	851	BCR	C10-C11-C12-C13
23	A1	851	BCR	C16-C17-C18-C19
23	A1	851	BCR	C16-C17-C18-C36
23	A1	851	BCR	C36-C18-C19-C20
23	A1	851	BCR	C18-C19-C20-C21
23	A1	851	BCR	C20-C21-C22-C37
23	A1	851	BCR	C37-C22-C23-C24
23	A1	851	BCR	C22-C23-C24-C25
23	A1	853	BCR	C11-C12-C13-C35
23	A1	853	BCR	C16-C17-C18-C36
23	A1	853	BCR	C36-C18-C19-C20
23	A1	853	BCR	C18-C19-C20-C21
23	A1	853	BCR	C20-C21-C22-C37
23	B1	838	BCR	C1-C6-C7-C8
23	B1	838	BCR	C5-C6-C7-C8
23	B1	838	BCR	C7-C8-C9-C10
23	B1	838	BCR	C11-C12-C13-C35
23	B1	838	BCR	C16-C17-C18-C36
23	B1	838	BCR	C17-C18-C19-C20
23	B1	838	BCR	C20-C21-C22-C37
23	B1	839	BCR	C35-C13-C14-C15
23	B1	839	BCR	C20-C21-C22-C37
23	B1	839	BCR	C37-C22-C23-C24
23	B1	841	BCR	C6-C7-C8-C9
23	B1	841	BCR	C11-C12-C13-C35
23	B1	841	BCR	C35-C13-C14-C15
23	B1	841	BCR	C16-C17-C18-C19
23	B1	841	BCR	C36-C18-C19-C20
23	B1	841	BCR	C18-C19-C20-C21
23	B1	841	BCR	C21-C22-C23-C24
23	B1	841	BCR	C37-C22-C23-C24
23	B1	841	BCR	C23-C24-C25-C26
23	B1	841	BCR	C23-C24-C25-C30
23	B1	842	BCR	C6-C7-C8-C9
23	B1	842	BCR	C7-C8-C9-C10
23	B1	842	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	B1	842	BCR	C11-C10-C9-C8
23	B1	842	BCR	C11-C12-C13-C14
23	B1	842	BCR	C11-C12-C13-C35
23	B1	842	BCR	C17-C18-C19-C20
23	B1	842	BCR	C36-C18-C19-C20
23	B1	842	BCR	C20-C21-C22-C23
23	B1	842	BCR	C20-C21-C22-C37
23	B1	843	BCR	C1-C6-C7-C8
23	B1	843	BCR	C11-C12-C13-C35
23	B1	843	BCR	C14-C15-C16-C17
23	B1	843	BCR	C16-C17-C18-C36
23	B1	843	BCR	C36-C18-C19-C20
23	B1	843	BCR	C20-C21-C22-C37
23	B1	843	BCR	C22-C23-C24-C25
23	F1	303	BCR	C7-C8-C9-C34
23	F1	303	BCR	C11-C10-C9-C8
23	F1	303	BCR	C11-C10-C9-C34
23	F1	303	BCR	C10-C11-C12-C13
23	F1	303	BCR	C11-C12-C13-C35
23	F1	303	BCR	C12-C13-C14-C15
23	F1	303	BCR	C16-C17-C18-C36
23	F1	303	BCR	C23-C24-C25-C30
23	F1	304	BCR	C7-C8-C9-C10
23	F1	304	BCR	C7-C8-C9-C34
23	F1	304	BCR	C11-C10-C9-C34
23	F1	304	BCR	C11-C12-C13-C35
23	F1	304	BCR	C36-C18-C19-C20
23	F1	304	BCR	C18-C19-C20-C21
23	F1	304	BCR	C20-C21-C22-C23
23	F1	304	BCR	C21-C22-C23-C24
23	F1	306	BCR	C1-C6-C7-C8
23	F1	306	BCR	C5-C6-C7-C8
23	F1	306	BCR	C6-C7-C8-C9
23	F1	306	BCR	C7-C8-C9-C10
23	F1	306	BCR	C11-C10-C9-C8
23	F1	306	BCR	C10-C11-C12-C13
23	F1	306	BCR	C11-C12-C13-C14
23	F1	306	BCR	C11-C12-C13-C35
23	F1	306	BCR	C16-C17-C18-C19
23	F1	306	BCR	C16-C17-C18-C36
23	F1	306	BCR	C36-C18-C19-C20
23	F1	306	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	F1	306	BCR	C21-C22-C23-C24
23	F1	306	BCR	C37-C22-C23-C24
23	F1	306	BCR	C22-C23-C24-C25
23	I1	101	BCR	C1-C6-C7-C8
23	I1	101	BCR	C11-C10-C9-C34
23	I1	101	BCR	C11-C12-C13-C35
23	I1	101	BCR	C16-C17-C18-C36
23	I1	101	BCR	C36-C18-C19-C20
23	I1	101	BCR	C20-C21-C22-C37
23	I1	101	BCR	C21-C22-C23-C24
23	J1	102	BCR	C7-C8-C9-C34
23	J1	102	BCR	C11-C10-C9-C34
23	J1	102	BCR	C11-C12-C13-C14
23	J1	102	BCR	C35-C13-C14-C15
23	J1	102	BCR	C16-C17-C18-C36
23	J1	102	BCR	C36-C18-C19-C20
23	J1	102	BCR	C21-C22-C23-C24
23	J1	102	BCR	C37-C22-C23-C24
23	J1	102	BCR	C23-C24-C25-C30
23	J1	104	BCR	C11-C10-C9-C34
23	J1	104	BCR	C11-C12-C13-C35
23	J1	104	BCR	C16-C17-C18-C36
23	J1	104	BCR	C36-C18-C19-C20
23	J1	104	BCR	C21-C22-C23-C24
23	J1	104	BCR	C23-C24-C25-C26
23	K1	104	BCR	C7-C8-C9-C34
23	K1	104	BCR	C11-C12-C13-C35
23	K1	104	BCR	C36-C18-C19-C20
23	K1	104	BCR	C20-C21-C22-C23
23	K1	104	BCR	C20-C21-C22-C37
23	K1	104	BCR	C21-C22-C23-C24
23	K1	106	BCR	C7-C8-C9-C10
23	K1	106	BCR	C35-C13-C14-C15
23	K1	106	BCR	C36-C18-C19-C20
23	K1	106	BCR	C18-C19-C20-C21
23	K1	106	BCR	C20-C21-C22-C37
23	K1	106	BCR	C22-C23-C24-C25
23	L1	201	BCR	C11-C12-C13-C35
23	L1	201	BCR	C17-C18-C19-C20
23	L1	201	BCR	C36-C18-C19-C20
23	L1	201	BCR	C37-C22-C23-C24
23	L1	208	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	L1	208	BCR	C7-C8-C9-C34
23	L1	208	BCR	C11-C10-C9-C34
23	L1	208	BCR	C11-C12-C13-C35
23	L1	208	BCR	C16-C17-C18-C36
23	L1	208	BCR	C37-C22-C23-C24
23	L1	208	BCR	C23-C24-C25-C26
23	L1	208	BCR	C23-C24-C25-C30
23	L1	209	BCR	C1-C6-C7-C8
23	L1	209	BCR	C5-C6-C7-C8
23	L1	209	BCR	C11-C10-C9-C8
23	L1	209	BCR	C11-C10-C9-C34
23	L1	209	BCR	C9-C10-C11-C12
23	L1	209	BCR	C10-C11-C12-C13
23	L1	209	BCR	C11-C12-C13-C14
23	L1	209	BCR	C11-C12-C13-C35
23	L1	209	BCR	C16-C17-C18-C36
23	L1	209	BCR	C20-C21-C22-C37
23	L1	209	BCR	C21-C22-C23-C24
23	M1	101	BCR	C6-C7-C8-C9
23	M1	101	BCR	C7-C8-C9-C10
23	M1	101	BCR	C7-C8-C9-C34
23	M1	101	BCR	C11-C10-C9-C8
23	M1	101	BCR	C11-C10-C9-C34
23	M1	101	BCR	C10-C11-C12-C13
23	M1	101	BCR	C12-C13-C14-C15
23	M1	101	BCR	C35-C13-C14-C15
23	M1	101	BCR	C14-C15-C16-C17
23	M1	101	BCR	C17-C18-C19-C20
23	M1	101	BCR	C36-C18-C19-C20
23	M1	101	BCR	C18-C19-C20-C21
23	M1	101	BCR	C21-C22-C23-C24
23	M1	101	BCR	C37-C22-C23-C24
23	A2	847	BCR	C11-C10-C9-C34
23	A2	847	BCR	C11-C12-C13-C35
23	A2	847	BCR	C36-C18-C19-C20
23	A2	848	BCR	C7-C8-C9-C10
23	A2	848	BCR	C11-C12-C13-C35
23	A2	848	BCR	C36-C18-C19-C20
23	A2	848	BCR	C37-C22-C23-C24
23	A2	849	BCR	C7-C8-C9-C34
23	A2	849	BCR	C11-C10-C9-C34
23	A2	849	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
23	A2	849	BCR	C18-C19-C20-C21
23	A2	849	BCR	C21-C22-C23-C24
23	A2	849	BCR	C37-C22-C23-C24
23	A2	849	BCR	C23-C24-C25-C30
23	A2	850	BCR	C7-C8-C9-C34
23	A2	850	BCR	C11-C10-C9-C8
23	A2	850	BCR	C11-C10-C9-C34
23	A2	850	BCR	C10-C11-C12-C13
23	A2	850	BCR	C11-C12-C13-C14
23	A2	850	BCR	C16-C17-C18-C19
23	A2	850	BCR	C16-C17-C18-C36
23	A2	850	BCR	C37-C22-C23-C24
23	A2	851	BCR	C7-C8-C9-C34
23	A2	851	BCR	C11-C10-C9-C8
23	A2	851	BCR	C11-C10-C9-C34
23	A2	851	BCR	C10-C11-C12-C13
23	A2	851	BCR	C35-C13-C14-C15
23	A2	851	BCR	C18-C19-C20-C21
23	A2	851	BCR	C20-C21-C22-C37
23	A2	851	BCR	C37-C22-C23-C24
23	A2	851	BCR	C22-C23-C24-C25
23	A2	853	BCR	C11-C12-C13-C35
23	A2	853	BCR	C16-C17-C18-C36
23	A2	853	BCR	C36-C18-C19-C20
23	A2	853	BCR	C18-C19-C20-C21
23	A2	853	BCR	C20-C21-C22-C37
23	B2	839	BCR	C1-C6-C7-C8
23	B2	839	BCR	C5-C6-C7-C8
23	B2	839	BCR	C7-C8-C9-C10
23	B2	839	BCR	C11-C12-C13-C35
23	B2	839	BCR	C16-C17-C18-C36
23	B2	839	BCR	C17-C18-C19-C20
23	B2	839	BCR	C20-C21-C22-C37
23	B2	840	BCR	C35-C13-C14-C15
23	B2	840	BCR	C16-C17-C18-C36
23	B2	840	BCR	C21-C22-C23-C24
23	B2	840	BCR	C37-C22-C23-C24
23	B2	842	BCR	C6-C7-C8-C9
23	B2	842	BCR	C7-C8-C9-C34
23	B2	842	BCR	C11-C10-C9-C34
23	B2	842	BCR	C10-C11-C12-C13
23	B2	842	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
23	B2	842	BCR	C35-C13-C14-C15
23	B2	842	BCR	C14-C15-C16-C17
23	B2	842	BCR	C18-C19-C20-C21
23	B2	842	BCR	C20-C21-C22-C37
23	B2	842	BCR	C22-C23-C24-C25
23	B2	843	BCR	C6-C7-C8-C9
23	B2	843	BCR	C7-C8-C9-C10
23	B2	843	BCR	C7-C8-C9-C34
23	B2	843	BCR	C11-C10-C9-C8
23	B2	843	BCR	C10-C11-C12-C13
23	B2	843	BCR	C11-C12-C13-C14
23	B2	843	BCR	C17-C18-C19-C20
23	B2	843	BCR	C36-C18-C19-C20
23	B2	843	BCR	C20-C21-C22-C37
23	B2	844	BCR	C1-C6-C7-C8
23	B2	844	BCR	C11-C12-C13-C35
23	B2	844	BCR	C16-C17-C18-C36
23	B2	844	BCR	C36-C18-C19-C20
23	B2	844	BCR	C20-C21-C22-C23
23	B2	844	BCR	C20-C21-C22-C37
23	B2	844	BCR	C22-C23-C24-C25
23	F2	303	BCR	C7-C8-C9-C34
23	F2	303	BCR	C11-C10-C9-C8
23	F2	303	BCR	C11-C10-C9-C34
23	F2	303	BCR	C10-C11-C12-C13
23	F2	303	BCR	C11-C12-C13-C35
23	F2	303	BCR	C16-C17-C18-C36
23	F2	303	BCR	C21-C22-C23-C24
23	F2	303	BCR	C23-C24-C25-C30
23	F2	304	BCR	C7-C8-C9-C10
23	F2	304	BCR	C7-C8-C9-C34
23	F2	304	BCR	C11-C10-C9-C8
23	F2	304	BCR	C11-C10-C9-C34
23	F2	304	BCR	C11-C12-C13-C35
23	F2	304	BCR	C18-C19-C20-C21
23	F2	304	BCR	C20-C21-C22-C23
23	F2	304	BCR	C21-C22-C23-C24
23	F2	305	BCR	C1-C6-C7-C8
23	F2	305	BCR	C5-C6-C7-C8
23	F2	305	BCR	C7-C8-C9-C10
23	F2	305	BCR	C7-C8-C9-C34
23	F2	305	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	F2	305	BCR	C10-C11-C12-C13
23	F2	305	BCR	C11-C12-C13-C14
23	F2	305	BCR	C11-C12-C13-C35
23	F2	305	BCR	C15-C16-C17-C18
23	F2	305	BCR	C16-C17-C18-C19
23	F2	305	BCR	C16-C17-C18-C36
23	F2	305	BCR	C17-C18-C19-C20
23	F2	305	BCR	C18-C19-C20-C21
23	F2	305	BCR	C20-C21-C22-C23
23	F2	305	BCR	C20-C21-C22-C37
23	F2	305	BCR	C22-C23-C24-C25
23	I2	101	BCR	C1-C6-C7-C8
23	I2	101	BCR	C11-C10-C9-C34
23	I2	101	BCR	C11-C12-C13-C35
23	I2	101	BCR	C16-C17-C18-C36
23	I2	101	BCR	C36-C18-C19-C20
23	I2	101	BCR	C20-C21-C22-C37
23	I2	101	BCR	C21-C22-C23-C24
23	I2	102	BCR	C11-C12-C13-C35
23	I2	102	BCR	C36-C18-C19-C20
23	I2	102	BCR	C37-C22-C23-C24
23	I2	103	BCR	C7-C8-C9-C10
23	I2	103	BCR	C7-C8-C9-C34
23	I2	103	BCR	C11-C10-C9-C34
23	I2	103	BCR	C10-C11-C12-C13
23	I2	103	BCR	C11-C12-C13-C35
23	I2	103	BCR	C16-C17-C18-C36
23	I2	103	BCR	C37-C22-C23-C24
23	I2	103	BCR	C23-C24-C25-C26
23	I2	103	BCR	C23-C24-C25-C30
23	J2	102	BCR	C7-C8-C9-C34
23	J2	102	BCR	C11-C10-C9-C34
23	J2	102	BCR	C11-C12-C13-C14
23	J2	102	BCR	C35-C13-C14-C15
23	J2	102	BCR	C36-C18-C19-C20
23	J2	102	BCR	C21-C22-C23-C24
23	J2	102	BCR	C37-C22-C23-C24
23	J2	102	BCR	C23-C24-C25-C30
23	J2	104	BCR	C6-C7-C8-C9
23	J2	104	BCR	C11-C10-C9-C34
23	J2	104	BCR	C11-C12-C13-C35
23	J2	104	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	J2	104	BCR	C16-C17-C18-C36
23	J2	104	BCR	C36-C18-C19-C20
23	J2	104	BCR	C21-C22-C23-C24
23	J2	104	BCR	C23-C24-C25-C26
23	K2	103	BCR	C11-C12-C13-C35
23	K2	103	BCR	C36-C18-C19-C20
23	K2	103	BCR	C18-C19-C20-C21
23	K2	103	BCR	C20-C21-C22-C23
23	K2	103	BCR	C20-C21-C22-C37
23	K2	105	BCR	C7-C8-C9-C10
23	K2	105	BCR	C35-C13-C14-C15
23	K2	105	BCR	C16-C17-C18-C36
23	K2	105	BCR	C17-C18-C19-C20
23	K2	105	BCR	C36-C18-C19-C20
23	K2	105	BCR	C18-C19-C20-C21
23	K2	105	BCR	C20-C21-C22-C23
23	K2	105	BCR	C20-C21-C22-C37
23	L2	207	BCR	C1-C6-C7-C8
23	L2	207	BCR	C5-C6-C7-C8
23	L2	207	BCR	C7-C8-C9-C34
23	L2	207	BCR	C11-C10-C9-C8
23	L2	207	BCR	C11-C10-C9-C34
23	L2	207	BCR	C10-C11-C12-C13
23	L2	207	BCR	C11-C12-C13-C14
23	L2	207	BCR	C11-C12-C13-C35
23	L2	207	BCR	C16-C17-C18-C36
23	L2	207	BCR	C20-C21-C22-C37
23	L2	207	BCR	C21-C22-C23-C24
23	M2	102	BCR	C6-C7-C8-C9
23	M2	102	BCR	C7-C8-C9-C10
23	M2	102	BCR	C7-C8-C9-C34
23	M2	102	BCR	C11-C10-C9-C8
23	M2	102	BCR	C11-C10-C9-C34
23	M2	102	BCR	C10-C11-C12-C13
23	M2	102	BCR	C12-C13-C14-C15
23	M2	102	BCR	C35-C13-C14-C15
23	M2	102	BCR	C14-C15-C16-C17
23	M2	102	BCR	C17-C18-C19-C20
23	M2	102	BCR	C36-C18-C19-C20
23	M2	102	BCR	C18-C19-C20-C21
23	M2	102	BCR	C37-C22-C23-C24
23	A	847	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	A	847	BCR	C11-C12-C13-C35
23	A	848	BCR	C7-C8-C9-C10
23	A	848	BCR	C11-C10-C9-C34
23	A	848	BCR	C11-C12-C13-C35
23	A	848	BCR	C16-C17-C18-C36
23	A	848	BCR	C36-C18-C19-C20
23	A	848	BCR	C21-C22-C23-C24
23	A	849	BCR	C7-C8-C9-C34
23	A	849	BCR	C11-C10-C9-C34
23	A	849	BCR	C35-C13-C14-C15
23	A	849	BCR	C17-C18-C19-C20
23	A	849	BCR	C20-C21-C22-C37
23	A	849	BCR	C37-C22-C23-C24
23	A	849	BCR	C23-C24-C25-C30
23	A	850	BCR	C7-C8-C9-C34
23	A	850	BCR	C11-C10-C9-C8
23	A	850	BCR	C11-C10-C9-C34
23	A	850	BCR	C11-C12-C13-C14
23	A	850	BCR	C11-C12-C13-C35
23	A	850	BCR	C16-C17-C18-C19
23	A	850	BCR	C16-C17-C18-C36
23	A	850	BCR	C20-C21-C22-C37
23	A	850	BCR	C37-C22-C23-C24
23	A	851	BCR	C7-C8-C9-C34
23	A	851	BCR	C11-C10-C9-C8
23	A	851	BCR	C10-C11-C12-C13
23	A	851	BCR	C12-C13-C14-C15
23	A	851	BCR	C16-C17-C18-C19
23	A	851	BCR	C16-C17-C18-C36
23	A	851	BCR	C18-C19-C20-C21
23	A	851	BCR	C20-C21-C22-C37
23	A	851	BCR	C37-C22-C23-C24
23	A	851	BCR	C22-C23-C24-C25
23	A	853	BCR	C11-C12-C13-C35
23	A	853	BCR	C13-C14-C15-C16
23	A	853	BCR	C16-C17-C18-C36
23	A	853	BCR	C36-C18-C19-C20
23	A	853	BCR	C18-C19-C20-C21
23	A	854	BCR	C7-C8-C9-C10
23	A	854	BCR	C35-C13-C14-C15
23	A	854	BCR	C14-C15-C16-C17
23	A	854	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	A	854	BCR	C36-C18-C19-C20
23	A	854	BCR	C18-C19-C20-C21
23	A	854	BCR	C19-C20-C21-C22
23	A	854	BCR	C20-C21-C22-C23
23	A	854	BCR	C20-C21-C22-C37
23	A	854	BCR	C37-C22-C23-C24
23	A	854	BCR	C23-C24-C25-C30
23	B	839	BCR	C1-C6-C7-C8
23	B	839	BCR	C5-C6-C7-C8
23	B	839	BCR	C7-C8-C9-C10
23	B	839	BCR	C11-C12-C13-C35
23	B	839	BCR	C16-C17-C18-C36
23	B	839	BCR	C17-C18-C19-C20
23	B	839	BCR	C18-C19-C20-C21
23	B	839	BCR	C20-C21-C22-C37
23	B	840	BCR	C37-C22-C23-C24
23	B	842	BCR	C6-C7-C8-C9
23	B	842	BCR	C11-C12-C13-C35
23	B	842	BCR	C35-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C36
23	B	842	BCR	C21-C22-C23-C24
23	B	842	BCR	C37-C22-C23-C24
23	B	842	BCR	C23-C24-C25-C26
23	B	842	BCR	C23-C24-C25-C30
23	B	843	BCR	C6-C7-C8-C9
23	B	843	BCR	C7-C8-C9-C10
23	B	843	BCR	C7-C8-C9-C34
23	B	843	BCR	C11-C10-C9-C8
23	B	843	BCR	C11-C10-C9-C34
23	B	843	BCR	C10-C11-C12-C13
23	B	843	BCR	C11-C12-C13-C14
23	B	843	BCR	C11-C12-C13-C35
23	B	843	BCR	C36-C18-C19-C20
23	B	843	BCR	C20-C21-C22-C23
23	B	843	BCR	C20-C21-C22-C37
23	B	843	BCR	C23-C24-C25-C30
23	B	844	BCR	C7-C8-C9-C34
23	B	844	BCR	C11-C12-C13-C35
23	B	844	BCR	C16-C17-C18-C36
23	B	844	BCR	C36-C18-C19-C20
23	B	844	BCR	C20-C21-C22-C23
23	B	844	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	B	844	BCR	C22-C23-C24-C25
23	B	848	BCR	C7-C8-C9-C10
23	B	848	BCR	C7-C8-C9-C34
23	B	848	BCR	C12-C13-C14-C15
23	B	848	BCR	C16-C17-C18-C36
23	B	848	BCR	C36-C18-C19-C20
23	B	848	BCR	C19-C20-C21-C22
23	F	303	BCR	C7-C8-C9-C34
23	F	303	BCR	C11-C10-C9-C8
23	F	303	BCR	C11-C10-C9-C34
23	F	303	BCR	C10-C11-C12-C13
23	F	303	BCR	C12-C13-C14-C15
23	F	303	BCR	C16-C17-C18-C36
23	F	303	BCR	C23-C24-C25-C30
23	F	304	BCR	C7-C8-C9-C10
23	F	304	BCR	C11-C10-C9-C8
23	F	304	BCR	C11-C12-C13-C35
23	F	304	BCR	C35-C13-C14-C15
23	F	304	BCR	C17-C18-C19-C20
23	F	304	BCR	C36-C18-C19-C20
23	F	304	BCR	C18-C19-C20-C21
23	F	304	BCR	C20-C21-C22-C23
23	F	304	BCR	C21-C22-C23-C24
23	F	305	BCR	C1-C6-C7-C8
23	F	305	BCR	C5-C6-C7-C8
23	F	305	BCR	C6-C7-C8-C9
23	F	305	BCR	C7-C8-C9-C10
23	F	305	BCR	C10-C11-C12-C13
23	F	305	BCR	C11-C12-C13-C14
23	F	305	BCR	C11-C12-C13-C35
23	F	305	BCR	C15-C16-C17-C18
23	F	305	BCR	C16-C17-C18-C19
23	F	305	BCR	C16-C17-C18-C36
23	F	305	BCR	C17-C18-C19-C20
23	F	305	BCR	C18-C19-C20-C21
23	F	305	BCR	C21-C22-C23-C24
23	F	305	BCR	C37-C22-C23-C24
23	F	305	BCR	C22-C23-C24-C25
23	I	101	BCR	C11-C10-C9-C34
23	I	101	BCR	C11-C12-C13-C35
23	I	101	BCR	C35-C13-C14-C15
23	I	101	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	I	101	BCR	C36-C18-C19-C20
23	I	101	BCR	C20-C21-C22-C37
23	I	101	BCR	C21-C22-C23-C24
23	I	101	BCR	C37-C22-C23-C24
23	I	102	BCR	C11-C12-C13-C35
23	I	102	BCR	C36-C18-C19-C20
23	J	102	BCR	C7-C8-C9-C34
23	J	102	BCR	C11-C10-C9-C34
23	J	102	BCR	C9-C10-C11-C12
23	J	102	BCR	C11-C12-C13-C14
23	J	102	BCR	C12-C13-C14-C15
23	J	102	BCR	C35-C13-C14-C15
23	J	102	BCR	C16-C17-C18-C36
23	J	102	BCR	C17-C18-C19-C20
23	J	102	BCR	C21-C22-C23-C24
23	J	102	BCR	C37-C22-C23-C24
23	J	102	BCR	C23-C24-C25-C30
23	J	104	BCR	C6-C7-C8-C9
23	J	104	BCR	C11-C10-C9-C34
23	J	104	BCR	C11-C12-C13-C35
23	J	104	BCR	C16-C17-C18-C36
23	J	104	BCR	C17-C18-C19-C20
23	J	104	BCR	C36-C18-C19-C20
23	J	104	BCR	C21-C22-C23-C24
23	J	104	BCR	C23-C24-C25-C26
23	K	103	BCR	C11-C10-C9-C34
23	K	103	BCR	C10-C11-C12-C13
23	K	103	BCR	C16-C17-C18-C36
23	K	103	BCR	C17-C18-C19-C20
23	K	103	BCR	C20-C21-C22-C37
23	K	103	BCR	C21-C22-C23-C24
23	K	103	BCR	C37-C22-C23-C24
23	K	103	BCR	C23-C24-C25-C30
23	L	205	BCR	C7-C8-C9-C10
23	L	205	BCR	C7-C8-C9-C34
23	L	205	BCR	C11-C10-C9-C34
23	L	205	BCR	C11-C12-C13-C35
23	L	205	BCR	C37-C22-C23-C24
23	L	205	BCR	C23-C24-C25-C26
23	L	205	BCR	C23-C24-C25-C30
23	L	206	BCR	C1-C6-C7-C8
23	L	206	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	L	206	BCR	C11-C10-C9-C8
23	L	206	BCR	C11-C10-C9-C34
23	L	206	BCR	C9-C10-C11-C12
23	L	206	BCR	C10-C11-C12-C13
23	L	206	BCR	C11-C12-C13-C14
23	L	206	BCR	C11-C12-C13-C35
23	L	206	BCR	C16-C17-C18-C36
23	L	206	BCR	C17-C18-C19-C20
23	L	206	BCR	C20-C21-C22-C37
23	L	206	BCR	C21-C22-C23-C24
23	M	101	BCR	C7-C8-C9-C10
23	M	101	BCR	C7-C8-C9-C34
23	M	101	BCR	C11-C10-C9-C8
23	M	101	BCR	C11-C10-C9-C34
23	M	101	BCR	C10-C11-C12-C13
23	M	101	BCR	C11-C12-C13-C14
23	M	101	BCR	C11-C12-C13-C35
23	M	101	BCR	C12-C13-C14-C15
23	M	101	BCR	C35-C13-C14-C15
23	M	101	BCR	C14-C15-C16-C17
23	M	101	BCR	C15-C16-C17-C18
23	M	101	BCR	C16-C17-C18-C19
23	M	101	BCR	C16-C17-C18-C36
23	M	101	BCR	C36-C18-C19-C20
23	M	101	BCR	C18-C19-C20-C21
23	M	101	BCR	C21-C22-C23-C24
23	M	101	BCR	C37-C22-C23-C24
23	M	101	BCR	C23-C24-C25-C26
23	AA	848	BCR	C11-C10-C9-C34
23	AA	848	BCR	C10-C11-C12-C13
23	AA	848	BCR	C11-C12-C13-C35
23	AA	849	BCR	C7-C8-C9-C10
23	AA	849	BCR	C11-C10-C9-C34
23	AA	849	BCR	C11-C12-C13-C35
23	AA	849	BCR	C16-C17-C18-C36
23	AA	849	BCR	C36-C18-C19-C20
23	AA	849	BCR	C21-C22-C23-C24
23	AA	850	BCR	C7-C8-C9-C34
23	AA	850	BCR	C11-C10-C9-C34
23	AA	850	BCR	C35-C13-C14-C15
23	AA	850	BCR	C17-C18-C19-C20
23	AA	850	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	AA	850	BCR	C20-C21-C22-C37
23	AA	850	BCR	C37-C22-C23-C24
23	AA	850	BCR	C23-C24-C25-C30
23	AA	851	BCR	C7-C8-C9-C34
23	AA	851	BCR	C11-C10-C9-C8
23	AA	851	BCR	C11-C10-C9-C34
23	AA	851	BCR	C10-C11-C12-C13
23	AA	851	BCR	C11-C12-C13-C14
23	AA	851	BCR	C11-C12-C13-C35
23	AA	851	BCR	C16-C17-C18-C19
23	AA	851	BCR	C16-C17-C18-C36
23	AA	851	BCR	C20-C21-C22-C37
23	AA	851	BCR	C37-C22-C23-C24
23	AA	852	BCR	C7-C8-C9-C34
23	AA	852	BCR	C11-C10-C9-C8
23	AA	852	BCR	C10-C11-C12-C13
23	AA	852	BCR	C12-C13-C14-C15
23	AA	852	BCR	C16-C17-C18-C19
23	AA	852	BCR	C16-C17-C18-C36
23	AA	852	BCR	C36-C18-C19-C20
23	AA	852	BCR	C18-C19-C20-C21
23	AA	852	BCR	C20-C21-C22-C37
23	AA	852	BCR	C37-C22-C23-C24
23	AA	852	BCR	C22-C23-C24-C25
23	AA	854	BCR	C11-C12-C13-C35
23	AA	854	BCR	C13-C14-C15-C16
23	AA	854	BCR	C16-C17-C18-C36
23	AA	854	BCR	C36-C18-C19-C20
23	AA	854	BCR	C18-C19-C20-C21
23	AA	854	BCR	C20-C21-C22-C37
23	AA	854	BCR	C21-C22-C23-C24
23	AA	855	BCR	C7-C8-C9-C10
23	AA	855	BCR	C35-C13-C14-C15
23	AA	855	BCR	C36-C18-C19-C20
23	AA	855	BCR	C18-C19-C20-C21
23	AA	855	BCR	C19-C20-C21-C22
23	AA	855	BCR	C20-C21-C22-C23
23	AA	855	BCR	C20-C21-C22-C37
23	AA	855	BCR	C37-C22-C23-C24
23	AA	855	BCR	C23-C24-C25-C30
23	BB	838	BCR	C1-C6-C7-C8
23	BB	838	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	BB	838	BCR	C7-C8-C9-C10
23	BB	838	BCR	C16-C17-C18-C36
23	BB	838	BCR	C18-C19-C20-C21
23	BB	838	BCR	C20-C21-C22-C23
23	BB	838	BCR	C20-C21-C22-C37
23	BB	839	BCR	C37-C22-C23-C24
23	BB	841	BCR	C6-C7-C8-C9
23	BB	841	BCR	C11-C12-C13-C35
23	BB	841	BCR	C35-C13-C14-C15
23	BB	841	BCR	C16-C17-C18-C36
23	BB	841	BCR	C17-C18-C19-C20
23	BB	841	BCR	C21-C22-C23-C24
23	BB	841	BCR	C37-C22-C23-C24
23	BB	841	BCR	C23-C24-C25-C26
23	BB	841	BCR	C23-C24-C25-C30
23	BB	842	BCR	C6-C7-C8-C9
23	BB	842	BCR	C7-C8-C9-C10
23	BB	842	BCR	C7-C8-C9-C34
23	BB	842	BCR	C11-C10-C9-C8
23	BB	842	BCR	C11-C10-C9-C34
23	BB	842	BCR	C11-C12-C13-C14
23	BB	842	BCR	C11-C12-C13-C35
23	BB	842	BCR	C16-C17-C18-C36
23	BB	842	BCR	C36-C18-C19-C20
23	BB	842	BCR	C20-C21-C22-C23
23	BB	842	BCR	C20-C21-C22-C37
23	BB	843	BCR	C7-C8-C9-C34
23	BB	843	BCR	C11-C12-C13-C35
23	BB	843	BCR	C35-C13-C14-C15
23	BB	843	BCR	C16-C17-C18-C36
23	BB	843	BCR	C36-C18-C19-C20
23	BB	843	BCR	C20-C21-C22-C23
23	BB	843	BCR	C20-C21-C22-C37
23	BB	843	BCR	C22-C23-C24-C25
23	BB	847	BCR	C1-C6-C7-C8
23	BB	847	BCR	C7-C8-C9-C10
23	BB	847	BCR	C7-C8-C9-C34
23	BB	847	BCR	C12-C13-C14-C15
23	BB	847	BCR	C36-C18-C19-C20
23	BB	847	BCR	C19-C20-C21-C22
23	FF	303	BCR	C6-C7-C8-C9
23	FF	303	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	FF	303	BCR	C11-C10-C9-C8
23	FF	303	BCR	C11-C10-C9-C34
23	FF	303	BCR	C10-C11-C12-C13
23	FF	303	BCR	C12-C13-C14-C15
23	FF	303	BCR	C16-C17-C18-C36
23	FF	303	BCR	C21-C22-C23-C24
23	FF	303	BCR	C23-C24-C25-C30
23	FF	304	BCR	C7-C8-C9-C10
23	FF	304	BCR	C7-C8-C9-C34
23	FF	304	BCR	C11-C10-C9-C8
23	FF	304	BCR	C11-C10-C9-C34
23	FF	304	BCR	C11-C12-C13-C35
23	FF	304	BCR	C35-C13-C14-C15
23	FF	304	BCR	C36-C18-C19-C20
23	FF	304	BCR	C18-C19-C20-C21
23	FF	304	BCR	C20-C21-C22-C23
23	FF	304	BCR	C21-C22-C23-C24
23	FF	306	BCR	C1-C6-C7-C8
23	FF	306	BCR	C5-C6-C7-C8
23	FF	306	BCR	C6-C7-C8-C9
23	FF	306	BCR	C7-C8-C9-C10
23	FF	306	BCR	C11-C10-C9-C8
23	FF	306	BCR	C10-C11-C12-C13
23	FF	306	BCR	C11-C12-C13-C14
23	FF	306	BCR	C11-C12-C13-C35
23	FF	306	BCR	C15-C16-C17-C18
23	FF	306	BCR	C16-C17-C18-C19
23	FF	306	BCR	C16-C17-C18-C36
23	FF	306	BCR	C17-C18-C19-C20
23	FF	306	BCR	C18-C19-C20-C21
23	FF	306	BCR	C21-C22-C23-C24
23	FF	306	BCR	C37-C22-C23-C24
23	FF	306	BCR	C22-C23-C24-C25
23	II	101	BCR	C11-C10-C9-C34
23	II	101	BCR	C11-C12-C13-C35
23	II	101	BCR	C16-C17-C18-C36
23	II	101	BCR	C36-C18-C19-C20
23	II	101	BCR	C21-C22-C23-C24
23	II	101	BCR	C37-C22-C23-C24
23	II	102	BCR	C11-C12-C13-C35
23	II	102	BCR	C35-C13-C14-C15
23	II	102	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	II	102	BCR	C36-C18-C19-C20
23	II	104	BCR	C7-C8-C9-C10
23	II	104	BCR	C7-C8-C9-C34
23	II	104	BCR	C11-C10-C9-C34
23	II	104	BCR	C11-C12-C13-C35
23	II	104	BCR	C16-C17-C18-C36
23	II	104	BCR	C37-C22-C23-C24
23	II	104	BCR	C23-C24-C25-C26
23	II	104	BCR	C23-C24-C25-C30
23	JJ	102	BCR	C7-C8-C9-C34
23	JJ	102	BCR	C11-C10-C9-C34
23	JJ	102	BCR	C9-C10-C11-C12
23	JJ	102	BCR	C11-C12-C13-C14
23	JJ	102	BCR	C35-C13-C14-C15
23	JJ	102	BCR	C16-C17-C18-C36
23	JJ	102	BCR	C36-C18-C19-C20
23	JJ	102	BCR	C21-C22-C23-C24
23	JJ	102	BCR	C37-C22-C23-C24
23	JJ	102	BCR	C23-C24-C25-C30
23	JJ	104	BCR	C11-C10-C9-C34
23	JJ	104	BCR	C11-C12-C13-C35
23	JJ	104	BCR	C16-C17-C18-C36
23	JJ	104	BCR	C17-C18-C19-C20
23	JJ	104	BCR	C36-C18-C19-C20
23	JJ	104	BCR	C23-C24-C25-C26
23	KK	103	BCR	C7-C8-C9-C34
23	KK	103	BCR	C11-C10-C9-C34
23	KK	103	BCR	C11-C12-C13-C35
23	KK	103	BCR	C16-C17-C18-C36
23	KK	103	BCR	C17-C18-C19-C20
23	KK	103	BCR	C20-C21-C22-C37
23	KK	103	BCR	C21-C22-C23-C24
23	KK	103	BCR	C37-C22-C23-C24
23	KK	103	BCR	C23-C24-C25-C30
23	LL	204	BCR	C1-C6-C7-C8
23	LL	204	BCR	C5-C6-C7-C8
23	LL	204	BCR	C6-C7-C8-C9
23	LL	204	BCR	C11-C10-C9-C8
23	LL	204	BCR	C11-C10-C9-C34
23	LL	204	BCR	C11-C12-C13-C14
23	LL	204	BCR	C11-C12-C13-C35
23	LL	204	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	LL	204	BCR	C17-C18-C19-C20
23	LL	204	BCR	C20-C21-C22-C37
23	LL	204	BCR	C21-C22-C23-C24
23	MM	101	BCR	C7-C8-C9-C10
23	MM	101	BCR	C11-C10-C9-C8
23	MM	101	BCR	C11-C10-C9-C34
23	MM	101	BCR	C10-C11-C12-C13
23	MM	101	BCR	C11-C12-C13-C14
23	MM	101	BCR	C12-C13-C14-C15
23	MM	101	BCR	C35-C13-C14-C15
23	MM	101	BCR	C14-C15-C16-C17
23	MM	101	BCR	C16-C17-C18-C19
23	MM	101	BCR	C16-C17-C18-C36
23	MM	101	BCR	C36-C18-C19-C20
23	MM	101	BCR	C18-C19-C20-C21
23	MM	101	BCR	C20-C21-C22-C23
23	MM	101	BCR	C20-C21-C22-C37
23	MM	101	BCR	C21-C22-C23-C24
23	MM	101	BCR	C37-C22-C23-C24
25	B1	844	LMG	C2-C1-O1-C7
25	B1	844	LMG	O6-C1-O1-C7
25	B1	846	LMG	C2-C1-O1-C7
25	B1	846	LMG	O6-C1-O1-C7
25	I1	102	LMG	C2-C1-O1-C7
25	I1	102	LMG	O6-C1-O1-C7
25	B2	845	LMG	C2-C1-O1-C7
25	B2	845	LMG	O6-C1-O1-C7
25	B2	847	LMG	C2-C1-O1-C7
25	B2	847	LMG	O6-C1-O1-C7
25	B	845	LMG	C2-C1-O1-C7
25	B	845	LMG	O6-C1-O1-C7
25	BB	844	LMG	C2-C1-O1-C7
25	BB	844	LMG	O6-C1-O1-C7
25	II	105	LMG	C11-C10-O7-C8
26	B1	840	ECH	C1-C6-C7-C8
26	B1	840	ECH	C5-C6-C7-C8
26	B1	840	ECH	C7-C8-C9-C10
26	B1	840	ECH	C7-C8-C9-C34
26	B1	840	ECH	C11-C12-C13-C14
26	B1	840	ECH	C11-C12-C13-C35
26	B2	841	ECH	C1-C6-C7-C8
26	B2	841	ECH	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	B2	841	ECH	C7-C8-C9-C10
26	B2	841	ECH	C7-C8-C9-C34
26	B2	841	ECH	C11-C12-C13-C14
26	B2	841	ECH	C11-C12-C13-C35
26	B	841	ECH	C1-C6-C7-C8
26	B	841	ECH	C5-C6-C7-C8
26	B	841	ECH	C7-C8-C9-C10
26	B	841	ECH	C7-C8-C9-C34
26	BB	840	ECH	C5-C6-C7-C8
26	BB	840	ECH	C7-C8-C9-C10
26	BB	840	ECH	C7-C8-C9-C34
26	BB	840	ECH	C11-C12-C13-C14
26	BB	840	ECH	C11-C12-C13-C35
26	BB	840	ECH	C13-C14-C15-C16
28	B	856	DGD	C2D-C1D-O3G-C3G
28	B	856	DGD	O6D-C1D-O3G-C3G
28	B	856	DGD	C2E-C1E-O5D-C6D
28	B	856	DGD	O6E-C1E-O5D-C6D
28	BB	854	DGD	C2D-C1D-O3G-C3G
28	BB	854	DGD	O6D-C1D-O3G-C3G
28	BB	854	DGD	C2E-C1E-O5D-C6D
28	BB	854	DGD	O6E-C1E-O5D-C6D
19	B1	833	CLA	C4C-C3C-CAC-CBC
19	BB	829	CLA	C4C-C3C-CAC-CBC
19	A1	827	CLA	O1D-CGD-O2D-CED
19	B1	803	CLA	O1D-CGD-O2D-CED
19	B1	832	CLA	O1D-CGD-O2D-CED
19	A2	801	CLA	O1D-CGD-O2D-CED
19	A2	812	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	O1D-CGD-O2D-CED
19	B	806	CLA	O1D-CGD-O2D-CED
19	B	854	CLA	O1D-CGD-O2D-CED
19	AA	812	CLA	O1D-CGD-O2D-CED
19	AA	823	CLA	O1D-CGD-O2D-CED
19	BB	806	CLA	O1D-CGD-O2D-CED
19	BB	816	CLA	O1D-CGD-O2D-CED
19	BB	832	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	C2C-C3C-CAC-CBC
19	BB	833	CLA	C2C-C3C-CAC-CBC
19	BB	833	CLA	C4C-C3C-CAC-CBC
19	A1	811	CLA	O1D-CGD-O2D-CED
19	A1	822	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B1	806	CLA	O1D-CGD-O2D-CED
19	B1	816	CLA	O1D-CGD-O2D-CED
19	B1	848	CLA	O1D-CGD-O2D-CED
19	F1	301	CLA	O1D-CGD-O2D-CED
19	A2	828	CLA	O1D-CGD-O2D-CED
19	B2	803	CLA	O1D-CGD-O2D-CED
19	B2	806	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O1D-CGD-O2D-CED
19	B	816	CLA	O1D-CGD-O2D-CED
19	B	833	CLA	O1D-CGD-O2D-CED
19	B	859	CLA	O1D-CGD-O2D-CED
19	AA	828	CLA	O1D-CGD-O2D-CED
19	BB	803	CLA	O1D-CGD-O2D-CED
19	BB	808	CLA	O1D-CGD-O2D-CED
19	BB	852	CLA	O1D-CGD-O2D-CED
19	BB	856	CLA	O1D-CGD-O2D-CED
19	A1	801	CLA	CBD-CGD-O2D-CED
19	A1	827	CLA	CBD-CGD-O2D-CED
19	A1	829	CLA	CBD-CGD-O2D-CED
19	A1	830	CLA	CBD-CGD-O2D-CED
19	A1	834	CLA	CBD-CGD-O2D-CED
19	A1	836	CLA	CBD-CGD-O2D-CED
19	B1	801	CLA	CBD-CGD-O2D-CED
19	B1	803	CLA	CBD-CGD-O2D-CED
19	B1	806	CLA	CBD-CGD-O2D-CED
19	B1	810	CLA	CBD-CGD-O2D-CED
19	B1	815	CLA	CBD-CGD-O2D-CED
19	B1	816	CLA	CBD-CGD-O2D-CED
19	B1	850	CLA	CBD-CGD-O2D-CED
19	F1	301	CLA	CBD-CGD-O2D-CED
19	J1	101	CLA	CBD-CGD-O2D-CED
19	L1	207	CLA	CBD-CGD-O2D-CED
19	A2	801	CLA	CBD-CGD-O2D-CED
19	A2	811	CLA	CBD-CGD-O2D-CED
19	A2	816	CLA	CBD-CGD-O2D-CED
19	A2	830	CLA	CBD-CGD-O2D-CED
19	A2	831	CLA	CBD-CGD-O2D-CED
19	A2	832	CLA	CBD-CGD-O2D-CED
19	A2	836	CLA	CBD-CGD-O2D-CED
19	A2	837	CLA	CBD-CGD-O2D-CED
19	B2	801	CLA	CBD-CGD-O2D-CED
19	B2	803	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B2	812	CLA	CBD-CGD-O2D-CED
19	B2	824	CLA	CBD-CGD-O2D-CED
19	B2	827	CLA	CBD-CGD-O2D-CED
19	B2	852	CLA	CBD-CGD-O2D-CED
19	F2	301	CLA	CBD-CGD-O2D-CED
19	J2	101	CLA	CBD-CGD-O2D-CED
19	A	801	CLA	CBD-CGD-O2D-CED
19	A	804	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	823	CLA	CBD-CGD-O2D-CED
19	A	824	CLA	CBD-CGD-O2D-CED
19	A	831	CLA	CBD-CGD-O2D-CED
19	B	806	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	B	816	CLA	CBD-CGD-O2D-CED
19	B	824	CLA	CBD-CGD-O2D-CED
19	B	827	CLA	CBD-CGD-O2D-CED
19	B	832	CLA	CBD-CGD-O2D-CED
19	B	854	CLA	CBD-CGD-O2D-CED
19	B	859	CLA	CBD-CGD-O2D-CED
19	F	301	CLA	CBD-CGD-O2D-CED
19	J	103	CLA	CBD-CGD-O2D-CED
19	AA	801	CLA	CBD-CGD-O2D-CED
19	AA	822	CLA	CBD-CGD-O2D-CED
19	AA	823	CLA	CBD-CGD-O2D-CED
19	AA	829	CLA	CBD-CGD-O2D-CED
19	BB	801	CLA	CBD-CGD-O2D-CED
19	BB	808	CLA	CBD-CGD-O2D-CED
19	BB	816	CLA	CBD-CGD-O2D-CED
19	BB	820	CLA	CBD-CGD-O2D-CED
19	BB	824	CLA	CBD-CGD-O2D-CED
19	BB	830	CLA	CBD-CGD-O2D-CED
19	BB	831	CLA	CBD-CGD-O2D-CED
19	BB	856	CLA	CBD-CGD-O2D-CED
19	FF	301	CLA	CBD-CGD-O2D-CED
19	LL	203	CLA	CBD-CGD-O2D-CED
19	B1	806	CLA	O1A-CGA-O2A-C1
19	B1	807	CLA	O1A-CGA-O2A-C1
19	B2	806	CLA	O1A-CGA-O2A-C1
19	B2	807	CLA	O1A-CGA-O2A-C1
19	B	806	CLA	O1A-CGA-O2A-C1
19	BB	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A1	802	CL0	O1A-CGA-O2A-C1
22	L1	211	LHG	O10-C23-O8-C6
19	K1	103	CLA	O1A-CGA-O2A-C1
19	A2	802	CLA	O1A-CGA-O2A-C1
19	KK	102	CLA	O1A-CGA-O2A-C1
25	I2	105	LMG	C4-C5-C6-O5
19	A1	815	CLA	O1D-CGD-O2D-CED
19	B1	810	CLA	O1D-CGD-O2D-CED
19	B1	850	CLA	O1D-CGD-O2D-CED
19	B2	849	CLA	O1D-CGD-O2D-CED
19	B	803	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
19	F	301	CLA	O1D-CGD-O2D-CED
19	BB	824	CLA	O1D-CGD-O2D-CED
19	FF	301	CLA	O1D-CGD-O2D-CED
19	LL	203	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	C4C-C3C-CAC-CBC
19	BB	829	CLA	C2C-C3C-CAC-CBC
19	A1	810	CLA	O1D-CGD-O2D-CED
19	A1	844	CLA	O1D-CGD-O2D-CED
19	K1	105	CLA	O1D-CGD-O2D-CED
19	L1	207	CLA	O1D-CGD-O2D-CED
19	A2	816	CLA	O1D-CGD-O2D-CED
19	A2	823	CLA	O1D-CGD-O2D-CED
19	A2	825	CLA	O1D-CGD-O2D-CED
19	A2	844	CLA	O1D-CGD-O2D-CED
19	B2	810	CLA	O1D-CGD-O2D-CED
19	B2	824	CLA	O1D-CGD-O2D-CED
19	F2	301	CLA	O1D-CGD-O2D-CED
19	F2	302	CLA	O1D-CGD-O2D-CED
19	L2	206	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	O1D-CGD-O2D-CED
19	A	816	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	B	824	CLA	O1D-CGD-O2D-CED
19	F	302	CLA	O1D-CGD-O2D-CED
19	L	204	CLA	O1D-CGD-O2D-CED
19	AA	811	CLA	O1D-CGD-O2D-CED
19	AA	816	CLA	O1D-CGD-O2D-CED
19	AA	845	CLA	O1D-CGD-O2D-CED
19	BB	810	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B1	807	CLA	CBA-CGA-O2A-C1
19	B2	806	CLA	CBA-CGA-O2A-C1
19	B2	807	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	BB	806	CLA	CBA-CGA-O2A-C1
25	B1	844	LMG	C29-C28-O8-C9
25	B1	852	LMG	C29-C28-O8-C9
25	B2	845	LMG	C29-C28-O8-C9
25	B2	854	LMG	C29-C28-O8-C9
25	B	845	LMG	C29-C28-O8-C9
19	A1	819	CLA	CBD-CGD-O2D-CED
19	A1	823	CLA	CBD-CGD-O2D-CED
19	A1	825	CLA	CBD-CGD-O2D-CED
19	A1	828	CLA	CBD-CGD-O2D-CED
19	A1	831	CLA	CBD-CGD-O2D-CED
19	A1	835	CLA	CBD-CGD-O2D-CED
19	A1	837	CLA	CBD-CGD-O2D-CED
19	A1	852	CLA	CBD-CGD-O2D-CED
19	B1	820	CLA	CBD-CGD-O2D-CED
19	B1	831	CLA	CBD-CGD-O2D-CED
19	B1	836	CLA	CBD-CGD-O2D-CED
19	A2	808	CLA	CBD-CGD-O2D-CED
19	A2	814	CLA	CBD-CGD-O2D-CED
19	A2	826	CLA	CBD-CGD-O2D-CED
19	A2	829	CLA	CBD-CGD-O2D-CED
19	A2	838	CLA	CBD-CGD-O2D-CED
19	B2	829	CLA	CBD-CGD-O2D-CED
19	B2	832	CLA	CBD-CGD-O2D-CED
19	B2	837	CLA	CBD-CGD-O2D-CED
19	A	813	CLA	CBD-CGD-O2D-CED
19	A	829	CLA	CBD-CGD-O2D-CED
19	A	834	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	A	844	CLA	CBD-CGD-O2D-CED
19	B	815	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED
19	J	101	CLA	CBD-CGD-O2D-CED
19	K	102	CLA	CBD-CGD-O2D-CED
19	AA	817	CLA	CBD-CGD-O2D-CED
19	AA	820	CLA	CBD-CGD-O2D-CED
19	AA	831	CLA	CBD-CGD-O2D-CED
19	AA	834	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	AA	836	CLA	CBD-CGD-O2D-CED
19	BB	815	CLA	CBD-CGD-O2D-CED
19	JJ	101	CLA	CBD-CGD-O2D-CED
19	KK	102	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	C2C-C3C-CAC-CBC
19	A1	814	CLA	O1A-CGA-O2A-C1
19	B1	833	CLA	O1A-CGA-O2A-C1
19	A2	815	CLA	O1A-CGA-O2A-C1
19	A2	839	CLA	O1A-CGA-O2A-C1
19	B2	802	CLA	O1A-CGA-O2A-C1
19	B2	834	CLA	O1A-CGA-O2A-C1
19	A	815	CLA	O1A-CGA-O2A-C1
19	A	839	CLA	O1A-CGA-O2A-C1
19	B	826	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	O1A-CGA-O2A-C1
19	AA	815	CLA	O1A-CGA-O2A-C1
19	AA	839	CLA	O1A-CGA-O2A-C1
19	BB	802	CLA	O1A-CGA-O2A-C1
19	BB	807	CLA	O1A-CGA-O2A-C1
19	BB	833	CLA	O1A-CGA-O2A-C1
19	FF	301	CLA	O1A-CGA-O2A-C1
20	AA	803	CL0	O1A-CGA-O2A-C1
22	L2	208	LHG	O10-C23-O8-C6
25	B1	846	LMG	O10-C28-O8-C9
25	B1	852	LMG	O10-C28-O8-C9
25	I1	102	LMG	O10-C28-O8-C9
25	B2	847	LMG	O10-C28-O8-C9
25	B2	854	LMG	O10-C28-O8-C9
28	B	856	DGD	O1A-C1A-O1G-C1G
28	BB	854	DGD	O1A-C1A-O1G-C1G
19	A1	803	CLA	O1D-CGD-O2D-CED
19	B1	824	CLA	O1D-CGD-O2D-CED
19	F1	302	CLA	O1D-CGD-O2D-CED
19	A2	804	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1D-CGD-O2D-CED
19	FF	302	CLA	O1D-CGD-O2D-CED
19	B2	834	CLA	C4C-C3C-CAC-CBC
19	A1	833	CLA	O1D-CGD-O2D-CED
19	B1	827	CLA	O1D-CGD-O2D-CED
19	A2	834	CLA	O1D-CGD-O2D-CED
19	B2	816	CLA	O1D-CGD-O2D-CED
19	B2	851	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	835	CLA	O1D-CGD-O2D-CED
19	AA	830	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	CBD-CGD-O2D-CED
19	A	817	CLA	CBD-CGD-O2D-CED
19	B	819	CLA	CBD-CGD-O2D-CED
19	AA	813	CLA	CBD-CGD-O2D-CED
19	A1	830	CLA	O1D-CGD-O2D-CED
19	A1	834	CLA	O1D-CGD-O2D-CED
19	A1	836	CLA	O1D-CGD-O2D-CED
19	A2	835	CLA	O1D-CGD-O2D-CED
19	B2	801	CLA	O1D-CGD-O2D-CED
19	B	801	CLA	O1D-CGD-O2D-CED
19	AA	804	CLA	O1D-CGD-O2D-CED
19	AA	835	CLA	O1D-CGD-O2D-CED
25	I1	102	LMG	O9-C10-O7-C8
25	II	105	LMG	O9-C10-O7-C8
28	B	856	DGD	O1B-C1B-O2G-C2G
28	BB	854	DGD	O1B-C1B-O2G-C2G
19	BB	826	CLA	O1A-CGA-O2A-C1
25	B	845	LMG	O10-C28-O8-C9
19	A1	822	CLA	C3-C5-C6-C7
19	A2	823	CLA	C3-C5-C6-C7
19	B2	804	CLA	C3-C5-C6-C7
19	L2	205	CLA	C3-C5-C6-C7
19	A	823	CLA	C3-C5-C6-C7
19	A	835	CLA	C3-C5-C6-C7
19	B	804	CLA	C3-C5-C6-C7
19	AA	808	CLA	C3-C5-C6-C7
19	AA	823	CLA	C3-C5-C6-C7
19	AA	835	CLA	C3-C5-C6-C7
19	BB	804	CLA	C3-C5-C6-C7
19	FF	301	CLA	C3-C5-C6-C7
19	A1	801	CLA	CBA-CGA-O2A-C1
19	A1	814	CLA	CBA-CGA-O2A-C1
19	A1	821	CLA	CBA-CGA-O2A-C1
19	B1	833	CLA	CBA-CGA-O2A-C1
19	A2	801	CLA	CBA-CGA-O2A-C1
19	A2	815	CLA	CBA-CGA-O2A-C1
19	B2	834	CLA	CBA-CGA-O2A-C1
19	A	801	CLA	CBA-CGA-O2A-C1
19	A	813	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	807	CLA	CBA-CGA-O2A-C1
19	B	834	CLA	CBA-CGA-O2A-C1
19	AA	813	CLA	CBA-CGA-O2A-C1
19	AA	815	CLA	CBA-CGA-O2A-C1
19	BB	816	CLA	CBA-CGA-O2A-C1
19	BB	833	CLA	CBA-CGA-O2A-C1
20	A1	802	CL0	CBA-CGA-O2A-C1
20	AA	803	CL0	CBA-CGA-O2A-C1
22	L1	211	LHG	C24-C23-O8-C6
22	L2	208	LHG	C24-C23-O8-C6
25	B1	846	LMG	C29-C28-O8-C9
25	B2	847	LMG	C29-C28-O8-C9
25	BB	844	LMG	C29-C28-O8-C9
22	L1	211	LHG	C8-C7-O7-C5
22	L2	208	LHG	C8-C7-O7-C5
22	L	207	LHG	C8-C7-O7-C5
22	LL	205	LHG	C8-C7-O7-C5
19	A2	811	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	O1D-CGD-O2D-CED
19	BB	801	CLA	O1D-CGD-O2D-CED
19	A1	812	CLA	CBD-CGD-O2D-CED
19	B1	808	CLA	CBD-CGD-O2D-CED
19	B1	812	CLA	CBD-CGD-O2D-CED
19	A2	820	CLA	CBD-CGD-O2D-CED
19	B2	831	CLA	CBD-CGD-O2D-CED
19	BB	812	CLA	CBD-CGD-O2D-CED
19	B2	834	CLA	C2C-C3C-CAC-CBC
19	A1	812	CLA	O1A-CGA-O2A-C1
19	A1	820	CLA	O1A-CGA-O2A-C1
25	I2	105	LMG	O6-C5-C6-O5
19	A	825	CLA	C3-C5-C6-C7
19	AA	825	CLA	C3-C5-C6-C7
19	B1	826	CLA	C4-C3-C5-C6
19	BB	833	CLA	C4-C3-C5-C6
19	B1	826	CLA	C2-C3-C5-C6
19	B	816	CLA	C2-C3-C5-C6
19	B	826	CLA	C2-C3-C5-C6
19	B	834	CLA	C2-C3-C5-C6
19	BB	852	CLA	C2-C3-C5-C6
21	A2	843	PQN	C12-C13-C15-C16
21	A	843	PQN	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A2	813	CLA	CBD-CGD-O2D-CED
19	B2	834	CLA	CBD-CGD-O2D-CED
19	AA	808	CLA	CBD-CGD-O2D-CED
19	AA	838	CLA	CBD-CGD-O2D-CED
19	A1	811	CLA	C2A-CAA-CBA-CGA
19	A1	828	CLA	C2A-CAA-CBA-CGA
19	A1	829	CLA	C2A-CAA-CBA-CGA
19	B1	835	CLA	C2A-CAA-CBA-CGA
19	A2	830	CLA	C2A-CAA-CBA-CGA
19	A2	852	CLA	C2A-CAA-CBA-CGA
19	B2	836	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2A-CAA-CBA-CGA
19	AA	830	CLA	C2A-CAA-CBA-CGA
19	BB	835	CLA	C2A-CAA-CBA-CGA
19	FF	301	CLA	C2A-CAA-CBA-CGA
19	A1	838	CLA	O1A-CGA-O2A-C1
19	A2	808	CLA	O1A-CGA-O2A-C1
19	B2	801	CLA	O1A-CGA-O2A-C1
19	AA	808	CLA	O1A-CGA-O2A-C1
25	B1	844	LMG	O10-C28-O8-C9
25	B2	845	LMG	O10-C28-O8-C9
19	A1	829	CLA	O1D-CGD-O2D-CED
19	A	820	CLA	O1D-CGD-O2D-CED
19	B1	804	CLA	C3-C5-C6-C7
19	A2	808	CLA	C3-C5-C6-C7
19	B	807	CLA	C3-C5-C6-C7
19	BB	807	CLA	C3-C5-C6-C7
20	A	803	CL0	C3-C5-C6-C7
19	A1	807	CLA	CBA-CGA-O2A-C1
19	A1	812	CLA	CBA-CGA-O2A-C1
19	A2	813	CLA	CBA-CGA-O2A-C1
19	A2	839	CLA	CBA-CGA-O2A-C1
19	B2	801	CLA	CBA-CGA-O2A-C1
19	B2	802	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	CBA-CGA-O2A-C1
19	A	819	CLA	CBA-CGA-O2A-C1
19	A	839	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	CBA-CGA-O2A-C1
19	B	826	CLA	CBA-CGA-O2A-C1
19	F	301	CLA	CBA-CGA-O2A-C1
19	AA	801	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	AA	819	CLA	CBA-CGA-O2A-C1
19	AA	839	CLA	CBA-CGA-O2A-C1
19	AA	843	CLA	CBA-CGA-O2A-C1
19	BB	801	CLA	CBA-CGA-O2A-C1
19	BB	802	CLA	CBA-CGA-O2A-C1
19	BB	807	CLA	CBA-CGA-O2A-C1
19	BB	826	CLA	CBA-CGA-O2A-C1
19	BB	832	CLA	CBA-CGA-O2A-C1
19	FF	301	CLA	CBA-CGA-O2A-C1
20	A	803	CL0	CBA-CGA-O2A-C1
25	II	105	LMG	C29-C28-O8-C9
28	B	856	DGD	C2A-C1A-O1G-C1G
28	BB	854	DGD	C2A-C1A-O1G-C1G
25	B1	846	LMG	C4-C5-C6-O5
19	A2	837	CLA	O1D-CGD-O2D-CED
19	B	832	CLA	O1D-CGD-O2D-CED
19	B2	820	CLA	CBD-CGD-O2D-CED
19	B	860	CLA	CBD-CGD-O2D-CED
19	AA	853	CLA	CBD-CGD-O2D-CED
19	BB	819	CLA	CBD-CGD-O2D-CED
19	XX	101	CLA	CBD-CGD-O2D-CED
19	A1	801	CLA	O1D-CGD-O2D-CED
19	B1	801	CLA	O1D-CGD-O2D-CED
19	J1	101	CLA	O1D-CGD-O2D-CED
19	B2	827	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	O1D-CGD-O2D-CED
19	J	103	CLA	O1D-CGD-O2D-CED
19	AA	822	CLA	O1D-CGD-O2D-CED
19	BB	820	CLA	O1D-CGD-O2D-CED
19	A1	818	CLA	O1A-CGA-O2A-C1
19	A1	821	CLA	O1A-CGA-O2A-C1
19	B1	801	CLA	O1A-CGA-O2A-C1
19	B1	802	CLA	O1A-CGA-O2A-C1
19	B1	826	CLA	O1A-CGA-O2A-C1
19	A2	813	CLA	O1A-CGA-O2A-C1
19	A2	819	CLA	O1A-CGA-O2A-C1
19	A2	821	CLA	O1A-CGA-O2A-C1
19	A2	822	CLA	O1A-CGA-O2A-C1
19	B2	826	CLA	O1A-CGA-O2A-C1
19	B2	852	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	O1A-CGA-O2A-C1
19	A	821	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	801	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	O1A-CGA-O2A-C1
19	B	860	CLA	O1A-CGA-O2A-C1
19	AA	819	CLA	O1A-CGA-O2A-C1
19	AA	821	CLA	O1A-CGA-O2A-C1
19	AA	843	CLA	O1A-CGA-O2A-C1
25	M	102	LMG	O10-C28-O8-C9
25	BB	844	LMG	O10-C28-O8-C9
19	BB	831	CLA	O1D-CGD-O2D-CED
23	A1	853	BCR	C13-C14-C15-C16
23	F1	306	BCR	C15-C16-C17-C18
23	A2	853	BCR	C13-C14-C15-C16
23	A2	853	BCR	C15-C16-C17-C18
23	I2	101	BCR	C9-C10-C11-C12
23	L2	207	BCR	C9-C10-C11-C12
23	A	853	BCR	C15-C16-C17-C18
23	AA	854	BCR	C15-C16-C17-C18
23	LL	204	BCR	C9-C10-C11-C12
23	MM	101	BCR	C19-C20-C21-C22
19	A1	807	CLA	CBD-CGD-O2D-CED
19	A1	814	CLA	CBD-CGD-O2D-CED
19	A1	842	CLA	CBD-CGD-O2D-CED
19	B1	819	CLA	CBD-CGD-O2D-CED
19	B1	830	CLA	CBD-CGD-O2D-CED
19	A2	815	CLA	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	CBD-CGD-O2D-CED
19	A	838	CLA	CBD-CGD-O2D-CED
19	A	852	CLA	CBD-CGD-O2D-CED
19	AA	815	CLA	CBD-CGD-O2D-CED
19	BB	813	CLA	CBD-CGD-O2D-CED
19	BB	836	CLA	CBD-CGD-O2D-CED
20	A2	803	CL0	CBD-CGD-O2D-CED
20	AA	803	CL0	CBD-CGD-O2D-CED
19	A2	830	CLA	O1D-CGD-O2D-CED
19	A	801	CLA	O1D-CGD-O2D-CED
19	BB	830	CLA	O1D-CGD-O2D-CED
22	A1	845	LHG	O2-C2-C3-O3
22	B1	847	LHG	O2-C2-C3-O3
22	B2	848	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	L2	208	LHG	O2-C2-C3-O3
22	B	853	LHG	O2-C2-C3-O3
22	BB	851	LHG	O2-C2-C3-O3
19	A1	809	CLA	CBA-CGA-O2A-C1
19	A1	822	CLA	CBA-CGA-O2A-C1
19	A1	835	CLA	CBA-CGA-O2A-C1
19	A1	838	CLA	CBA-CGA-O2A-C1
19	B1	830	CLA	CBA-CGA-O2A-C1
19	B1	832	CLA	CBA-CGA-O2A-C1
19	A2	808	CLA	CBA-CGA-O2A-C1
19	A2	819	CLA	CBA-CGA-O2A-C1
19	A2	820	CLA	CBA-CGA-O2A-C1
19	A2	823	CLA	CBA-CGA-O2A-C1
19	B2	823	CLA	CBA-CGA-O2A-C1
19	B2	826	CLA	CBA-CGA-O2A-C1
19	B2	831	CLA	CBA-CGA-O2A-C1
19	B2	833	CLA	CBA-CGA-O2A-C1
19	B2	852	CLA	CBA-CGA-O2A-C1
19	F2	301	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	CBA-CGA-O2A-C1
19	B	833	CLA	CBA-CGA-O2A-C1
19	B	860	CLA	CBA-CGA-O2A-C1
19	AA	808	CLA	CBA-CGA-O2A-C1
19	AA	820	CLA	CBA-CGA-O2A-C1
19	AA	821	CLA	CBA-CGA-O2A-C1
19	BB	823	CLA	CBA-CGA-O2A-C1
19	BB	830	CLA	CBA-CGA-O2A-C1
25	I1	102	LMG	C29-C28-O8-C9
25	M	102	LMG	C29-C28-O8-C9
19	A1	801	CLA	O1A-CGA-O2A-C1
19	A1	842	CLA	O1A-CGA-O2A-C1
19	A2	801	CLA	O1A-CGA-O2A-C1
19	A	801	CLA	O1A-CGA-O2A-C1
19	A	813	CLA	O1A-CGA-O2A-C1
19	F	301	CLA	O1A-CGA-O2A-C1
19	AA	801	CLA	O1A-CGA-O2A-C1
19	AA	813	CLA	O1A-CGA-O2A-C1
19	BB	816	CLA	O1A-CGA-O2A-C1
25	II	105	LMG	O10-C28-O8-C9
25	M	102	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
19	A2	831	CLA	O1D-CGD-O2D-CED
19	B	812	CLA	O1D-CGD-O2D-CED
19	AA	829	CLA	O1D-CGD-O2D-CED
19	A1	840	CLA	CBA-CGA-O2A-C1
19	A2	841	CLA	CBA-CGA-O2A-C1
19	B2	823	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	B	823	CLA	CBD-CGD-O2D-CED
19	AA	826	CLA	CBD-CGD-O2D-CED
19	BB	823	CLA	CBD-CGD-O2D-CED
23	B2	844	BCR	C14-C15-C16-C17
23	A	848	BCR	C14-C15-C16-C17
23	AA	849	BCR	C14-C15-C16-C17
25	M	102	LMG	C4-C5-C6-O5
19	B1	815	CLA	O1D-CGD-O2D-CED
19	A2	832	CLA	O1D-CGD-O2D-CED
19	A2	836	CLA	O1D-CGD-O2D-CED
19	A1	826	CLA	CBD-CGD-O2D-CED
19	AA	843	CLA	CBD-CGD-O2D-CED
19	B1	815	CLA	C3-C5-C6-C7
19	A2	805	CLA	C3-C5-C6-C7
19	B2	815	CLA	C3-C5-C6-C7
19	A1	818	CLA	CBA-CGA-O2A-C1
19	A1	820	CLA	CBA-CGA-O2A-C1
19	A1	842	CLA	CBA-CGA-O2A-C1
19	B1	801	CLA	CBA-CGA-O2A-C1
19	B1	802	CLA	CBA-CGA-O2A-C1
19	B1	826	CLA	CBA-CGA-O2A-C1
19	A2	821	CLA	CBA-CGA-O2A-C1
19	A2	822	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	CBA-CGA-O2A-C1
19	B	801	CLA	CBA-CGA-O2A-C1
19	B	802	CLA	CBA-CGA-O2A-C1
19	AA	823	CLA	CBA-CGA-O2A-C1
19	J2	101	CLA	O1D-CGD-O2D-CED
25	B1	846	LMG	O6-C5-C6-O5
19	A1	809	CLA	O1A-CGA-O2A-C1
19	B1	832	CLA	O1A-CGA-O2A-C1
19	B2	823	CLA	O1A-CGA-O2A-C1
19	B2	833	CLA	O1A-CGA-O2A-C1
19	B	816	CLA	O1A-CGA-O2A-C1
19	B	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	831	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	O1A-CGA-O2A-C1
19	AA	820	CLA	O1A-CGA-O2A-C1
19	BB	801	CLA	O1A-CGA-O2A-C1
19	BB	823	CLA	O1A-CGA-O2A-C1
25	L1	210	LMG	O10-C28-O8-C9
19	AA	812	CLA	CBA-CGA-O2A-C1
19	A1	818	CLA	C4-C3-C5-C6
19	A1	828	CLA	C4-C3-C5-C6
19	B1	811	CLA	C4-C3-C5-C6
19	B1	816	CLA	C4-C3-C5-C6
19	B1	823	CLA	C4-C3-C5-C6
19	B1	833	CLA	C4-C3-C5-C6
19	B1	850	CLA	C4-C3-C5-C6
19	A2	819	CLA	C4-C3-C5-C6
19	B2	811	CLA	C4-C3-C5-C6
19	B2	816	CLA	C4-C3-C5-C6
19	B2	823	CLA	C4-C3-C5-C6
19	B2	834	CLA	C4-C3-C5-C6
19	B2	851	CLA	C4-C3-C5-C6
19	A	810	CLA	C4-C3-C5-C6
19	A	819	CLA	C4-C3-C5-C6
19	A	842	CLA	C4-C3-C5-C6
19	B	811	CLA	C4-C3-C5-C6
19	B	823	CLA	C4-C3-C5-C6
19	B	859	CLA	C4-C3-C5-C6
19	L	202	CLA	C4-C3-C5-C6
19	AA	810	CLA	C4-C3-C5-C6
19	AA	819	CLA	C4-C3-C5-C6
19	AA	842	CLA	C4-C3-C5-C6
19	BB	811	CLA	C4-C3-C5-C6
19	BB	816	CLA	C4-C3-C5-C6
19	BB	823	CLA	C4-C3-C5-C6
19	BB	856	CLA	C4-C3-C5-C6
19	LL	201	CLA	C4-C3-C5-C6
20	AA	803	CL0	C4-C3-C5-C6
19	A1	818	CLA	C2-C3-C5-C6
19	A1	828	CLA	C2-C3-C5-C6
19	A1	841	CLA	C2-C3-C5-C6
19	B1	811	CLA	C2-C3-C5-C6
19	B1	816	CLA	C2-C3-C5-C6
19	B1	823	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B1	833	CLA	C2-C3-C5-C6
19	B1	850	CLA	C2-C3-C5-C6
19	A2	819	CLA	C2-C3-C5-C6
19	A2	842	CLA	C2-C3-C5-C6
19	B2	811	CLA	C2-C3-C5-C6
19	B2	816	CLA	C2-C3-C5-C6
19	B2	823	CLA	C2-C3-C5-C6
19	B2	834	CLA	C2-C3-C5-C6
19	B2	851	CLA	C2-C3-C5-C6
19	A	810	CLA	C2-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	A	842	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	B	823	CLA	C2-C3-C5-C6
19	B	859	CLA	C2-C3-C5-C6
19	L	202	CLA	C2-C3-C5-C6
19	AA	810	CLA	C2-C3-C5-C6
19	AA	819	CLA	C2-C3-C5-C6
19	AA	842	CLA	C2-C3-C5-C6
19	BB	811	CLA	C2-C3-C5-C6
19	BB	816	CLA	C2-C3-C5-C6
19	BB	823	CLA	C2-C3-C5-C6
19	BB	833	CLA	C2-C3-C5-C6
19	BB	856	CLA	C2-C3-C5-C6
19	LL	201	CLA	C2-C3-C5-C6
20	AA	803	CL0	C2-C3-C5-C6
19	A2	812	CLA	C2A-CAA-CBA-CGA
19	B	836	CLA	C2A-CAA-CBA-CGA
19	AA	829	CLA	C2A-CAA-CBA-CGA
19	A1	835	CLA	O1D-CGD-O2D-CED
19	B2	852	CLA	O1D-CGD-O2D-CED
19	AA	831	CLA	O1D-CGD-O2D-CED
19	AA	834	CLA	O1D-CGD-O2D-CED
19	A1	822	CLA	O1A-CGA-O2A-C1
19	A1	835	CLA	O1A-CGA-O2A-C1
19	B1	830	CLA	O1A-CGA-O2A-C1
19	A2	823	CLA	O1A-CGA-O2A-C1
19	B2	831	CLA	O1A-CGA-O2A-C1
19	F2	301	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	O1A-CGA-O2A-C1
19	BB	830	CLA	O1A-CGA-O2A-C1
19	BB	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	803	CL0	O1A-CGA-O2A-C1
19	A1	819	CLA	CBA-CGA-O2A-C1
19	F1	301	CLA	CBA-CGA-O2A-C1
19	B2	811	CLA	CBA-CGA-O2A-C1
19	B	811	CLA	CBA-CGA-O2A-C1
19	L	202	CLA	CBA-CGA-O2A-C1
20	A2	803	CL0	CBA-CGA-O2A-C1
22	A2	846	LHG	C24-C23-O8-C6
22	B2	848	LHG	C24-C23-O8-C6
19	A2	830	CLA	C2C-C3C-CAC-CBC
19	A1	823	CLA	O1D-CGD-O2D-CED
19	B2	812	CLA	O1D-CGD-O2D-CED
19	B	837	CLA	O1D-CGD-O2D-CED
19	AA	801	CLA	O1D-CGD-O2D-CED
19	A2	820	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	O1A-CGA-O2A-C1
19	AA	823	CLA	O1A-CGA-O2A-C1
19	A1	825	CLA	O1D-CGD-O2D-CED
19	A1	831	CLA	O1D-CGD-O2D-CED
19	A1	837	CLA	O1D-CGD-O2D-CED
19	A1	852	CLA	O1D-CGD-O2D-CED
19	B1	831	CLA	O1D-CGD-O2D-CED
19	A2	808	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	O1D-CGD-O2D-CED
19	AA	820	CLA	O1D-CGD-O2D-CED
19	A1	813	CLA	CBD-CGD-O2D-CED
22	B1	847	LHG	C1-C2-C3-O3
25	II	105	LMG	O6-C5-C6-O5
19	A1	819	CLA	O1A-CGA-O2A-C1
19	F1	301	CLA	O1A-CGA-O2A-C1
20	A2	803	CL0	O1A-CGA-O2A-C1
19	F1	301	CLA	C3-C5-C6-C7
19	A2	815	CLA	C3-C5-C6-C7
19	B	815	CLA	C3-C5-C6-C7
19	B1	820	CLA	O1D-CGD-O2D-CED
19	A2	838	CLA	O1D-CGD-O2D-CED
19	A1	804	CLA	CBA-CGA-O2A-C1
19	B1	821	CLA	CBA-CGA-O2A-C1
19	B1	823	CLA	CBA-CGA-O2A-C1
19	A2	805	CLA	CBA-CGA-O2A-C1
19	A2	810	CLA	CBA-CGA-O2A-C1
19	A2	836	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B2	821	CLA	CBA-CGA-O2A-C1
19	A	805	CLA	CBA-CGA-O2A-C1
19	A	810	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	CBA-CGA-O2A-C1
19	AA	805	CLA	CBA-CGA-O2A-C1
19	AA	810	CLA	CBA-CGA-O2A-C1
19	AA	827	CLA	CBA-CGA-O2A-C1
19	BB	803	CLA	CBA-CGA-O2A-C1
19	LL	201	CLA	CBA-CGA-O2A-C1
22	A1	846	LHG	C24-C23-O8-C6
22	X2	103	LHG	C24-C23-O8-C6
22	B	853	LHG	C24-C23-O8-C6
22	BB	851	LHG	C24-C23-O8-C6
25	L1	210	LMG	C29-C28-O8-C9
19	A	821	CLA	C8-C10-C11-C12
19	B1	835	CLA	CBD-CGD-O2D-CED
19	B	836	CLA	CBD-CGD-O2D-CED
19	K	102	CLA	O1D-CGD-O2D-CED
23	A1	853	BCR	C15-C16-C17-C18
23	B1	841	BCR	C13-C14-C15-C16
23	I1	101	BCR	C9-C10-C11-C12
23	B	842	BCR	C13-C14-C15-C16
26	BB	840	ECH	C15-C16-C17-C18
19	A1	801	CLA	C8-C10-C11-C12
19	K1	105	CLA	C2C-C3C-CAC-CBC
28	B	856	DGD	O6E-C5E-C6E-O5E
19	B1	807	CLA	C15-C16-C17-C18
19	A2	821	CLA	C8-C10-C11-C12
19	A2	829	CLA	C10-C11-C12-C13
19	B2	807	CLA	C15-C16-C17-C18
19	A	808	CLA	C10-C11-C12-C13
19	B	815	CLA	C10-C11-C12-C13
19	AA	808	CLA	C10-C11-C12-C13
19	BB	803	CLA	C8-C10-C11-C12
19	B1	823	CLA	O1A-CGA-O2A-C1
19	A2	810	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	O1A-CGA-O2A-C1
25	B	851	LMG	O10-C28-O8-C9
19	B1	821	CLA	C4-C3-C5-C6
19	A1	803	CLA	C6-C7-C8-C9
19	A1	852	CLA	C11-C10-C8-C9
19	B1	816	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B1	823	CLA	C6-C7-C8-C9
19	B1	825	CLA	C14-C13-C15-C16
19	B1	833	CLA	C14-C13-C15-C16
19	A2	804	CLA	C6-C7-C8-C9
19	A2	813	CLA	C6-C7-C8-C9
19	A2	829	CLA	C11-C10-C8-C9
19	A2	852	CLA	C11-C10-C8-C9
19	B2	807	CLA	C6-C7-C8-C9
19	B2	816	CLA	C6-C7-C8-C9
19	B2	825	CLA	C14-C13-C15-C16
19	B2	836	CLA	C6-C7-C8-C9
19	L2	205	CLA	C6-C7-C8-C9
19	A	804	CLA	C6-C7-C8-C9
19	A	827	CLA	C14-C13-C15-C16
19	A	829	CLA	C11-C10-C8-C9
19	A	852	CLA	C11-C10-C8-C9
19	B	807	CLA	C6-C7-C8-C9
19	B	807	CLA	C14-C13-C15-C16
19	B	825	CLA	C14-C13-C15-C16
19	B	834	CLA	C14-C13-C15-C16
19	B	836	CLA	C6-C7-C8-C9
19	AA	804	CLA	C6-C7-C8-C9
19	AA	829	CLA	C11-C10-C8-C9
19	AA	853	CLA	C11-C10-C8-C9
19	BB	807	CLA	C6-C7-C8-C9
19	BB	807	CLA	C14-C13-C15-C16
19	BB	815	CLA	C14-C13-C15-C16
19	BB	823	CLA	C6-C7-C8-C9
19	BB	825	CLA	C14-C13-C15-C16
19	BB	835	CLA	C6-C7-C8-C9
20	A2	803	CL0	C11-C10-C8-C9
20	AA	803	CL0	C6-C7-C8-C9
19	A1	828	CLA	O1D-CGD-O2D-CED
19	A2	826	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	O1D-CGD-O2D-CED
19	A	844	CLA	O1D-CGD-O2D-CED
19	J	101	CLA	O1D-CGD-O2D-CED
19	AA	836	CLA	O1D-CGD-O2D-CED
19	JJ	101	CLA	O1D-CGD-O2D-CED
19	B2	819	CLA	CBD-CGD-O2D-CED
19	A	837	CLA	CBD-CGD-O2D-CED
19	B1	801	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	822	CLA	C13-C15-C16-C17
19	AA	821	CLA	C8-C10-C11-C12
19	B1	836	CLA	C2A-CAA-CBA-CGA
19	F1	301	CLA	C2A-CAA-CBA-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
19	AA	843	CLA	C2A-CAA-CBA-CGA
20	A	803	CL0	C2A-CAA-CBA-CGA
23	A1	848	BCR	C7-C8-C9-C34
23	A1	850	BCR	C11-C12-C13-C35
23	A1	853	BCR	C7-C8-C9-C34
23	A1	853	BCR	C37-C22-C23-C24
23	B1	838	BCR	C7-C8-C9-C34
23	B1	838	BCR	C37-C22-C23-C24
23	B1	841	BCR	C7-C8-C9-C34
23	F1	306	BCR	C7-C8-C9-C34
23	J1	102	BCR	C11-C12-C13-C35
23	K1	104	BCR	C37-C22-C23-C24
23	K1	106	BCR	C7-C8-C9-C34
23	L1	201	BCR	C7-C8-C9-C34
23	A2	848	BCR	C7-C8-C9-C34
23	A2	850	BCR	C11-C12-C13-C35
23	A2	853	BCR	C7-C8-C9-C34
23	A2	853	BCR	C37-C22-C23-C24
23	B2	839	BCR	C7-C8-C9-C34
23	B2	839	BCR	C37-C22-C23-C24
23	B2	843	BCR	C11-C12-C13-C35
23	F2	305	BCR	C36-C18-C19-C20
23	F2	305	BCR	C37-C22-C23-C24
23	J2	102	BCR	C11-C12-C13-C35
23	J2	104	BCR	C37-C22-C23-C24
23	K2	105	BCR	C7-C8-C9-C34
23	A	847	BCR	C7-C8-C9-C34
23	A	848	BCR	C37-C22-C23-C24
23	A	851	BCR	C11-C12-C13-C35
23	A	854	BCR	C7-C8-C9-C34
23	B	839	BCR	C7-C8-C9-C34
23	B	839	BCR	C37-C22-C23-C24
23	B	842	BCR	C7-C8-C9-C34
23	B	848	BCR	C11-C12-C13-C35
23	B	848	BCR	C37-C22-C23-C24
23	F	304	BCR	C7-C8-C9-C34
23	F	305	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	I	102	BCR	C7-C8-C9-C34
23	J	102	BCR	C11-C12-C13-C35
23	J	102	BCR	C36-C18-C19-C20
23	K	103	BCR	C36-C18-C19-C20
23	AA	849	BCR	C37-C22-C23-C24
23	AA	852	BCR	C11-C12-C13-C35
23	AA	855	BCR	C7-C8-C9-C34
23	BB	838	BCR	C7-C8-C9-C34
23	BB	838	BCR	C37-C22-C23-C24
23	BB	841	BCR	C7-C8-C9-C34
23	BB	847	BCR	C11-C12-C13-C35
23	BB	847	BCR	C37-C22-C23-C24
23	FF	303	BCR	C11-C12-C13-C35
23	FF	306	BCR	C7-C8-C9-C34
23	II	102	BCR	C7-C8-C9-C34
23	II	102	BCR	C37-C22-C23-C24
23	JJ	102	BCR	C11-C12-C13-C35
23	JJ	104	BCR	C37-C22-C23-C24
23	KK	103	BCR	C36-C18-C19-C20
23	MM	101	BCR	C7-C8-C9-C34
26	B	841	ECH	C11-C12-C13-C35
23	A1	853	BCR	C7-C8-C9-C10
23	A1	853	BCR	C21-C22-C23-C24
23	B1	838	BCR	C21-C22-C23-C24
23	B1	841	BCR	C7-C8-C9-C10
23	F1	306	BCR	C17-C18-C19-C20
23	K1	106	BCR	C17-C18-C19-C20
23	L1	201	BCR	C7-C8-C9-C10
23	A2	853	BCR	C7-C8-C9-C10
23	A2	853	BCR	C21-C22-C23-C24
23	B2	839	BCR	C21-C22-C23-C24
23	F2	305	BCR	C21-C22-C23-C24
23	I2	102	BCR	C7-C8-C9-C10
23	M2	102	BCR	C21-C22-C23-C24
23	A	853	BCR	C7-C8-C9-C10
23	A	853	BCR	C21-C22-C23-C24
23	B	839	BCR	C21-C22-C23-C24
23	B	842	BCR	C7-C8-C9-C10
23	B	848	BCR	C17-C18-C19-C20
23	B	848	BCR	C21-C22-C23-C24
23	I	102	BCR	C7-C8-C9-C10
23	AA	854	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	AA	855	BCR	C17-C18-C19-C20
23	BB	838	BCR	C21-C22-C23-C24
23	BB	841	BCR	C7-C8-C9-C10
23	BB	847	BCR	C17-C18-C19-C20
23	BB	847	BCR	C21-C22-C23-C24
23	II	102	BCR	C7-C8-C9-C10
23	JJ	104	BCR	C21-C22-C23-C24
25	I1	102	LMG	C11-C10-O7-C8
28	B	856	DGD	C2B-C1B-O2G-C2G
28	BB	854	DGD	C2B-C1B-O2G-C2G
19	B	837	CLA	C2C-C3C-CAC-CBC
19	LL	203	CLA	C2C-C3C-CAC-CBC
19	A1	804	CLA	O1A-CGA-O2A-C1
19	B1	821	CLA	O1A-CGA-O2A-C1
19	A2	805	CLA	O1A-CGA-O2A-C1
19	B2	821	CLA	O1A-CGA-O2A-C1
19	A	805	CLA	O1A-CGA-O2A-C1
19	AA	810	CLA	O1A-CGA-O2A-C1
19	A2	807	CLA	C5-C6-C7-C8
19	B2	801	CLA	C10-C11-C12-C13
19	B2	803	CLA	C8-C10-C11-C12
19	AA	804	CLA	C10-C11-C12-C13
19	A1	819	CLA	O1D-CGD-O2D-CED
19	A2	814	CLA	O1D-CGD-O2D-CED
19	B	815	CLA	O1D-CGD-O2D-CED
19	B2	808	CLA	CBD-CGD-O2D-CED
19	KK	102	CLA	O1D-CGD-O2D-CED
19	BB	815	CLA	C3-C5-C6-C7
19	A1	831	CLA	CBA-CGA-O2A-C1
19	B1	803	CLA	CBA-CGA-O2A-C1
19	A2	827	CLA	CBA-CGA-O2A-C1
19	BB	811	CLA	CBA-CGA-O2A-C1
22	A	846	LHG	C24-C23-O8-C6
25	B	851	LMG	C29-C28-O8-C9
19	A1	803	CLA	C13-C15-C16-C17
19	A1	807	CLA	C10-C11-C12-C13
19	A1	835	CLA	C5-C6-C7-C8
19	B1	801	CLA	C10-C11-C12-C13
19	B1	803	CLA	C13-C15-C16-C17
19	B1	806	CLA	C8-C10-C11-C12
19	B1	822	CLA	C13-C15-C16-C17
19	B1	826	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B1	832	CLA	C15-C16-C17-C18
19	A2	801	CLA	C10-C11-C12-C13
19	B2	801	CLA	C5-C6-C7-C8
19	B2	806	CLA	C8-C10-C11-C12
19	B2	823	CLA	C13-C15-C16-C17
19	B2	825	CLA	C10-C11-C12-C13
19	A	801	CLA	C10-C11-C12-C13
19	B	803	CLA	C8-C10-C11-C12
19	B	806	CLA	C8-C10-C11-C12
19	AA	807	CLA	C5-C6-C7-C8
19	BB	803	CLA	C13-C15-C16-C17
19	BB	815	CLA	C10-C11-C12-C13
19	BB	822	CLA	C13-C15-C16-C17
21	B2	838	PQN	C25-C26-C27-C28
21	A	843	PQN	C23-C25-C26-C27
22	A2	846	LHG	C7-C8-C9-C10
22	X	102	LHG	C7-C8-C9-C10
19	BB	815	CLA	O1D-CGD-O2D-CED
19	B1	813	CLA	CBD-CGD-O2D-CED
19	B1	823	CLA	CBD-CGD-O2D-CED
19	B	813	CLA	CBD-CGD-O2D-CED
19	B	825	CLA	CBD-CGD-O2D-CED
23	AA	855	BCR	C14-C15-C16-C17
19	A1	801	CLA	C10-C11-C12-C13
19	A1	803	CLA	C10-C11-C12-C13
19	A1	806	CLA	C5-C6-C7-C8
19	A1	842	CLA	C13-C15-C16-C17
19	B1	803	CLA	C8-C10-C11-C12
19	B1	823	CLA	C8-C10-C11-C12
19	A2	801	CLA	C8-C10-C11-C12
19	A2	840	CLA	C5-C6-C7-C8
19	B2	803	CLA	C13-C15-C16-C17
19	B2	822	CLA	C13-C15-C16-C17
19	B2	833	CLA	C15-C16-C17-C18
19	A	801	CLA	C8-C10-C11-C12
19	A	804	CLA	C8-C10-C11-C12
19	A	804	CLA	C10-C11-C12-C13
19	A	807	CLA	C5-C6-C7-C8
19	A	829	CLA	C10-C11-C12-C13
19	B	814	CLA	C5-C6-C7-C8
19	B	826	CLA	C10-C11-C12-C13
19	B	860	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	AA	801	CLA	C8-C10-C11-C12
19	AA	804	CLA	C13-C15-C16-C17
19	AA	819	CLA	C8-C10-C11-C12
19	AA	829	CLA	C10-C11-C12-C13
19	AA	853	CLA	C13-C15-C16-C17
19	BB	801	CLA	C5-C6-C7-C8
19	BB	806	CLA	C8-C10-C11-C12
20	AA	803	CL0	C13-C15-C16-C17
21	B1	837	PQN	C25-C26-C27-C28
19	B1	836	CLA	O1D-CGD-O2D-CED
19	A2	829	CLA	O1D-CGD-O2D-CED
19	B2	832	CLA	O1D-CGD-O2D-CED
19	A	813	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
22	A1	846	LHG	O10-C23-O8-C6
22	A1	846	LHG	C7-C8-C9-C10
22	X1	102	LHG	C7-C8-C9-C10
22	AA	847	LHG	C7-C8-C9-C10
22	XX	102	LHG	C7-C8-C9-C10
25	I1	102	LMG	C10-C11-C12-C13
25	B	851	LMG	C28-C29-C30-C31
19	BB	822	CLA	CBD-CGD-O2D-CED
19	B2	829	CLA	O1D-CGD-O2D-CED
19	B1	825	CLA	C10-C11-C12-C13
19	L1	207	CLA	C13-C15-C16-C17
19	A2	804	CLA	C10-C11-C12-C13
19	A2	808	CLA	C10-C11-C12-C13
19	B	829	CLA	C13-C15-C16-C17
19	AA	801	CLA	C10-C11-C12-C13
19	AA	804	CLA	C8-C10-C11-C12
19	A1	826	CLA	CBA-CGA-O2A-C1
19	B1	811	CLA	CBA-CGA-O2A-C1
19	A	836	CLA	CBA-CGA-O2A-C1
22	X1	103	LHG	C24-C23-O8-C6
28	BB	854	DGD	O6E-C5E-C6E-O5E
19	A1	807	CLA	C2-C1-O2A-CGA
19	A1	826	CLA	C2-C1-O2A-CGA
19	B1	807	CLA	C2-C1-O2A-CGA
19	A2	827	CLA	C2-C1-O2A-CGA
19	B2	807	CLA	C2-C1-O2A-CGA
19	A	808	CLA	C2-C1-O2A-CGA
19	A1	828	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B2	834	CLA	C13-C15-C16-C17
19	B	801	CLA	C5-C6-C7-C8
19	B	836	CLA	C13-C15-C16-C17
19	AA	831	CLA	C5-C6-C7-C8
19	BB	832	CLA	C15-C16-C17-C18
20	A1	802	CL0	C13-C15-C16-C17
20	A	803	CL0	C8-C10-C11-C12
21	B	838	PQN	C25-C26-C27-C28
22	X2	102	LHG	C7-C8-C9-C10
19	AA	841	CLA	CBA-CGA-O2A-C1
19	A1	852	CLA	C13-C15-C16-C17
19	B1	815	CLA	C10-C11-C12-C13
19	A2	807	CLA	C13-C15-C16-C17
19	A	819	CLA	C8-C10-C11-C12
19	B	825	CLA	C10-C11-C12-C13
19	B	833	CLA	C15-C16-C17-C18
19	B	819	CLA	O1D-CGD-O2D-CED
19	A1	820	CLA	C11-C10-C8-C7
19	A1	826	CLA	C11-C10-C8-C7
19	A2	801	CLA	C11-C10-C8-C7
19	B2	829	CLA	C12-C13-C15-C16
19	A	807	CLA	C11-C10-C8-C7
19	B	811	CLA	C6-C7-C8-C10
19	BB	811	CLA	C6-C7-C8-C10
19	BB	811	CLA	C11-C12-C13-C15
21	A1	843	PQN	C16-C17-C18-C20
21	A1	843	PQN	C21-C22-C23-C25
21	A2	843	PQN	C16-C17-C18-C20
21	A2	843	PQN	C21-C22-C23-C25
19	A1	834	CLA	C3-C5-C6-C7
19	A2	835	CLA	C3-C5-C6-C7
19	A2	836	CLA	O1A-CGA-O2A-C1
19	B2	811	CLA	O1A-CGA-O2A-C1
19	AA	805	CLA	O1A-CGA-O2A-C1
19	BB	803	CLA	O1A-CGA-O2A-C1
19	LL	201	CLA	O1A-CGA-O2A-C1
22	X2	103	LHG	O10-C23-O8-C6
22	BB	851	LHG	O10-C23-O8-C6
23	F1	306	BCR	C9-C10-C11-C12
23	F1	306	BCR	C19-C20-C21-C22
23	J1	102	BCR	C9-C10-C11-C12
23	K1	106	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	J2	102	BCR	C9-C10-C11-C12
23	K2	105	BCR	C13-C14-C15-C16
23	A	853	BCR	C19-C20-C21-C22
23	F	305	BCR	C9-C10-C11-C12
23	AA	854	BCR	C19-C20-C21-C22
23	FF	306	BCR	C9-C10-C11-C12
23	II	101	BCR	C9-C10-C11-C12
23	MM	101	BCR	C15-C16-C17-C18
26	B	841	ECH	C13-C14-C15-C16
19	B2	822	CLA	C2A-CAA-CBA-CGA
19	B2	837	CLA	C2A-CAA-CBA-CGA
19	B	822	CLA	C2A-CAA-CBA-CGA
19	B	858	CLA	C2A-CAA-CBA-CGA
19	B	860	CLA	C2A-CAA-CBA-CGA
19	F	301	CLA	C2A-CAA-CBA-CGA
19	BB	814	CLA	C2A-CAA-CBA-CGA
19	BB	822	CLA	C2A-CAA-CBA-CGA
19	BB	836	CLA	C2A-CAA-CBA-CGA
20	A1	802	CL0	C2A-CAA-CBA-CGA
19	B2	831	CLA	O1D-CGD-O2D-CED
19	B2	837	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	O1D-CGD-O2D-CED
19	AA	813	CLA	O1D-CGD-O2D-CED
19	AA	817	CLA	O1D-CGD-O2D-CED
19	BB	812	CLA	O1D-CGD-O2D-CED
19	A1	839	CLA	C5-C6-C7-C8
19	B1	826	CLA	C5-C6-C7-C8
19	B1	835	CLA	C8-C10-C11-C12
19	A2	829	CLA	C5-C6-C7-C8
19	B2	826	CLA	C5-C6-C7-C8
19	A	804	CLA	C13-C15-C16-C17
19	BB	825	CLA	C10-C11-C12-C13
19	FF	305	CLA	C13-C15-C16-C17
23	J1	104	BCR	C6-C7-C8-C9
23	M1	101	BCR	C22-C23-C24-C25
23	F2	305	BCR	C6-C7-C8-C9
23	M2	102	BCR	C22-C23-C24-C25
19	A	827	CLA	O1A-CGA-O2A-C1
19	L	202	CLA	O1A-CGA-O2A-C1
19	AA	827	CLA	O1A-CGA-O2A-C1
19	B2	836	CLA	CBD-CGD-O2D-CED
19	A1	822	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A2	804	CLA	C13-C15-C16-C17
19	A	808	CLA	C15-C16-C17-C18
19	A	823	CLA	C5-C6-C7-C8
19	AA	823	CLA	C5-C6-C7-C8
23	A1	847	BCR	C10-C11-C12-C13
23	A1	847	BCR	C18-C19-C20-C21
23	A1	849	BCR	C18-C19-C20-C21
23	B1	838	BCR	C18-C19-C20-C21
23	B1	842	BCR	C10-C11-C12-C13
23	I1	101	BCR	C18-C19-C20-C21
23	K1	104	BCR	C18-C19-C20-C21
23	L1	208	BCR	C10-C11-C12-C13
23	A2	847	BCR	C10-C11-C12-C13
23	A2	847	BCR	C18-C19-C20-C21
23	B2	839	BCR	C18-C19-C20-C21
23	I2	102	BCR	C18-C19-C20-C21
23	A	847	BCR	C10-C11-C12-C13
23	A	847	BCR	C18-C19-C20-C21
23	A	848	BCR	C10-C11-C12-C13
23	A	849	BCR	C10-C11-C12-C13
23	A	849	BCR	C18-C19-C20-C21
23	A	850	BCR	C10-C11-C12-C13
23	B	842	BCR	C18-C19-C20-C21
23	B	844	BCR	C18-C19-C20-C21
23	I	101	BCR	C18-C19-C20-C21
23	K	103	BCR	C18-C19-C20-C21
23	L	205	BCR	C10-C11-C12-C13
23	AA	848	BCR	C18-C19-C20-C21
23	AA	849	BCR	C10-C11-C12-C13
23	AA	850	BCR	C10-C11-C12-C13
23	AA	850	BCR	C18-C19-C20-C21
23	BB	841	BCR	C18-C19-C20-C21
23	BB	842	BCR	C10-C11-C12-C13
23	II	101	BCR	C18-C19-C20-C21
23	II	104	BCR	C10-C11-C12-C13
23	KK	103	BCR	C10-C11-C12-C13
23	LL	204	BCR	C10-C11-C12-C13
19	A1	840	CLA	O1A-CGA-O2A-C1
19	A2	841	CLA	O1A-CGA-O2A-C1
19	B1	805	CLA	C3-C5-C6-C7
19	B	805	CLA	C3-C5-C6-C7
19	A1	820	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A1	830	CLA	C5-C6-C7-C8
19	B1	828	CLA	C13-C15-C16-C17
19	B1	832	CLA	C5-C6-C7-C8
19	B2	826	CLA	C10-C11-C12-C13
19	B2	833	CLA	C5-C6-C7-C8
19	A	831	CLA	C5-C6-C7-C8
19	A	852	CLA	C13-C15-C16-C17
19	B	801	CLA	C10-C11-C12-C13
19	B	836	CLA	C8-C10-C11-C12
19	AA	804	CLA	C5-C6-C7-C8
19	AA	827	CLA	C5-C6-C7-C8
19	BB	814	CLA	C5-C6-C7-C8
19	BB	826	CLA	C10-C11-C12-C13
21	A1	843	PQN	C23-C25-C26-C27
21	B	838	PQN	C15-C16-C17-C18
19	BB	821	CLA	CBA-CGA-O2A-C1
19	B1	803	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	O1A-CGA-O2A-C1
19	BB	811	CLA	O1A-CGA-O2A-C1
22	A2	846	LHG	O10-C23-O8-C6
22	B2	848	LHG	O10-C23-O8-C6
22	B	853	LHG	O10-C23-O8-C6
19	A	841	CLA	CBA-CGA-O2A-C1
19	A1	806	CLA	C13-C15-C16-C17
19	A1	807	CLA	C15-C16-C17-C18
19	A1	831	CLA	C8-C10-C11-C12
19	B1	810	CLA	C8-C10-C11-C12
19	B1	814	CLA	C5-C6-C7-C8
19	B1	814	CLA	C8-C10-C11-C12
19	A2	823	CLA	C5-C6-C7-C8
19	A2	832	CLA	C8-C10-C11-C12
19	B2	814	CLA	C8-C10-C11-C12
19	L2	204	CLA	C5-C6-C7-C8
19	A	804	CLA	C5-C6-C7-C8
19	A	807	CLA	C10-C11-C12-C13
19	A	823	CLA	C8-C10-C11-C12
19	B	823	CLA	C15-C16-C17-C18
19	B	833	CLA	C5-C6-C7-C8
19	B	834	CLA	C10-C11-C12-C13
19	AA	807	CLA	C13-C15-C16-C17
19	BB	814	CLA	C8-C10-C11-C12
21	BB	837	PQN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	A1	812	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	O1D-CGD-O2D-CED
19	AA	838	CLA	O1D-CGD-O2D-CED
19	B	818	CLA	CBD-CGD-O2D-CED
19	B1	811	CLA	O1A-CGA-O2A-C1
19	A2	827	CLA	O1A-CGA-O2A-C1
22	X1	103	LHG	O10-C23-O8-C6
25	I2	105	LMG	C11-C10-O7-C8
19	A1	818	CLA	C8-C10-C11-C12
19	A1	820	CLA	C15-C16-C17-C18
19	B1	806	CLA	C15-C16-C17-C18
19	B1	823	CLA	C13-C15-C16-C17
19	A2	808	CLA	C15-C16-C17-C18
19	A2	819	CLA	C8-C10-C11-C12
19	A2	852	CLA	C13-C15-C16-C17
19	B2	806	CLA	C15-C16-C17-C18
19	B2	810	CLA	C8-C10-C11-C12
19	B2	852	CLA	C13-C15-C16-C17
19	L2	206	CLA	C13-C15-C16-C17
19	A	807	CLA	C13-C15-C16-C17
19	B	803	CLA	C13-C15-C16-C17
19	AA	823	CLA	C8-C10-C11-C12
19	AA	843	CLA	C13-C15-C16-C17
19	BB	801	CLA	C10-C11-C12-C13
19	BB	823	CLA	C15-C16-C17-C18
21	A2	843	PQN	C23-C25-C26-C27
21	A2	843	PQN	C25-C26-C27-C28
22	L1	211	LHG	C3-O3-P-O6
22	L2	208	LHG	C4-O6-P-O3
22	X	102	LHG	C4-O6-P-O3
19	B2	805	CLA	C3-C5-C6-C7
19	BB	805	CLA	C3-C5-C6-C7
19	A1	827	CLA	CBA-CGA-O2A-C1
19	B1	816	CLA	CBA-CGA-O2A-C1
19	L1	205	CLA	CBA-CGA-O2A-C1
19	A2	832	CLA	CBA-CGA-O2A-C1
19	B2	808	CLA	CBA-CGA-O2A-C1
19	L2	204	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBA-CGA-O2A-C1
22	AA	847	LHG	C24-C23-O8-C6
25	I1	102	LMG	O6-C5-C6-O5
19	A1	804	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A2	823	CLA	C8-C10-C11-C12
19	B2	834	CLA	C10-C11-C12-C13
19	A	832	CLA	C8-C10-C11-C12
19	B	823	CLA	C8-C10-C11-C12
19	AA	808	CLA	C15-C16-C17-C18
19	AA	832	CLA	C8-C10-C11-C12
19	BB	832	CLA	C5-C6-C7-C8
19	BB	835	CLA	C13-C15-C16-C17
21	A1	843	PQN	C25-C26-C27-C28
19	A1	826	CLA	O1A-CGA-O2A-C1
19	A1	831	CLA	O1A-CGA-O2A-C1
25	B2	845	LMG	C4-C5-C6-O5
19	B1	808	CLA	O1D-CGD-O2D-CED
22	A1	845	LHG	C7-C8-C9-C10
22	A	846	LHG	C7-C8-C9-C10
19	A2	813	CLA	O1D-CGD-O2D-CED
25	L1	210	LMG	O9-C10-O7-C8
25	I2	105	LMG	O9-C10-O7-C8
19	B1	849	CLA	C4-C3-C5-C6
19	A	827	CLA	C4-C3-C5-C6
19	A1	803	CLA	C5-C6-C7-C8
19	B1	833	CLA	C10-C11-C12-C13
19	BB	833	CLA	C10-C11-C12-C13
21	A	843	PQN	C25-C26-C27-C28
19	A1	820	CLA	CBD-CGD-O2D-CED
19	A1	842	CLA	C2A-CAA-CBA-CGA
19	B1	814	CLA	C2A-CAA-CBA-CGA
19	A2	801	CLA	C2A-CAA-CBA-CGA
19	A2	804	CLA	C2A-CAA-CBA-CGA
19	B2	814	CLA	C2A-CAA-CBA-CGA
19	B2	852	CLA	C2A-CAA-CBA-CGA
19	F2	301	CLA	C2A-CAA-CBA-CGA
19	A	804	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	C2A-CAA-CBA-CGA
19	AA	804	CLA	C2A-CAA-CBA-CGA
19	BB	855	CLA	C2A-CAA-CBA-CGA
19	B2	814	CLA	C3-C5-C6-C7
19	F2	301	CLA	C3-C5-C6-C7
19	A2	820	CLA	O1D-CGD-O2D-CED
19	B1	808	CLA	CBA-CGA-O2A-C1
19	A2	828	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	AA	832	CLA	CBA-CGA-O2A-C1
19	AA	836	CLA	CBA-CGA-O2A-C1
22	B1	847	LHG	C24-C23-O8-C6
19	A	829	CLA	C5-C6-C7-C8
19	AA	812	CLA	O1A-CGA-O2A-C1
19	B1	835	CLA	C13-C15-C16-C17
21	BB	837	PQN	C15-C16-C17-C18
23	A1	853	BCR	C19-C20-C21-C22
23	A2	853	BCR	C19-C20-C21-C22
23	F2	305	BCR	C9-C10-C11-C12
23	A	854	BCR	C13-C14-C15-C16
23	B	848	BCR	C15-C16-C17-C18
23	AA	855	BCR	C13-C14-C15-C16
23	BB	841	BCR	C13-C14-C15-C16
23	BB	847	BCR	C15-C16-C17-C18
26	B1	840	ECH	C15-C16-C17-C18
26	B2	841	ECH	C15-C16-C17-C18
26	B	841	ECH	C15-C16-C17-C18
22	A	845	LHG	C27-C28-C29-C30
19	B1	812	CLA	O1D-CGD-O2D-CED
19	B2	834	CLA	O1D-CGD-O2D-CED
22	A1	845	LHG	C8-C7-O7-C5
19	B2	815	CLA	C10-C11-C12-C13
20	A2	803	CL0	C15-C16-C17-C18
23	A1	847	BCR	C16-C17-C18-C36
23	A1	848	BCR	C11-C10-C9-C34
23	A1	848	BCR	C20-C21-C22-C37
23	A1	850	BCR	C20-C21-C22-C37
23	A1	851	BCR	C35-C13-C14-C15
23	A1	853	BCR	C35-C13-C14-C15
23	B1	839	BCR	C11-C10-C9-C34
23	B1	839	BCR	C16-C17-C18-C36
23	B1	841	BCR	C16-C17-C18-C36
23	B1	842	BCR	C11-C10-C9-C34
23	B1	843	BCR	C35-C13-C14-C15
23	F1	303	BCR	C20-C21-C22-C37
23	F1	304	BCR	C35-C13-C14-C15
23	F1	304	BCR	C16-C17-C18-C36
23	F1	306	BCR	C20-C21-C22-C37
23	I1	101	BCR	C35-C13-C14-C15
23	J1	102	BCR	C20-C21-C22-C37
23	J1	104	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	K1	104	BCR	C35-C13-C14-C15
23	K1	104	BCR	C16-C17-C18-C36
23	K1	106	BCR	C16-C17-C18-C36
23	L1	201	BCR	C35-C13-C14-C15
23	L1	208	BCR	C35-C13-C14-C15
23	L1	208	BCR	C20-C21-C22-C37
23	A2	847	BCR	C16-C17-C18-C36
23	A2	848	BCR	C11-C10-C9-C34
23	A2	848	BCR	C16-C17-C18-C36
23	A2	848	BCR	C20-C21-C22-C37
23	A2	849	BCR	C20-C21-C22-C37
23	A2	850	BCR	C20-C21-C22-C37
23	A2	853	BCR	C35-C13-C14-C15
23	B2	840	BCR	C11-C10-C9-C34
23	B2	843	BCR	C11-C10-C9-C34
23	B2	843	BCR	C16-C17-C18-C36
23	B2	844	BCR	C35-C13-C14-C15
23	F2	303	BCR	C20-C21-C22-C37
23	F2	304	BCR	C35-C13-C14-C15
23	F2	304	BCR	C16-C17-C18-C36
23	F2	305	BCR	C11-C10-C9-C34
23	I2	101	BCR	C35-C13-C14-C15
23	I2	102	BCR	C11-C10-C9-C34
23	I2	102	BCR	C35-C13-C14-C15
23	I2	103	BCR	C35-C13-C14-C15
23	I2	103	BCR	C20-C21-C22-C37
23	J2	102	BCR	C16-C17-C18-C36
23	J2	104	BCR	C20-C21-C22-C37
23	K2	103	BCR	C11-C10-C9-C34
23	K2	103	BCR	C16-C17-C18-C36
23	A	847	BCR	C35-C13-C14-C15
23	A	847	BCR	C16-C17-C18-C36
23	A	848	BCR	C35-C13-C14-C15
23	A	849	BCR	C16-C17-C18-C36
23	A	851	BCR	C11-C10-C9-C34
23	A	851	BCR	C35-C13-C14-C15
23	A	853	BCR	C35-C13-C14-C15
23	A	853	BCR	C20-C21-C22-C37
23	B	839	BCR	C11-C10-C9-C34
23	B	840	BCR	C11-C10-C9-C34
23	B	840	BCR	C35-C13-C14-C15
23	B	840	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	B	843	BCR	C16-C17-C18-C36
23	B	844	BCR	C35-C13-C14-C15
23	B	848	BCR	C35-C13-C14-C15
23	F	303	BCR	C35-C13-C14-C15
23	F	303	BCR	C20-C21-C22-C37
23	F	305	BCR	C20-C21-C22-C37
23	I	102	BCR	C35-C13-C14-C15
23	J	104	BCR	C20-C21-C22-C37
23	K	103	BCR	C35-C13-C14-C15
23	L	205	BCR	C16-C17-C18-C36
23	L	205	BCR	C20-C21-C22-C37
23	AA	848	BCR	C35-C13-C14-C15
23	AA	848	BCR	C16-C17-C18-C36
23	AA	849	BCR	C35-C13-C14-C15
23	AA	852	BCR	C11-C10-C9-C34
23	AA	852	BCR	C35-C13-C14-C15
23	AA	854	BCR	C35-C13-C14-C15
23	BB	839	BCR	C11-C10-C9-C34
23	BB	839	BCR	C35-C13-C14-C15
23	BB	839	BCR	C16-C17-C18-C36
23	BB	841	BCR	C20-C21-C22-C37
23	BB	847	BCR	C35-C13-C14-C15
23	BB	847	BCR	C16-C17-C18-C36
23	FF	303	BCR	C35-C13-C14-C15
23	FF	303	BCR	C20-C21-C22-C37
23	II	101	BCR	C20-C21-C22-C37
19	A1	814	CLA	C3-C5-C6-C7
19	A1	842	CLA	C3-C5-C6-C7
19	K1	105	CLA	C4C-C3C-CAC-CBC
22	X2	103	LHG	C14-C15-C16-C17
22	A	845	LHG	C26-C27-C28-C29
25	B1	844	LMG	C22-C23-C24-C25
25	B1	844	LMG	C30-C31-C32-C33
19	A	836	CLA	O1A-CGA-O2A-C1
19	B2	820	CLA	O1D-CGD-O2D-CED
19	AA	808	CLA	O1D-CGD-O2D-CED
19	BB	819	CLA	O1D-CGD-O2D-CED
19	A1	812	CLA	C16-C17-C18-C20
19	A1	822	CLA	C11-C12-C13-C15
19	A2	823	CLA	C11-C12-C13-C15
19	A	823	CLA	C11-C12-C13-C15
19	AA	813	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	AA	823	CLA	C11-C12-C13-C15
19	BB	825	CLA	C16-C17-C18-C19
21	B2	838	PQN	C26-C27-C28-C30
19	B1	829	CLA	CBA-CGA-O2A-C1
19	A2	831	CLA	CBA-CGA-O2A-C1
19	B	859	CLA	CBA-CGA-O2A-C1
22	B	853	LHG	C30-C31-C32-C33
22	AA	846	LHG	C26-C27-C28-C29
22	AA	846	LHG	C27-C28-C29-C30
25	I2	105	LMG	C16-C17-C18-C19
25	B	851	LMG	C19-C20-C21-C22
25	M	102	LMG	C32-C33-C34-C35
25	B2	847	LMG	O9-C10-O7-C8
25	B	851	LMG	O9-C10-O7-C8
22	LL	205	LHG	C23-C24-C25-C26
19	AA	840	CLA	CBD-CGD-O2D-CED
22	X1	103	LHG	C30-C31-C32-C33
22	BB	851	LHG	C30-C31-C32-C33
19	B1	819	CLA	O1D-CGD-O2D-CED
19	XX	101	CLA	O1D-CGD-O2D-CED
22	A1	845	LHG	C27-C28-C29-C30
22	B	853	LHG	C11-C10-C9-C8
22	LL	205	LHG	C11-C12-C13-C14
25	B	851	LMG	C30-C31-C32-C33
19	A	822	CLA	O1D-CGD-O2D-CED
19	AA	853	CLA	O1D-CGD-O2D-CED
22	X1	103	LHG	O2-C2-C3-O3
22	X1	103	LHG	C14-C15-C16-C17
22	L	207	LHG	C11-C12-C13-C14
25	M	102	LMG	C34-C35-C36-C37
19	F	301	CLA	C3-C5-C6-C7
28	B	856	DGD	C1B-C2B-C3B-C4B
28	BB	854	DGD	C1B-C2B-C3B-C4B
19	B	860	CLA	O1D-CGD-O2D-CED
23	A1	847	BCR	C11-C10-C9-C8
23	A1	849	BCR	C11-C10-C9-C8
23	A1	851	BCR	C12-C13-C14-C15
23	A1	853	BCR	C16-C17-C18-C19
23	B1	838	BCR	C16-C17-C18-C19
23	B1	838	BCR	C20-C21-C22-C23
23	B1	839	BCR	C16-C17-C18-C19
23	B1	843	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	F1	303	BCR	C16-C17-C18-C19
23	F1	304	BCR	C11-C10-C9-C8
23	F1	304	BCR	C16-C17-C18-C19
23	F1	306	BCR	C20-C21-C22-C23
23	I1	101	BCR	C16-C17-C18-C19
23	J1	102	BCR	C12-C13-C14-C15
23	J1	102	BCR	C20-C21-C22-C23
23	J1	104	BCR	C11-C10-C9-C8
23	J1	104	BCR	C12-C13-C14-C15
23	J1	104	BCR	C16-C17-C18-C19
23	K1	106	BCR	C12-C13-C14-C15
23	K1	106	BCR	C16-C17-C18-C19
23	K1	106	BCR	C20-C21-C22-C23
23	L1	208	BCR	C11-C10-C9-C8
23	L1	209	BCR	C20-C21-C22-C23
23	A2	847	BCR	C11-C10-C9-C8
23	A2	849	BCR	C11-C10-C9-C8
23	A2	851	BCR	C12-C13-C14-C15
23	A2	851	BCR	C20-C21-C22-C23
23	A2	853	BCR	C16-C17-C18-C19
23	B2	839	BCR	C20-C21-C22-C23
23	B2	840	BCR	C16-C17-C18-C19
23	B2	842	BCR	C11-C10-C9-C8
23	B2	842	BCR	C12-C13-C14-C15
23	F2	303	BCR	C12-C13-C14-C15
23	F2	303	BCR	C16-C17-C18-C19
23	F2	304	BCR	C16-C17-C18-C19
23	I2	101	BCR	C16-C17-C18-C19
23	I2	102	BCR	C20-C21-C22-C23
23	I2	103	BCR	C11-C10-C9-C8
23	J2	102	BCR	C12-C13-C14-C15
23	J2	104	BCR	C11-C10-C9-C8
23	K2	105	BCR	C12-C13-C14-C15
23	K2	105	BCR	C16-C17-C18-C19
23	L2	207	BCR	C16-C17-C18-C19
23	L2	207	BCR	C20-C21-C22-C23
23	A	847	BCR	C11-C10-C9-C8
23	A	849	BCR	C12-C13-C14-C15
23	A	849	BCR	C20-C21-C22-C23
23	A	853	BCR	C16-C17-C18-C19
23	A	854	BCR	C12-C13-C14-C15
23	B	839	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	B	842	BCR	C12-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C19
23	F	303	BCR	C16-C17-C18-C19
23	F	304	BCR	C12-C13-C14-C15
23	F	305	BCR	C11-C10-C9-C8
23	I	101	BCR	C11-C10-C9-C8
23	I	101	BCR	C12-C13-C14-C15
23	I	101	BCR	C16-C17-C18-C19
23	I	101	BCR	C20-C21-C22-C23
23	J	104	BCR	C11-C10-C9-C8
23	J	104	BCR	C16-C17-C18-C19
23	K	103	BCR	C16-C17-C18-C19
23	L	205	BCR	C11-C10-C9-C8
23	L	206	BCR	C16-C17-C18-C19
23	L	206	BCR	C20-C21-C22-C23
23	AA	848	BCR	C11-C10-C9-C8
23	AA	850	BCR	C12-C13-C14-C15
23	AA	850	BCR	C20-C21-C22-C23
23	AA	854	BCR	C16-C17-C18-C19
23	AA	855	BCR	C12-C13-C14-C15
23	BB	838	BCR	C16-C17-C18-C19
23	BB	841	BCR	C16-C17-C18-C19
23	FF	303	BCR	C16-C17-C18-C19
23	II	101	BCR	C11-C10-C9-C8
23	II	101	BCR	C16-C17-C18-C19
23	II	101	BCR	C20-C21-C22-C23
23	II	104	BCR	C11-C10-C9-C8
23	JJ	102	BCR	C11-C10-C9-C8
23	JJ	102	BCR	C12-C13-C14-C15
23	JJ	102	BCR	C20-C21-C22-C23
23	JJ	104	BCR	C11-C10-C9-C8
23	JJ	104	BCR	C16-C17-C18-C19
23	KK	103	BCR	C16-C17-C18-C19
23	LL	204	BCR	C16-C17-C18-C19
23	LL	204	BCR	C20-C21-C22-C23
19	A1	830	CLA	CBA-CGA-O2A-C1
19	B2	815	CLA	CBA-CGA-O2A-C1
19	B2	830	CLA	CBA-CGA-O2A-C1
19	AA	828	CLA	CBA-CGA-O2A-C1
25	B	845	LMG	C22-C23-C24-C25
25	B	851	LMG	C18-C19-C20-C21
19	L1	205	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	814	CLA	C8-C10-C11-C12
19	BB	823	CLA	C8-C10-C11-C12
21	AA	844	PQN	C25-C26-C27-C28
19	B1	816	CLA	O1A-CGA-O2A-C1
19	A2	828	CLA	O1A-CGA-O2A-C1
19	B2	808	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	O1A-CGA-O2A-C1
22	A	846	LHG	O10-C23-O8-C6
19	A2	813	CLA	C16-C17-C18-C20
19	A	804	CLA	C16-C17-C18-C19
19	AA	823	CLA	C11-C12-C13-C14
21	B	838	PQN	C26-C27-C28-C29
21	BB	837	PQN	C26-C27-C28-C29
19	A	832	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	O1D-CGD-O2D-CED
19	A1	820	CLA	C4-C3-C5-C6
19	L1	207	CLA	C4-C3-C5-C6
19	B2	808	CLA	C4-C3-C5-C6
19	B2	814	CLA	C4-C3-C5-C6
19	L2	206	CLA	C4-C3-C5-C6
19	B	810	CLA	C4-C3-C5-C6
19	AA	827	CLA	C4-C3-C5-C6
19	BB	810	CLA	C4-C3-C5-C6
22	X2	103	LHG	C11-C10-C9-C8
22	BB	851	LHG	C14-C15-C16-C17
25	B2	845	LMG	C22-C23-C24-C25
25	B2	845	LMG	C41-C42-C43-C44
25	BB	844	LMG	C22-C23-C24-C25
19	B1	849	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
19	A1	820	CLA	C11-C12-C13-C14
19	A1	820	CLA	C14-C13-C15-C16
19	A1	841	CLA	C6-C7-C8-C9
19	B1	803	CLA	C11-C12-C13-C14
19	B1	811	CLA	C6-C7-C8-C9
19	B1	811	CLA	C11-C12-C13-C14
19	B1	825	CLA	C11-C10-C8-C9
19	B1	828	CLA	C14-C13-C15-C16
19	A2	801	CLA	C11-C10-C8-C9
19	B2	803	CLA	C11-C12-C13-C14
19	B2	811	CLA	C6-C7-C8-C9
19	B2	811	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B2	829	CLA	C14-C13-C15-C16
19	B2	849	CLA	C6-C7-C8-C9
19	A	842	CLA	C6-C7-C8-C9
19	B	815	CLA	C11-C10-C8-C9
19	AA	827	CLA	C11-C10-C8-C9
19	BB	803	CLA	C11-C12-C13-C14
19	BB	810	CLA	C6-C7-C8-C9
19	BB	833	CLA	C14-C13-C15-C16
20	A1	802	CL0	C6-C7-C8-C9
21	A2	843	PQN	C21-C22-C23-C24
19	A1	814	CLA	O1D-CGD-O2D-CED
19	B1	830	CLA	O1D-CGD-O2D-CED
19	A	815	CLA	O1D-CGD-O2D-CED
19	BB	813	CLA	O1D-CGD-O2D-CED
22	L	207	LHG	C23-C24-C25-C26
22	X	102	LHG	C23-C24-C25-C26
22	XX	102	LHG	C23-C24-C25-C26
22	A2	845	LHG	C27-C28-C29-C30
22	B	853	LHG	C14-C15-C16-C17
25	I1	102	LMG	C12-C13-C14-C15
25	B2	845	LMG	C30-C31-C32-C33
19	A1	822	CLA	C5-C6-C7-C8
19	A2	831	CLA	C5-C6-C7-C8
19	A	827	CLA	C15-C16-C17-C18
19	A1	801	CLA	C2A-CAA-CBA-CGA
19	A2	824	CLA	C2A-CAA-CBA-CGA
19	A	801	CLA	C2A-CAA-CBA-CGA
19	B	837	CLA	C2A-CAA-CBA-CGA
19	AA	801	CLA	C2A-CAA-CBA-CGA
19	L1	205	CLA	O1A-CGA-O2A-C1
19	A2	832	CLA	O1A-CGA-O2A-C1
19	L2	204	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	O1A-CGA-O2A-C1
19	BB	821	CLA	O1A-CGA-O2A-C1
23	F1	304	BCR	C37-C22-C23-C24
23	J1	104	BCR	C37-C22-C23-C24
23	F2	304	BCR	C37-C22-C23-C24
23	I2	102	BCR	C7-C8-C9-C34
23	A	848	BCR	C7-C8-C9-C34
23	A	853	BCR	C7-C8-C9-C34
23	A	853	BCR	C37-C22-C23-C24
23	F	304	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	J	104	BCR	C37-C22-C23-C24
23	AA	849	BCR	C7-C8-C9-C34
23	AA	854	BCR	C7-C8-C9-C34
23	AA	854	BCR	C37-C22-C23-C24
23	FF	304	BCR	C37-C22-C23-C24
22	B	853	LHG	C17-C18-C19-C20
22	BB	851	LHG	C17-C18-C19-C20
25	L1	210	LMG	C19-C20-C21-C22
23	L1	208	BCR	C21-C22-C23-C24
23	L1	209	BCR	C17-C18-C19-C20
23	A2	849	BCR	C11-C12-C13-C14
23	I2	102	BCR	C17-C18-C19-C20
23	I2	103	BCR	C21-C22-C23-C24
23	F	303	BCR	C21-C22-C23-C24
23	I	102	BCR	C17-C18-C19-C20
23	L	205	BCR	C21-C22-C23-C24
23	II	104	BCR	C21-C22-C23-C24
19	A1	807	CLA	C3-C5-C6-C7
19	B2	852	CLA	C3-C5-C6-C7
22	A1	845	LHG	O9-C7-O7-C5
19	BB	810	CLA	C10-C11-C12-C13
19	B2	830	CLA	C4C-C3C-CAC-CBC
22	X1	103	LHG	C17-C18-C19-C20
22	A2	845	LHG	C13-C14-C15-C16
22	B	852	LHG	C11-C12-C13-C14
22	BB	850	LHG	C11-C12-C13-C14
22	BB	851	LHG	C11-C10-C9-C8
22	BB	851	LHG	C15-C16-C17-C18
25	L1	210	LMG	C30-C31-C32-C33
25	B	845	LMG	C29-C30-C31-C32
19	A2	823	CLA	C11-C12-C13-C14
19	A	813	CLA	C16-C17-C18-C20
19	A	823	CLA	C11-C12-C13-C14
21	B1	837	PQN	C26-C27-C28-C30
21	B2	838	PQN	C26-C27-C28-C29
19	B	810	CLA	C10-C11-C12-C13
22	L1	211	LHG	C9-C10-C11-C12
22	X2	103	LHG	C15-C16-C17-C18
25	B1	844	LMG	C18-C19-C20-C21
25	II	105	LMG	C34-C35-C36-C37
19	BB	836	CLA	O1D-CGD-O2D-CED
25	L1	210	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
25	L1	210	LMG	C28-C29-C30-C31
19	A1	828	CLA	C5-C6-C7-C8
19	A1	827	CLA	O1A-CGA-O2A-C1
19	B	859	CLA	O1A-CGA-O2A-C1
22	AA	847	LHG	O10-C23-O8-C6
22	B2	848	LHG	C11-C10-C9-C8
22	AA	846	LHG	C13-C14-C15-C16
19	AA	843	CLA	C3-C5-C6-C7
19	BB	801	CLA	C3-C5-C6-C7
19	B2	803	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	CBA-CGA-O2A-C1
19	BB	856	CLA	CBA-CGA-O2A-C1
25	B	845	LMG	C41-C42-C43-C44
19	A1	807	CLA	O1D-CGD-O2D-CED
19	A1	842	CLA	O1D-CGD-O2D-CED
19	A	852	CLA	O1D-CGD-O2D-CED
19	A1	807	CLA	C3A-C2A-CAA-CBA
19	A1	810	CLA	C3A-C2A-CAA-CBA
19	A1	826	CLA	C3A-C2A-CAA-CBA
19	A1	838	CLA	C3A-C2A-CAA-CBA
19	B1	802	CLA	C3A-C2A-CAA-CBA
19	B1	820	CLA	C3A-C2A-CAA-CBA
19	B1	850	CLA	C3A-C2A-CAA-CBA
19	A2	808	CLA	C3A-C2A-CAA-CBA
19	A2	826	CLA	C3A-C2A-CAA-CBA
19	A2	827	CLA	C3A-C2A-CAA-CBA
19	A2	839	CLA	C3A-C2A-CAA-CBA
19	B2	802	CLA	C3A-C2A-CAA-CBA
19	B2	820	CLA	C3A-C2A-CAA-CBA
19	B2	834	CLA	C3A-C2A-CAA-CBA
19	B2	851	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	C3A-C2A-CAA-CBA
19	A	811	CLA	C3A-C2A-CAA-CBA
19	A	827	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
19	A	839	CLA	C3A-C2A-CAA-CBA
19	A	852	CLA	C3A-C2A-CAA-CBA
19	B	802	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C3A-C2A-CAA-CBA
19	AA	808	CLA	C3A-C2A-CAA-CBA
19	AA	811	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	AA	827	CLA	C3A-C2A-CAA-CBA
19	AA	839	CLA	C3A-C2A-CAA-CBA
19	AA	853	CLA	C3A-C2A-CAA-CBA
19	BB	820	CLA	C3A-C2A-CAA-CBA
19	BB	824	CLA	C3A-C2A-CAA-CBA
19	BB	856	CLA	C3A-C2A-CAA-CBA
19	FF	301	CLA	C3A-C2A-CAA-CBA
20	A	803	CL0	C3A-C2A-CAA-CBA
19	B2	814	CLA	C5-C6-C7-C8
19	B	810	CLA	C8-C10-C11-C12
19	BB	806	CLA	C15-C16-C17-C18
23	I	101	BCR	C9-C10-C11-C12
22	X1	103	LHG	C11-C10-C9-C8
22	B	853	LHG	C15-C16-C17-C18
25	BB	844	LMG	C29-C30-C31-C32
19	A	812	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	O1D-CGD-O2D-CED
19	AA	832	CLA	O1A-CGA-O2A-C1
19	A1	822	CLA	C11-C12-C13-C14
21	B1	837	PQN	C26-C27-C28-C29
21	B	838	PQN	C26-C27-C28-C30
22	X2	103	LHG	C30-C31-C32-C33
19	A	826	CLA	O1D-CGD-O2D-CED
19	AA	815	CLA	O1D-CGD-O2D-CED
28	BB	854	DGD	C1G-C2G-C3G-O3G
23	B	844	BCR	C14-C15-C16-C17
23	F	305	BCR	C14-C15-C16-C17
23	BB	843	BCR	C14-C15-C16-C17
23	KK	103	BCR	C14-C15-C16-C17
19	A2	815	CLA	O1D-CGD-O2D-CED
19	B2	837	CLA	C3-C5-C6-C7
19	L	202	CLA	C3-C5-C6-C7
22	X2	103	LHG	C17-C18-C19-C20
19	A1	826	CLA	C4-C3-C5-C6
19	A1	835	CLA	C4-C3-C5-C6
19	B1	814	CLA	C4-C3-C5-C6
19	A2	827	CLA	C4-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	BB	808	CLA	C4-C3-C5-C6
19	B2	851	CLA	CBA-CGA-O2A-C1
19	A1	826	CLA	C2-C3-C5-C6
19	L1	207	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A2	827	CLA	C2-C3-C5-C6
19	L2	206	CLA	C2-C3-C5-C6
19	A	827	CLA	C2-C3-C5-C6
19	B	808	CLA	C2-C3-C5-C6
19	B	858	CLA	C2-C3-C5-C6
19	BB	808	CLA	C2-C3-C5-C6
19	BB	810	CLA	C2-C3-C5-C6
19	BB	855	CLA	C2-C3-C5-C6
22	AA	846	LHG	C8-C7-O7-C5
19	AA	826	CLA	O1D-CGD-O2D-CED
22	B1	847	LHG	C11-C12-C13-C14
22	A	845	LHG	C13-C14-C15-C16
22	A1	846	LHG	O1-C1-C2-O2
22	A	846	LHG	O1-C1-C2-O2
22	AA	847	LHG	O1-C1-C2-O2
19	B2	836	CLA	C13-C15-C16-C17
25	L1	210	LMG	C15-C16-C17-C18
21	BB	837	PQN	C26-C27-C28-C30
19	A	821	CLA	C15-C16-C17-C18
25	BB	844	LMG	C41-C42-C43-C44
19	B	808	CLA	CBA-CGA-O2A-C1
19	BB	829	CLA	CBA-CGA-O2A-C1
19	B1	829	CLA	C4C-C3C-CAC-CBC
25	B	845	LMG	C13-C14-C15-C16
28	B	856	DGD	C2B-C3B-C4B-C5B
19	B1	808	CLA	O1A-CGA-O2A-C1
19	A2	831	CLA	O1A-CGA-O2A-C1
19	B2	851	CLA	O1A-CGA-O2A-C1
19	AA	828	CLA	O1A-CGA-O2A-C1
19	AA	836	CLA	O1A-CGA-O2A-C1
19	BB	856	CLA	O1A-CGA-O2A-C1
19	AA	829	CLA	C5-C6-C7-C8
22	BB	851	LHG	C1-C2-C3-O3
22	B1	847	LHG	C11-C10-C9-C8
22	A	845	LHG	C12-C13-C14-C15
19	B1	806	CLA	C2-C1-O2A-CGA
19	B1	828	CLA	C2-C1-O2A-CGA
19	B2	806	CLA	C2-C1-O2A-CGA
19	B2	829	CLA	C2-C1-O2A-CGA
19	A	827	CLA	C2-C1-O2A-CGA
19	B	806	CLA	C2-C1-O2A-CGA
19	B	807	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	B	829	CLA	C2-C1-O2A-CGA
19	AA	827	CLA	C2-C1-O2A-CGA
19	BB	806	CLA	C2-C1-O2A-CGA
19	BB	807	CLA	C2-C1-O2A-CGA
19	FF	305	CLA	C2-C1-O2A-CGA
20	A2	803	CL0	C2-C1-O2A-CGA
22	X1	103	LHG	C15-C16-C17-C18
25	B1	844	LMG	C29-C30-C31-C32
25	B2	845	LMG	C18-C19-C20-C21
19	B1	810	CLA	C10-C11-C12-C13
19	A2	831	CLA	C13-C15-C16-C17
19	A	852	CLA	C8-C10-C11-C12
19	B	826	CLA	C5-C6-C7-C8
19	BB	810	CLA	C8-C10-C11-C12
19	A1	830	CLA	O1A-CGA-O2A-C1
19	B1	829	CLA	O1A-CGA-O2A-C1
19	B2	815	CLA	O1A-CGA-O2A-C1
19	B2	830	CLA	O1A-CGA-O2A-C1
19	B	824	CLA	O1A-CGA-O2A-C1
22	B1	847	LHG	O10-C23-O8-C6
25	L1	210	LMG	C11-C12-C13-C14
25	B2	845	LMG	C29-C30-C31-C32
19	AA	813	CLA	C16-C17-C18-C19
20	A	803	CL0	CBD-CGD-O2D-CED
19	B1	836	CLA	C3-C5-C6-C7
19	A	805	CLA	C3-C5-C6-C7
19	AA	805	CLA	C3-C5-C6-C7
23	A1	849	BCR	C23-C24-C25-C26
23	A1	851	BCR	C23-C24-C25-C26
23	A1	851	BCR	C23-C24-C25-C30
23	B1	843	BCR	C5-C6-C7-C8
23	I1	101	BCR	C5-C6-C7-C8
23	J1	102	BCR	C23-C24-C25-C26
23	J1	104	BCR	C23-C24-C25-C30
23	K1	106	BCR	C23-C24-C25-C26
23	K1	106	BCR	C23-C24-C25-C30
23	A2	849	BCR	C23-C24-C25-C26
23	A2	851	BCR	C23-C24-C25-C26
23	A2	851	BCR	C23-C24-C25-C30
23	B2	842	BCR	C23-C24-C25-C26
23	B2	842	BCR	C23-C24-C25-C30
23	B2	844	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	F2	303	BCR	C23-C24-C25-C26
23	F2	305	BCR	C23-C24-C25-C26
23	F2	305	BCR	C23-C24-C25-C30
23	I2	101	BCR	C5-C6-C7-C8
23	J2	102	BCR	C23-C24-C25-C26
23	J2	104	BCR	C23-C24-C25-C30
23	A	849	BCR	C23-C24-C25-C26
23	A	851	BCR	C23-C24-C25-C26
23	A	851	BCR	C23-C24-C25-C30
23	A	854	BCR	C23-C24-C25-C26
23	B	843	BCR	C23-C24-C25-C26
23	B	844	BCR	C1-C6-C7-C8
23	B	844	BCR	C5-C6-C7-C8
23	F	303	BCR	C23-C24-C25-C26
23	I	101	BCR	C1-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C30
23	K	103	BCR	C23-C24-C25-C26
23	M	101	BCR	C23-C24-C25-C30
23	AA	850	BCR	C23-C24-C25-C26
23	AA	855	BCR	C23-C24-C25-C26
23	BB	842	BCR	C23-C24-C25-C30
23	BB	843	BCR	C1-C6-C7-C8
23	BB	843	BCR	C5-C6-C7-C8
23	BB	847	BCR	C5-C6-C7-C8
23	FF	303	BCR	C23-C24-C25-C26
23	JJ	104	BCR	C23-C24-C25-C30
23	KK	103	BCR	C23-C24-C25-C26
26	B1	840	ECH	C23-C24-C25-C26
26	B2	841	ECH	C23-C24-C25-C26
26	B	841	ECH	C23-C24-C25-C26
26	BB	840	ECH	C1-C6-C7-C8
26	BB	840	ECH	C23-C24-C25-C26
19	A2	830	CLA	C4C-C3C-CAC-CBC
19	AA	830	CLA	C2C-C3C-CAC-CBC
19	B1	815	CLA	CBA-CGA-O2A-C1
19	B1	850	CLA	CBA-CGA-O2A-C1
19	B2	816	CLA	CBA-CGA-O2A-C1
19	A	833	CLA	CBA-CGA-O2A-C1
19	AA	831	CLA	CBA-CGA-O2A-C1
19	BB	824	CLA	CBA-CGA-O2A-C1
19	A1	803	CLA	C8-C10-C11-C12
19	B1	848	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B2	836	CLA	C8-C10-C11-C12
19	B2	849	CLA	C13-C15-C16-C17
19	A	805	CLA	C8-C10-C11-C12
19	BB	826	CLA	C5-C6-C7-C8
22	A	845	LHG	C8-C7-O7-C5
25	B2	847	LMG	C11-C10-O7-C8
19	B1	850	CLA	O1A-CGA-O2A-C1
19	B2	803	CLA	O1A-CGA-O2A-C1
22	X1	102	LHG	C23-C24-C25-C26
22	X2	102	LHG	C23-C24-C25-C26
22	A1	845	LHG	C12-C13-C14-C15
19	B2	806	CLA	C5-C6-C7-C8
19	A	836	CLA	C13-C15-C16-C17
19	BB	835	CLA	C8-C10-C11-C12
22	A1	845	LHG	C13-C14-C15-C16
19	B1	808	CLA	C4-C3-C5-C6
19	B2	829	CLA	C4-C3-C5-C6
19	BB	855	CLA	C4-C3-C5-C6
19	FF	305	CLA	C4-C3-C5-C6
19	A1	801	CLA	C11-C10-C8-C7
19	A1	803	CLA	C6-C7-C8-C10
19	A1	820	CLA	C2-C3-C5-C6
19	A1	835	CLA	C2-C3-C5-C6
19	B1	805	CLA	C6-C7-C8-C10
19	B1	811	CLA	C6-C7-C8-C10
19	B1	811	CLA	C11-C12-C13-C15
19	B1	814	CLA	C2-C3-C5-C6
19	B1	828	CLA	C2-C3-C5-C6
19	B1	828	CLA	C12-C13-C15-C16
19	B1	833	CLA	C6-C7-C8-C10
19	L1	206	CLA	C11-C12-C13-C15
19	A2	804	CLA	C12-C13-C15-C16
19	A2	827	CLA	C11-C10-C8-C7
19	A2	836	CLA	C2-C3-C5-C6
19	B2	805	CLA	C6-C7-C8-C10
19	B2	808	CLA	C2-C3-C5-C6
19	B2	811	CLA	C6-C7-C8-C10
19	B2	811	CLA	C11-C12-C13-C15
19	B2	814	CLA	C2-C3-C5-C6
19	B2	829	CLA	C2-C3-C5-C6
19	B2	834	CLA	C6-C7-C8-C10
19	A	801	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	804	CLA	C6-C7-C8-C10
19	A	827	CLA	C11-C10-C8-C7
19	A	842	CLA	C6-C7-C8-C10
19	B	805	CLA	C6-C7-C8-C10
19	B	810	CLA	C6-C7-C8-C10
19	B	811	CLA	C11-C12-C13-C15
19	B	829	CLA	C2-C3-C5-C6
19	B	829	CLA	C12-C13-C15-C16
19	B	834	CLA	C6-C7-C8-C10
19	L	203	CLA	C11-C12-C13-C15
19	AA	804	CLA	C6-C7-C8-C10
19	AA	827	CLA	C2-C3-C5-C6
19	AA	842	CLA	C6-C7-C8-C10
19	BB	805	CLA	C6-C7-C8-C10
19	BB	810	CLA	C6-C7-C8-C10
19	BB	833	CLA	C6-C7-C8-C10
19	FF	305	CLA	C2-C3-C5-C6
19	FF	305	CLA	C12-C13-C15-C16
19	LL	202	CLA	C11-C12-C13-C15
21	A	843	PQN	C16-C17-C18-C20
19	A2	828	CLA	C3-C5-C6-C7
19	BB	824	CLA	O1A-CGA-O2A-C1
19	A	830	CLA	C2C-C3C-CAC-CBC
22	L2	208	LHG	C11-C10-C9-C8
19	B2	829	CLA	C13-C15-C16-C17
19	A	827	CLA	C5-C6-C7-C8
19	B	829	CLA	C5-C6-C7-C8
23	A	853	BCR	C9-C10-C11-C12
23	B	842	BCR	C9-C10-C11-C12
23	AA	854	BCR	C9-C10-C11-C12
23	BB	841	BCR	C9-C10-C11-C12
23	KK	103	BCR	C9-C10-C11-C12
19	A1	813	CLA	O1D-CGD-O2D-CED
19	B2	823	CLA	O1D-CGD-O2D-CED
19	BB	823	CLA	O1D-CGD-O2D-CED
22	A1	846	LHG	O9-C7-O7-C5
22	AA	846	LHG	O9-C7-O7-C5
19	B1	824	CLA	CBA-CGA-O2A-C1
19	B1	828	CLA	CBA-CGA-O2A-C1
19	B2	829	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	829	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	AA	833	CLA	CBA-CGA-O2A-C1
19	FF	305	CLA	CBA-CGA-O2A-C1
25	B1	844	LMG	C4-C5-C6-O5
19	A1	803	CLA	C2A-CAA-CBA-CGA
19	A1	823	CLA	C2A-CAA-CBA-CGA
19	B1	849	CLA	C2A-CAA-CBA-CGA
19	A2	808	CLA	C2A-CAA-CBA-CGA
19	B2	850	CLA	C2A-CAA-CBA-CGA
19	A	812	CLA	C2A-CAA-CBA-CGA
19	A	824	CLA	C2A-CAA-CBA-CGA
19	A1	809	CLA	C10-C11-C12-C13
19	B1	828	CLA	C5-C6-C7-C8
19	BB	852	CLA	C13-C15-C16-C17
19	FF	305	CLA	C5-C6-C7-C8
21	B1	837	PQN	C15-C16-C17-C18
19	B	808	CLA	O1A-CGA-O2A-C1
19	B	823	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	C5-C6-C7-C8
22	AA	846	LHG	C12-C13-C14-C15
19	A	815	CLA	C3-C5-C6-C7
19	B	860	CLA	C3-C5-C6-C7
25	BB	844	LMG	C30-C31-C32-C33
23	K2	105	BCR	C22-C23-C24-C25
23	L2	207	BCR	C6-C7-C8-C9
23	A	854	BCR	C22-C23-C24-C25
23	B	839	BCR	C6-C7-C8-C9
23	L	206	BCR	C6-C7-C8-C9
23	AA	855	BCR	C22-C23-C24-C25
23	JJ	104	BCR	C6-C7-C8-C9
19	AA	824	CLA	CBD-CGD-O2D-CED
19	BB	833	CLA	CBD-CGD-O2D-CED
19	B	814	CLA	CBA-CGA-O2A-C1
19	AA	804	CLA	CBA-CGA-O2A-C1
22	AA	846	LHG	C24-C23-O8-C6
19	B1	825	CLA	C16-C17-C18-C19
19	B	825	CLA	C16-C17-C18-C19
19	A2	852	CLA	C8-C10-C11-C12
19	B2	829	CLA	C5-C6-C7-C8
19	BB	806	CLA	C5-C6-C7-C8
25	B	845	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
28	BB	854	DGD	C2B-C3B-C4B-C5B
22	A1	846	LHG	C8-C7-O7-C5
22	A2	846	LHG	C8-C7-O7-C5
22	A	846	LHG	C8-C7-O7-C5
22	AA	847	LHG	C8-C7-O7-C5
25	L1	210	LMG	C11-C10-O7-C8
22	A2	846	LHG	O6-C4-C5-O7
22	A	846	LHG	O6-C4-C5-O7
22	AA	847	LHG	O6-C4-C5-O7
22	BB	850	LHG	O6-C4-C5-O7
23	L2	207	BCR	C18-C19-C20-C21
23	KK	103	BCR	C18-C19-C20-C21
25	B1	844	LMG	C41-C42-C43-C44
23	K1	104	BCR	C14-C15-C16-C17
19	BB	855	CLA	C15-C16-C17-C18
19	A1	832	CLA	CBD-CGD-O2D-CED
19	B2	813	CLA	CBD-CGD-O2D-CED
22	A	845	LHG	O9-C7-O7-C5
19	B2	829	CLA	C3-C5-C6-C7
25	B1	852	LMG	C2-C1-O1-C7
25	B2	854	LMG	C2-C1-O1-C7
25	B1	852	LMG	O6-C5-C6-O5
19	L2	205	CLA	CBA-CGA-O2A-C1
19	B	803	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
25	I1	102	LMG	C11-C12-C13-C14
19	B1	815	CLA	O1A-CGA-O2A-C1
19	B2	816	CLA	O1A-CGA-O2A-C1
19	BB	829	CLA	O1A-CGA-O2A-C1
19	A1	812	CLA	C16-C17-C18-C19
22	A1	845	LHG	C26-C27-C28-C29
25	BB	844	LMG	C18-C19-C20-C21
19	B1	850	CLA	C5-C6-C7-C8
19	A2	821	CLA	C15-C16-C17-C18
19	B2	851	CLA	C5-C6-C7-C8
19	B	823	CLA	C13-C15-C16-C17
21	B2	838	PQN	C15-C16-C17-C18
19	A2	836	CLA	C4-C3-C5-C6
19	B2	821	CLA	C4-C3-C5-C6
19	B	829	CLA	C4-C3-C5-C6
19	B	858	CLA	C4-C3-C5-C6
19	B1	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A2	821	CLA	C2-C3-C5-C6
19	A1	801	CLA	C11-C10-C8-C9
19	A1	803	CLA	C14-C13-C15-C16
19	A1	806	CLA	C11-C12-C13-C14
19	A1	820	CLA	C11-C10-C8-C9
19	A1	826	CLA	C11-C10-C8-C9
19	B1	806	CLA	C6-C7-C8-C9
19	B1	833	CLA	C6-C7-C8-C9
19	L1	205	CLA	C6-C7-C8-C9
19	L1	206	CLA	C11-C12-C13-C14
19	A2	804	CLA	C14-C13-C15-C16
19	A2	827	CLA	C11-C10-C8-C9
19	A2	831	CLA	C6-C7-C8-C9
19	B2	806	CLA	C6-C7-C8-C9
19	B2	834	CLA	C6-C7-C8-C9
19	L2	204	CLA	C6-C7-C8-C9
19	A	801	CLA	C11-C10-C8-C9
19	A	827	CLA	C11-C10-C8-C9
19	A	831	CLA	C6-C7-C8-C9
19	B	806	CLA	C6-C7-C8-C9
19	B	810	CLA	C6-C7-C8-C9
19	B	811	CLA	C6-C7-C8-C9
19	B	811	CLA	C11-C12-C13-C14
19	B	829	CLA	C14-C13-C15-C16
19	B	834	CLA	C6-C7-C8-C9
19	L	203	CLA	C11-C12-C13-C14
19	L	204	CLA	C6-C7-C8-C9
19	AA	801	CLA	C11-C10-C8-C9
19	AA	807	CLA	C11-C12-C13-C14
19	AA	831	CLA	C6-C7-C8-C9
19	AA	842	CLA	C6-C7-C8-C9
19	BB	806	CLA	C6-C7-C8-C9
19	BB	811	CLA	C6-C7-C8-C9
19	BB	811	CLA	C11-C12-C13-C14
19	BB	821	CLA	C6-C7-C8-C9
19	BB	833	CLA	C6-C7-C8-C9
19	FF	305	CLA	C14-C13-C15-C16
19	LL	202	CLA	C11-C12-C13-C14
21	A1	843	PQN	C21-C22-C23-C24
25	B2	847	LMG	O6-C5-C6-O5
25	B2	854	LMG	O6-C5-C6-O5
19	LL	203	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	B1	828	CLA	C3-C5-C6-C7
19	AA	815	CLA	C3-C5-C6-C7
19	LL	201	CLA	C3-C5-C6-C7
19	A	837	CLA	O1D-CGD-O2D-CED
19	B1	822	CLA	C2A-CAA-CBA-CGA
19	A2	826	CLA	C2A-CAA-CBA-CGA
19	AA	812	CLA	C2A-CAA-CBA-CGA
19	BB	815	CLA	CBA-CGA-O2A-C1
23	F1	303	BCR	C36-C18-C19-C20
23	L1	209	BCR	C7-C8-C9-C34
23	A	847	BCR	C36-C18-C19-C20
23	A	849	BCR	C36-C18-C19-C20
23	K	103	BCR	C7-C8-C9-C34
19	A1	826	CLA	O1D-CGD-O2D-CED
19	A2	827	CLA	C15-C16-C17-C18
19	AA	820	CLA	C8-C10-C11-C12
19	BB	856	CLA	C5-C6-C7-C8
25	B	845	LMG	C33-C34-C35-C36
23	A1	849	BCR	C21-C22-C23-C24
23	F1	304	BCR	C17-C18-C19-C20
23	A2	848	BCR	C11-C12-C13-C14
23	I2	101	BCR	C17-C18-C19-C20
23	A	854	BCR	C21-C22-C23-C24
23	B	842	BCR	C17-C18-C19-C20
23	FF	304	BCR	C17-C18-C19-C20
23	II	101	BCR	C17-C18-C19-C20
19	B1	824	CLA	O1A-CGA-O2A-C1
19	A	833	CLA	O1A-CGA-O2A-C1
19	AA	831	CLA	O1A-CGA-O2A-C1
19	A1	807	CLA	C1A-C2A-CAA-CBA
19	A1	809	CLA	C1A-C2A-CAA-CBA
19	A1	810	CLA	C1A-C2A-CAA-CBA
19	A1	817	CLA	C1A-C2A-CAA-CBA
19	A1	819	CLA	C1A-C2A-CAA-CBA
19	A1	822	CLA	C1A-C2A-CAA-CBA
19	A1	826	CLA	C1A-C2A-CAA-CBA
19	A1	838	CLA	C1A-C2A-CAA-CBA
19	B1	804	CLA	C1A-C2A-CAA-CBA
19	B1	815	CLA	C1A-C2A-CAA-CBA
19	B1	820	CLA	C1A-C2A-CAA-CBA
19	B1	825	CLA	C1A-C2A-CAA-CBA
19	B1	827	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B1	828	CLA	C1A-C2A-CAA-CBA
19	B1	834	CLA	C1A-C2A-CAA-CBA
19	B1	850	CLA	C1A-C2A-CAA-CBA
19	A2	808	CLA	C1A-C2A-CAA-CBA
19	A2	811	CLA	C1A-C2A-CAA-CBA
19	A2	818	CLA	C1A-C2A-CAA-CBA
19	A2	820	CLA	C1A-C2A-CAA-CBA
19	A2	823	CLA	C1A-C2A-CAA-CBA
19	A2	827	CLA	C1A-C2A-CAA-CBA
19	A2	839	CLA	C1A-C2A-CAA-CBA
19	B2	802	CLA	C1A-C2A-CAA-CBA
19	B2	804	CLA	C1A-C2A-CAA-CBA
19	B2	815	CLA	C1A-C2A-CAA-CBA
19	B2	820	CLA	C1A-C2A-CAA-CBA
19	B2	825	CLA	C1A-C2A-CAA-CBA
19	B2	827	CLA	C1A-C2A-CAA-CBA
19	B2	835	CLA	C1A-C2A-CAA-CBA
19	B2	851	CLA	C1A-C2A-CAA-CBA
19	K2	104	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C1A-C2A-CAA-CBA
19	A	810	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C1A-C2A-CAA-CBA
19	A	827	CLA	C1A-C2A-CAA-CBA
19	A	828	CLA	C1A-C2A-CAA-CBA
19	A	829	CLA	C1A-C2A-CAA-CBA
19	A	839	CLA	C1A-C2A-CAA-CBA
19	A	852	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	859	CLA	C1A-C2A-CAA-CBA
19	AA	805	CLA	C1A-C2A-CAA-CBA
19	AA	811	CLA	C1A-C2A-CAA-CBA
19	AA	818	CLA	C1A-C2A-CAA-CBA
19	AA	820	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	AA	822	CLA	C1A-C2A-CAA-CBA
19	AA	825	CLA	C1A-C2A-CAA-CBA
19	AA	827	CLA	C1A-C2A-CAA-CBA
19	AA	839	CLA	C1A-C2A-CAA-CBA
19	BB	804	CLA	C1A-C2A-CAA-CBA
19	BB	808	CLA	C1A-C2A-CAA-CBA
19	BB	824	CLA	C1A-C2A-CAA-CBA
19	BB	825	CLA	C1A-C2A-CAA-CBA
19	BB	827	CLA	C1A-C2A-CAA-CBA
19	BB	856	CLA	C1A-C2A-CAA-CBA
19	FF	301	CLA	C1A-C2A-CAA-CBA
19	A	813	CLA	C16-C17-C18-C19
22	A2	846	LHG	O9-C7-O7-C5
22	A	846	LHG	O9-C7-O7-C5
22	AA	847	LHG	O9-C7-O7-C5
23	B1	841	BCR	C9-C10-C11-C12
23	B2	842	BCR	C19-C20-C21-C22
23	KK	103	BCR	C15-C16-C17-C18
19	A	827	CLA	C10-C11-C12-C13
19	AA	805	CLA	C8-C10-C11-C12
22	X1	103	LHG	C3-O3-P-O6
25	II	105	LMG	C28-C29-C30-C31
19	A1	827	CLA	C3-C5-C6-C7
19	B2	822	CLA	C3-C5-C6-C7
19	AA	843	CLA	O1D-CGD-O2D-CED
19	B1	802	CLA	C15-C16-C17-C18
19	A2	801	CLA	C5-C6-C7-C8
19	A2	804	CLA	C5-C6-C7-C8
19	B2	823	CLA	C8-C10-C11-C12
19	B	806	CLA	C5-C6-C7-C8
19	B2	824	CLA	CBA-CGA-O2A-C1
22	L1	211	LHG	O6-C4-C5-C6
22	A	846	LHG	O6-C4-C5-C6
22	B	853	LHG	C23-C24-C25-C26
25	B2	845	LMG	O6-C5-C6-O5
19	B1	835	CLA	O1D-CGD-O2D-CED
19	A2	810	CLA	C10-C11-C12-C13
19	A	820	CLA	C8-C10-C11-C12
22	A1	845	LHG	C1-C2-C3-O3
19	B1	828	CLA	C4-C3-C5-C6
19	A2	821	CLA	C4-C3-C5-C6
19	A1	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B1	808	CLA	C2-C3-C5-C6
19	B1	813	CLA	C3A-C2A-CAA-CBA
19	A2	814	CLA	C3A-C2A-CAA-CBA
19	B2	813	CLA	C3A-C2A-CAA-CBA
19	A	814	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	AA	814	CLA	C3A-C2A-CAA-CBA
19	BB	813	CLA	C3A-C2A-CAA-CBA
19	B2	850	CLA	C15-C16-C17-C18
19	B	834	CLA	C13-C15-C16-C17
19	AA	810	CLA	C10-C11-C12-C13
19	BB	823	CLA	C13-C15-C16-C17
22	BB	850	LHG	C8-C7-O7-C5
19	A	828	CLA	O1A-CGA-O2A-C1
19	A	840	CLA	O1A-CGA-O2A-C1
19	B	803	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	B	830	CLA	O1A-CGA-O2A-C1
19	AA	833	CLA	O1A-CGA-O2A-C1
19	FF	305	CLA	O1A-CGA-O2A-C1
19	K1	103	CLA	C2A-CAA-CBA-CGA
19	B2	819	CLA	O1D-CGD-O2D-CED
19	B	829	CLA	C3-C5-C6-C7
19	FF	305	CLA	C3-C5-C6-C7
22	B1	847	LHG	C4-C5-C6-O8
22	L1	211	LHG	C4-C5-C6-O8
22	B2	848	LHG	C4-C5-C6-O8
22	L2	208	LHG	C4-C5-C6-O8
25	B2	847	LMG	O1-C7-C8-C9
25	M	102	LMG	O1-C7-C8-C9
28	B	856	DGD	C1G-C2G-C3G-O3G
25	B	845	LMG	C30-C31-C32-C33
19	B2	824	CLA	O1A-CGA-O2A-C1
19	B2	829	CLA	O1A-CGA-O2A-C1
19	L2	205	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	O1A-CGA-O2A-C1
23	A1	847	BCR	C14-C15-C16-C17
25	I1	102	LMG	C8-C7-O1-C1
19	B	808	CLA	CBD-CGD-O2D-CED
19	B1	849	CLA	C15-C16-C17-C18
19	B	826	CLA	C15-C16-C17-C18
19	BB	826	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B2	854	LMG	C14-C15-C16-C17
25	B	851	LMG	C37-C38-C39-C40
19	B2	808	CLA	O1D-CGD-O2D-CED
19	B	836	CLA	O1D-CGD-O2D-CED
19	B1	828	CLA	O1A-CGA-O2A-C1
19	B1	833	CLA	C13-C15-C16-C17
19	A	801	CLA	C5-C6-C7-C8
22	A2	846	LHG	O1-C1-C2-O2
25	B2	845	LMG	C33-C34-C35-C36
25	II	105	LMG	C16-C17-C18-C19
25	II	105	LMG	C4-C5-C6-O5
19	B	830	CLA	C4C-C3C-CAC-CBC
25	M	102	LMG	C15-C16-C17-C18
22	A2	845	LHG	C8-C7-O7-C5
22	X	102	LHG	C8-C7-O7-C5
25	B	851	LMG	C11-C10-O7-C8
19	B1	801	CLA	C13-C15-C16-C17
19	L1	207	CLA	C10-C11-C12-C13
19	AA	821	CLA	C15-C16-C17-C18
23	B1	841	BCR	C20-C21-C22-C37
23	F1	306	BCR	C11-C10-C9-C34
23	K2	103	BCR	C35-C13-C14-C15
23	L	205	BCR	C35-C13-C14-C15
23	AA	849	BCR	C20-C21-C22-C37
23	BB	838	BCR	C35-C13-C14-C15
23	II	104	BCR	C20-C21-C22-C37
19	A	841	CLA	O1A-CGA-O2A-C1
19	BB	814	CLA	C4-C3-C5-C6
19	B	815	CLA	O1A-CGA-O2A-C1
22	BB	850	LHG	C23-C24-C25-C26
19	A2	807	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C19
22	LL	205	LHG	C24-C23-O8-C6
19	A1	830	CLA	C13-C15-C16-C17
25	L1	210	LMG	C9-C8-O7-C10
25	B	851	LMG	C9-C8-O7-C10
28	B	856	DGD	C1G-C2G-O2G-C1B
28	BB	854	DGD	C1G-C2G-O2G-C1B
19	BB	822	CLA	O1D-CGD-O2D-CED
19	A2	802	CLA	C2A-CAA-CBA-CGA
19	B1	823	CLA	C15-C16-C17-C18
19	B2	801	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	BB	802	CLA	C15-C16-C17-C18
22	L2	208	LHG	C24-C25-C26-C27
25	B1	852	LMG	C14-C15-C16-C17
19	B1	813	CLA	O1D-CGD-O2D-CED
19	A1	804	CLA	C3-C5-C6-C7
19	B2	830	CLA	C2C-C3C-CAC-CBC
25	B2	845	LMG	C35-C36-C37-C38
19	B	813	CLA	O1D-CGD-O2D-CED
19	B2	803	CLA	C5-C6-C7-C8
19	B	858	CLA	C15-C16-C17-C18
22	X2	102	LHG	C25-C26-C27-C28
19	A1	832	CLA	CBA-CGA-O2A-C1
19	A1	839	CLA	CBA-CGA-O2A-C1
19	A2	804	CLA	CBA-CGA-O2A-C1
19	AA	840	CLA	CBA-CGA-O2A-C1
19	AA	853	CLA	CBA-CGA-O2A-C1
19	BB	808	CLA	CBA-CGA-O2A-C1
22	L	207	LHG	C24-C23-O8-C6
19	AA	804	CLA	O1A-CGA-O2A-C1
22	A1	846	LHG	O6-C4-C5-O7
19	B2	825	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C20
20	AA	803	CL0	C2C-C3C-CAC-CBC
22	X1	102	LHG	C25-C26-C27-C28
19	B1	803	CLA	C5-C6-C7-C8
19	A2	807	CLA	C10-C11-C12-C13
19	B2	810	CLA	C10-C11-C12-C13
25	M	102	LMG	C12-C13-C14-C15
19	B1	823	CLA	O1D-CGD-O2D-CED
19	BB	815	CLA	O1A-CGA-O2A-C1
22	AA	846	LHG	O10-C23-O8-C6
25	M	102	LMG	C17-C18-C19-C20
19	A	810	CLA	C10-C11-C12-C13
19	B	859	CLA	C5-C6-C7-C8
19	A1	820	CLA	O1D-CGD-O2D-CED
23	A1	851	BCR	C20-C21-C22-C23
23	B1	841	BCR	C11-C10-C9-C8
23	B1	841	BCR	C12-C13-C14-C15
23	L1	209	BCR	C16-C17-C18-C19
23	B2	839	BCR	C16-C17-C18-C19
23	B2	842	BCR	C20-C21-C22-C23
23	M2	102	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	B	839	BCR	C16-C17-C18-C19
23	B	840	BCR	C16-C17-C18-C19
23	J	102	BCR	C11-C10-C9-C8
23	AA	849	BCR	C16-C17-C18-C19
23	FF	304	BCR	C12-C13-C14-C15
25	M	102	LMG	C2-C1-O1-C7
25	I2	105	LMG	O1-C7-C8-O7
22	A2	845	LHG	C12-C13-C14-C15
25	L1	210	LMG	C37-C38-C39-C40
19	A	810	CLA	C8-C10-C11-C12
19	L	204	CLA	C8-C10-C11-C12
21	B1	837	PQN	C18-C20-C21-C22
19	A2	813	CLA	C16-C17-C18-C19
22	L2	208	LHG	C13-C14-C15-C16
25	L1	210	LMG	C21-C22-C23-C24
25	B2	845	LMG	C13-C14-C15-C16
25	B2	845	LMG	C38-C39-C40-C41
19	AA	821	CLA	C4-C3-C5-C6
19	A1	807	CLA	C5-C6-C7-C8
19	A1	803	CLA	C12-C13-C15-C16
19	A1	806	CLA	C11-C12-C13-C15
19	A1	820	CLA	C12-C13-C15-C16
19	A1	822	CLA	C6-C7-C8-C10
19	A1	829	CLA	C11-C10-C8-C7
19	A1	830	CLA	C6-C7-C8-C10
19	B1	801	CLA	C12-C13-C15-C16
19	B1	806	CLA	C6-C7-C8-C10
19	B1	811	CLA	C11-C10-C8-C7
19	B1	815	CLA	C11-C10-C8-C7
19	B1	815	CLA	C12-C13-C15-C16
19	B1	821	CLA	C6-C7-C8-C10
19	B1	832	CLA	C6-C7-C8-C10
19	L1	205	CLA	C6-C7-C8-C10
19	A2	804	CLA	C6-C7-C8-C10
19	A2	807	CLA	C11-C12-C13-C15
19	A2	807	CLA	C12-C13-C15-C16
19	A2	813	CLA	C11-C12-C13-C15
19	A2	823	CLA	C6-C7-C8-C10
19	A2	830	CLA	C11-C10-C8-C7
19	A2	831	CLA	C6-C7-C8-C10
19	B2	806	CLA	C6-C7-C8-C10
19	B2	810	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B2	811	CLA	C11-C10-C8-C7
19	B2	821	CLA	C6-C7-C8-C10
19	B2	826	CLA	C6-C7-C8-C10
19	B2	833	CLA	C6-C7-C8-C10
19	B2	836	CLA	C6-C7-C8-C10
19	B2	849	CLA	C6-C7-C8-C10
19	L2	204	CLA	C6-C7-C8-C10
19	A	807	CLA	C11-C12-C13-C15
19	A	807	CLA	C12-C13-C15-C16
19	A	813	CLA	C11-C12-C13-C15
19	A	821	CLA	C11-C12-C13-C15
19	A	823	CLA	C6-C7-C8-C10
19	A	830	CLA	C11-C10-C8-C7
19	A	831	CLA	C6-C7-C8-C10
19	A	835	CLA	C12-C13-C15-C16
19	B	806	CLA	C6-C7-C8-C10
19	B	815	CLA	C12-C13-C15-C16
19	B	821	CLA	C6-C7-C8-C10
19	B	826	CLA	C6-C7-C8-C10
19	B	836	CLA	C6-C7-C8-C10
19	AA	801	CLA	C11-C10-C8-C7
19	AA	804	CLA	C12-C13-C15-C16
19	AA	807	CLA	C11-C12-C13-C15
19	AA	813	CLA	C11-C12-C13-C15
19	AA	821	CLA	C11-C12-C13-C15
19	AA	823	CLA	C6-C7-C8-C10
19	AA	829	CLA	C11-C10-C8-C7
19	AA	830	CLA	C11-C10-C8-C7
19	AA	831	CLA	C6-C7-C8-C10
19	BB	806	CLA	C6-C7-C8-C10
19	BB	821	CLA	C6-C7-C8-C10
19	BB	826	CLA	C6-C7-C8-C10
19	BB	832	CLA	C6-C7-C8-C10
19	BB	835	CLA	C6-C7-C8-C10
20	A	803	CL0	C12-C13-C15-C16
21	B2	838	PQN	C21-C22-C23-C25
21	A	843	PQN	C21-C22-C23-C25
21	B	838	PQN	C21-C22-C23-C25
19	AA	841	CLA	O1A-CGA-O2A-C1
19	A	828	CLA	C3-C5-C6-C7
19	A	830	CLA	C3-C5-C6-C7
25	II	105	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
19	A1	822	CLA	C6-C7-C8-C9
19	A1	830	CLA	C6-C7-C8-C9
19	B1	801	CLA	C14-C13-C15-C16
19	B1	810	CLA	C11-C10-C8-C9
19	B1	815	CLA	C11-C10-C8-C9
19	B1	821	CLA	C6-C7-C8-C9
19	B1	832	CLA	C6-C7-C8-C9
19	B1	848	CLA	C11-C10-C8-C9
19	A2	807	CLA	C11-C12-C13-C14
19	A2	807	CLA	C14-C13-C15-C16
19	A2	821	CLA	C11-C12-C13-C14
19	A2	823	CLA	C6-C7-C8-C9
19	A2	830	CLA	C11-C12-C13-C14
19	B2	810	CLA	C6-C7-C8-C9
19	B2	815	CLA	C11-C10-C8-C9
19	B2	821	CLA	C6-C7-C8-C9
19	B2	823	CLA	C11-C12-C13-C14
19	B2	826	CLA	C6-C7-C8-C9
19	B2	833	CLA	C6-C7-C8-C9
19	B2	849	CLA	C11-C10-C8-C9
19	A	804	CLA	C14-C13-C15-C16
19	A	807	CLA	C11-C10-C8-C9
19	A	807	CLA	C11-C12-C13-C14
19	A	807	CLA	C14-C13-C15-C16
19	A	813	CLA	C11-C12-C13-C14
19	A	821	CLA	C11-C12-C13-C14
19	A	823	CLA	C6-C7-C8-C9
19	A	836	CLA	C14-C13-C15-C16
19	B	801	CLA	C14-C13-C15-C16
19	B	803	CLA	C11-C12-C13-C14
19	B	821	CLA	C6-C7-C8-C9
19	B	826	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	B	854	CLA	C11-C10-C8-C9
19	AA	804	CLA	C14-C13-C15-C16
19	AA	813	CLA	C11-C12-C13-C14
19	AA	821	CLA	C11-C12-C13-C14
19	AA	823	CLA	C6-C7-C8-C9
19	AA	836	CLA	C14-C13-C15-C16
19	AA	853	CLA	C11-C12-C13-C14
19	BB	801	CLA	C14-C13-C15-C16
19	BB	815	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	BB	826	CLA	C6-C7-C8-C9
19	BB	832	CLA	C6-C7-C8-C9
19	BB	852	CLA	C11-C10-C8-C9
20	A	803	CL0	C6-C7-C8-C9
21	A2	843	PQN	C16-C17-C18-C19
21	A	843	PQN	C21-C22-C23-C24
23	A2	848	BCR	C14-C15-C16-C17
23	F2	303	BCR	C14-C15-C16-C17
23	L	205	BCR	C14-C15-C16-C17
23	FF	306	BCR	C14-C15-C16-C17
19	A1	803	CLA	CBA-CGA-O2A-C1
22	A	845	LHG	C24-C23-O8-C6
19	F1	301	CLA	C10-C11-C12-C13
19	K	102	CLA	C2A-CAA-CBA-CGA
28	B	856	DGD	C4B-C5B-C6B-C7B
23	I1	101	BCR	C37-C22-C23-C24
23	I2	101	BCR	C37-C22-C23-C24
23	L	206	BCR	C7-C8-C9-C34
23	L	206	BCR	C37-C22-C23-C24
26	B1	840	ECH	C37-C22-C23-C24
26	B2	841	ECH	C37-C22-C23-C24
26	B	841	ECH	C37-C22-C23-C24
26	BB	840	ECH	C37-C22-C23-C24
19	A1	803	CLA	C16-C17-C18-C19
25	B1	844	LMG	C16-C17-C18-C19
19	B2	836	CLA	O1D-CGD-O2D-CED
23	A1	848	BCR	C21-C22-C23-C24
23	A2	849	BCR	C17-C18-C19-C20
23	A2	850	BCR	C21-C22-C23-C24
23	B2	842	BCR	C11-C12-C13-C14
23	F2	304	BCR	C17-C18-C19-C20
23	L2	207	BCR	C17-C18-C19-C20
23	A	853	BCR	C17-C18-C19-C20
23	AA	854	BCR	C17-C18-C19-C20
23	JJ	102	BCR	C17-C18-C19-C20
26	B1	840	ECH	C21-C22-C23-C24
26	B2	841	ECH	C17-C18-C19-C20
26	B2	841	ECH	C21-C22-C23-C24
26	B	841	ECH	C21-C22-C23-C24
26	BB	840	ECH	C21-C22-C23-C24
19	B	818	CLA	O1D-CGD-O2D-CED
22	B2	848	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
19	A1	801	CLA	C5-C6-C7-C8
19	A1	852	CLA	C8-C10-C11-C12
19	AA	810	CLA	C8-C10-C11-C12
19	A2	833	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	CBA-CGA-O2A-C1
22	B	852	LHG	C23-C24-C25-C26
19	L2	206	CLA	C10-C11-C12-C13
19	B	803	CLA	C5-C6-C7-C8
19	AA	827	CLA	C15-C16-C17-C18
19	AA	830	CLA	C5-C6-C7-C8
19	BB	803	CLA	C5-C6-C7-C8
19	BB	823	CLA	C10-C11-C12-C13
23	K1	104	BCR	C22-C23-C24-C25
19	A2	807	CLA	C16-C17-C18-C20
19	B1	810	CLA	C5-C6-C7-C8
19	A	830	CLA	C5-C6-C7-C8
19	AA	801	CLA	C5-C6-C7-C8
19	AA	843	CLA	C15-C16-C17-C18
22	A1	846	LHG	O6-C4-C5-C6
22	A2	846	LHG	O6-C4-C5-C6
22	AA	847	LHG	O6-C4-C5-C6
19	AA	830	CLA	C3-C5-C6-C7
19	B	825	CLA	O1D-CGD-O2D-CED
25	BB	844	LMG	C13-C14-C15-C16
19	A1	815	CLA	CBA-CGA-O2A-C1
19	B	804	CLA	CBA-CGA-O2A-C1
19	BB	804	CLA	CBA-CGA-O2A-C1
23	B	848	BCR	C18-C19-C20-C21
19	A2	830	CLA	C5-C6-C7-C8
19	AA	831	CLA	C13-C15-C16-C17
19	BB	801	CLA	C8-C10-C11-C12
25	B	851	LMG	C21-C22-C23-C24
19	B2	850	CLA	C4-C3-C5-C6
19	A	821	CLA	C4-C3-C5-C6
19	AA	828	CLA	C4-C3-C5-C6
19	BB	821	CLA	C4-C3-C5-C6
19	AA	821	CLA	C2-C3-C5-C6
19	AA	828	CLA	C2-C3-C5-C6
19	A1	826	CLA	C15-C16-C17-C18
19	BB	801	CLA	C15-C16-C17-C18
19	AA	804	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	A	803	CL0	C16-C17-C18-C19
19	A1	829	CLA	C5-C6-C7-C8
19	B2	852	CLA	C15-C16-C17-C18
20	A2	803	CL0	C2A-CAA-CBA-CGA
19	A1	805	CLA	CBA-CGA-O2A-C1
19	B2	804	CLA	CBA-CGA-O2A-C1
28	B	856	DGD	C1A-C2A-C3A-C4A
19	A1	829	CLA	C2C-C3C-CAC-CBC
25	L1	210	LMG	C34-C35-C36-C37
25	B	851	LMG	C11-C12-C13-C14
19	AA	840	CLA	O1D-CGD-O2D-CED
19	A1	814	CLA	C3A-C2A-CAA-CBA
19	A1	827	CLA	C3A-C2A-CAA-CBA
19	B1	804	CLA	C3A-C2A-CAA-CBA
19	B1	821	CLA	C3A-C2A-CAA-CBA
19	A2	806	CLA	C3A-C2A-CAA-CBA
19	A2	815	CLA	C3A-C2A-CAA-CBA
19	A2	828	CLA	C3A-C2A-CAA-CBA
19	A	815	CLA	C3A-C2A-CAA-CBA
19	A	824	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	C3A-C2A-CAA-CBA
19	B	804	CLA	C3A-C2A-CAA-CBA
19	B	821	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	B	859	CLA	C3A-C2A-CAA-CBA
19	AA	815	CLA	C3A-C2A-CAA-CBA
19	AA	828	CLA	C3A-C2A-CAA-CBA
19	BB	804	CLA	C3A-C2A-CAA-CBA
19	BB	821	CLA	C3A-C2A-CAA-CBA
19	LL	201	CLA	C3A-C2A-CAA-CBA
19	BB	833	CLA	C13-C15-C16-C17
22	A2	845	LHG	C29-C30-C31-C32
25	BB	844	LMG	C16-C17-C18-C19
23	K2	105	BCR	C19-C20-C21-C22
23	B	844	BCR	C9-C10-C11-C12
23	J	102	BCR	C15-C16-C17-C18
23	K	103	BCR	C15-C16-C17-C18
23	L	205	BCR	C15-C16-C17-C18
26	B1	840	ECH	C13-C14-C15-C16
26	B2	841	ECH	C13-C14-C15-C16
25	BB	844	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
19	A1	803	CLA	C3-C5-C6-C7
19	B1	814	CLA	C3-C5-C6-C7
19	B1	825	CLA	C3-C5-C6-C7
22	B	853	LHG	C34-C35-C36-C37
25	B1	844	LMG	C38-C39-C40-C41
25	II	105	LMG	C11-C12-C13-C14
19	AA	804	CLA	C16-C17-C18-C20
19	B1	804	CLA	CBA-CGA-O2A-C1
19	BB	814	CLA	CBA-CGA-O2A-C1
19	BB	852	CLA	CBA-CGA-O2A-C1
19	B	837	CLA	C4C-C3C-CAC-CBC
22	A	846	LHG	C14-C15-C16-C17
28	BB	854	DGD	C4B-C5B-C6B-C7B
19	A1	809	CLA	C8-C10-C11-C12
19	F2	301	CLA	C10-C11-C12-C13
19	AA	836	CLA	C13-C15-C16-C17
22	X1	102	LHG	C4-C5-C6-O8
25	B1	846	LMG	O1-C7-C8-C9
25	I1	102	LMG	O1-C7-C8-C9
19	AA	853	CLA	O1A-CGA-O2A-C1
19	A	828	CLA	C4-C3-C5-C6
20	A	803	CL0	C16-C17-C18-C20
22	AA	847	LHG	C14-C15-C16-C17
19	A2	804	CLA	C3-C5-C6-C7
19	AA	828	CLA	C3-C5-C6-C7
19	L	202	CLA	C2A-CAA-CBA-CGA
22	B	853	LHG	O1-C1-C2-O2
19	B	805	CLA	C5-C6-C7-C8
19	B	811	CLA	C8-C10-C11-C12
19	BB	805	CLA	C5-C6-C7-C8
22	B	852	LHG	O6-C4-C5-O7
22	BB	850	LHG	O9-C7-O7-C5
19	B2	849	CLA	CBA-CGA-O2A-C1
19	AA	816	CLA	CBA-CGA-O2A-C1
19	A1	832	CLA	O1A-CGA-O2A-C1
19	A1	839	CLA	O1A-CGA-O2A-C1
19	A2	804	CLA	O1A-CGA-O2A-C1
19	AA	840	CLA	O1A-CGA-O2A-C1
19	BB	808	CLA	O1A-CGA-O2A-C1
22	LL	205	LHG	O10-C23-O8-C6
22	A	845	LHG	C7-C8-C9-C10
19	A2	804	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	B2	825	CLA	C16-C17-C18-C20
19	L2	204	CLA	C10-C11-C12-C13
22	BB	851	LHG	C34-C35-C36-C37
25	B	845	LMG	C35-C36-C37-C38
19	A2	810	CLA	C8-C10-C11-C12
19	A	808	CLA	C5-C6-C7-C8
22	L	207	LHG	O10-C23-O8-C6
25	B2	845	LMG	C16-C17-C18-C19
19	AA	832	CLA	C3-C5-C6-C7
25	B1	844	LMG	O6-C5-C6-O5
25	I1	102	LMG	O1-C7-C8-O7
25	M	102	LMG	O1-C7-C8-O7
25	M	102	LMG	O7-C8-C9-O8
28	B	856	DGD	O2G-C2G-C3G-O3G
19	BB	825	CLA	CBD-CGD-O2D-CED
19	A2	816	CLA	CBA-CGA-O2A-C1
19	B1	820	CLA	C2C-C3C-CAC-CBC
22	B	852	LHG	C8-C7-O7-C5
19	A1	803	CLA	C16-C17-C18-C20
19	B1	825	CLA	C16-C17-C18-C20
19	B	801	CLA	C16-C17-C18-C20
19	A1	852	CLA	C5-C6-C7-C8
19	B1	801	CLA	C15-C16-C17-C18
19	A	831	CLA	C13-C15-C16-C17
19	B	860	CLA	C15-C16-C17-C18
19	L	202	CLA	C5-C6-C7-C8
19	BB	815	CLA	C13-C15-C16-C17
22	B	853	LHG	C1-C2-C3-O3
25	B	845	LMG	C38-C39-C40-C41
22	A2	845	LHG	O9-C7-O7-C5
22	X	102	LHG	O9-C7-O7-C5
19	A1	827	CLA	C4-C3-C5-C6
19	L1	205	CLA	C2-C1-O2A-CGA
19	L2	204	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C2-C1-O2A-CGA
19	B	824	CLA	C2-C1-O2A-CGA
19	BB	801	CLA	C2-C1-O2A-CGA
19	LL	201	CLA	C2-C1-O2A-CGA
19	AA	824	CLA	O1D-CGD-O2D-CED
19	B2	850	CLA	C2-C3-C5-C6
19	A	821	CLA	C2-C3-C5-C6
19	L1	205	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	A1	806	CLA	C14-C13-C15-C16
19	A1	812	CLA	C11-C12-C13-C14
19	B1	805	CLA	C11-C12-C13-C14
19	B1	826	CLA	C6-C7-C8-C9
19	A2	813	CLA	C11-C12-C13-C14
19	A2	827	CLA	C14-C13-C15-C16
19	A2	842	CLA	C6-C7-C8-C9
19	B2	801	CLA	C14-C13-C15-C16
19	B2	805	CLA	C11-C12-C13-C14
19	B2	836	CLA	C14-C13-C15-C16
19	A	835	CLA	C14-C13-C15-C16
19	B	805	CLA	C11-C12-C13-C14
19	AA	813	CLA	C6-C7-C8-C9
19	BB	803	CLA	C6-C7-C8-C9
19	BB	805	CLA	C11-C12-C13-C14
19	BB	816	CLA	C6-C7-C8-C9
19	B1	805	CLA	C5-C6-C7-C8
19	B2	805	CLA	C5-C6-C7-C8
22	X2	103	LHG	C2-C3-O3-P
22	B	853	LHG	C2-C3-O3-P
19	A	804	CLA	O1A-CGA-O2A-C1
22	X1	103	LHG	C10-C11-C12-C13
25	B1	844	LMG	C13-C14-C15-C16
25	B	851	LMG	C32-C33-C34-C35
19	A1	825	CLA	C2A-CAA-CBA-CGA
19	A	826	CLA	C2A-CAA-CBA-CGA
19	AA	808	CLA	C2A-CAA-CBA-CGA
19	B	825	CLA	C16-C17-C18-C20
19	BB	826	CLA	CBD-CGD-O2D-CED
19	AA	804	CLA	C3-C5-C6-C7
23	A1	850	BCR	C5-C6-C7-C8
23	A1	851	BCR	C5-C6-C7-C8
23	B1	842	BCR	C23-C24-C25-C30
23	F1	303	BCR	C1-C6-C7-C8
23	F1	303	BCR	C23-C24-C25-C26
23	K1	104	BCR	C23-C24-C25-C26
23	K1	104	BCR	C23-C24-C25-C30
23	L1	209	BCR	C23-C24-C25-C26
23	L1	209	BCR	C23-C24-C25-C30
23	A2	850	BCR	C5-C6-C7-C8
23	A2	851	BCR	C5-C6-C7-C8
23	B2	843	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	B2	843	BCR	C23-C24-C25-C30
23	F2	303	BCR	C1-C6-C7-C8
23	F2	303	BCR	C5-C6-C7-C8
23	K2	105	BCR	C23-C24-C25-C30
23	L2	207	BCR	C23-C24-C25-C26
23	L2	207	BCR	C23-C24-C25-C30
23	A	850	BCR	C5-C6-C7-C8
23	A	851	BCR	C5-C6-C7-C8
23	F	303	BCR	C1-C6-C7-C8
23	F	303	BCR	C5-C6-C7-C8
23	F	305	BCR	C23-C24-C25-C26
23	F	305	BCR	C23-C24-C25-C30
23	I	101	BCR	C5-C6-C7-C8
23	J	102	BCR	C1-C6-C7-C8
23	J	102	BCR	C5-C6-C7-C8
23	J	102	BCR	C23-C24-C25-C26
23	L	205	BCR	C5-C6-C7-C8
23	M	101	BCR	C1-C6-C7-C8
23	AA	851	BCR	C5-C6-C7-C8
23	AA	852	BCR	C5-C6-C7-C8
23	AA	852	BCR	C23-C24-C25-C26
23	BB	842	BCR	C23-C24-C25-C26
23	FF	303	BCR	C1-C6-C7-C8
23	FF	303	BCR	C5-C6-C7-C8
23	II	101	BCR	C1-C6-C7-C8
23	II	101	BCR	C5-C6-C7-C8
23	II	104	BCR	C5-C6-C7-C8
23	JJ	102	BCR	C1-C6-C7-C8
23	JJ	102	BCR	C5-C6-C7-C8
23	JJ	102	BCR	C23-C24-C25-C26
23	MM	101	BCR	C1-C6-C7-C8
23	MM	101	BCR	C5-C6-C7-C8
19	F	301	CLA	C10-C11-C12-C13
21	B2	838	PQN	C18-C20-C21-C22
23	K2	103	BCR	C7-C8-C9-C34
23	AA	848	BCR	C36-C18-C19-C20
26	B2	841	ECH	C36-C18-C19-C20
28	B	856	DGD	C4E-C5E-C6E-O5E
19	A1	803	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	O10-C23-O8-C6
19	A2	825	CLA	C1A-C2A-CAA-CBA
23	A1	850	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	J1	102	BCR	C17-C18-C19-C20
23	J1	104	BCR	C11-C12-C13-C14
23	L1	201	BCR	C11-C12-C13-C14
23	L1	201	BCR	C21-C22-C23-C24
23	M1	101	BCR	C11-C12-C13-C14
23	A2	848	BCR	C21-C22-C23-C24
23	J2	102	BCR	C17-C18-C19-C20
23	M2	102	BCR	C11-C12-C13-C14
23	B	843	BCR	C17-C18-C19-C20
23	AA	851	BCR	C21-C22-C23-C24
23	AA	852	BCR	C7-C8-C9-C10
23	FF	303	BCR	C7-C8-C9-C10
19	A2	804	CLA	C8-C10-C11-C12
25	BB	844	LMG	C33-C34-C35-C36
23	A1	848	BCR	C14-C15-C16-C17
23	A	847	BCR	C20-C21-C22-C23
23	A	849	BCR	C14-C15-C16-C17
23	B	848	BCR	C14-C15-C16-C17
23	AA	848	BCR	C20-C21-C22-C23
23	BB	847	BCR	C14-C15-C16-C17
19	B1	829	CLA	C2C-C3C-CAC-CBC
25	B1	844	LMG	C35-C36-C37-C38
19	A	804	CLA	C16-C17-C18-C20
19	BB	825	CLA	C16-C17-C18-C20
19	BB	836	CLA	C3-C5-C6-C7
22	B1	847	LHG	C12-C13-C14-C15
25	B	851	LMG	C15-C16-C17-C18
25	II	105	LMG	C30-C31-C32-C33
19	AA	830	CLA	C13-C15-C16-C17
19	A1	806	CLA	C12-C13-C15-C16
19	A1	807	CLA	C6-C7-C8-C10
19	A1	820	CLA	C11-C12-C13-C15
19	A1	827	CLA	C2-C3-C5-C6
19	A1	828	CLA	C11-C10-C8-C7
19	A1	834	CLA	C12-C13-C15-C16
19	A1	835	CLA	C12-C13-C15-C16
19	A1	852	CLA	C11-C10-C8-C7
19	B1	803	CLA	C6-C7-C8-C10
19	B1	806	CLA	C12-C13-C15-C16
19	B1	807	CLA	C6-C7-C8-C10
19	B1	810	CLA	C11-C10-C8-C7
19	B1	823	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B1	825	CLA	C11-C10-C8-C7
19	B1	826	CLA	C6-C7-C8-C10
19	B1	826	CLA	C12-C13-C15-C16
19	B1	835	CLA	C6-C7-C8-C10
19	B1	848	CLA	C11-C10-C8-C7
19	A2	808	CLA	C6-C7-C8-C10
19	A2	813	CLA	C6-C7-C8-C10
19	A2	821	CLA	C11-C12-C13-C15
19	A2	835	CLA	C12-C13-C15-C16
19	B2	801	CLA	C12-C13-C15-C16
19	B2	806	CLA	C12-C13-C15-C16
19	B2	815	CLA	C11-C10-C8-C7
19	B2	815	CLA	C12-C13-C15-C16
19	B2	823	CLA	C6-C7-C8-C10
19	B2	826	CLA	C12-C13-C15-C16
19	B2	836	CLA	C12-C13-C15-C16
19	B2	849	CLA	C11-C10-C8-C7
19	L2	205	CLA	C6-C7-C8-C10
19	A	804	CLA	C12-C13-C15-C16
19	A	808	CLA	C6-C7-C8-C10
19	A	828	CLA	C2-C3-C5-C6
19	B	801	CLA	C12-C13-C15-C16
19	B	803	CLA	C6-C7-C8-C10
19	B	815	CLA	C11-C10-C8-C7
19	B	823	CLA	C6-C7-C8-C10
19	B	825	CLA	C12-C13-C15-C16
19	B	833	CLA	C6-C7-C8-C10
19	B	854	CLA	C11-C10-C8-C7
19	AA	808	CLA	C6-C7-C8-C10
19	AA	835	CLA	C12-C13-C15-C16
19	AA	836	CLA	C12-C13-C15-C16
19	AA	853	CLA	C11-C12-C13-C15
19	BB	801	CLA	C12-C13-C15-C16
19	BB	803	CLA	C6-C7-C8-C10
19	BB	806	CLA	C12-C13-C15-C16
19	BB	810	CLA	C11-C10-C8-C7
19	BB	815	CLA	C12-C13-C15-C16
19	BB	823	CLA	C6-C7-C8-C10
19	BB	826	CLA	C12-C13-C15-C16
19	BB	835	CLA	C12-C13-C15-C16
19	BB	852	CLA	C11-C10-C8-C7
20	A	803	CL0	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	AA	803	CL0	C11-C10-C8-C7
21	BB	837	PQN	C21-C22-C23-C25
23	B1	843	BCR	C9-C10-C11-C12
23	K1	106	BCR	C19-C20-C21-C22
23	A	848	BCR	C9-C10-C11-C12
23	F	305	BCR	C19-C20-C21-C22
23	J	104	BCR	C9-C10-C11-C12
23	K	103	BCR	C19-C20-C21-C22
23	FF	306	BCR	C19-C20-C21-C22
23	JJ	104	BCR	C9-C10-C11-C12
23	KK	103	BCR	C19-C20-C21-C22
23	MM	101	BCR	C13-C14-C15-C16
26	B1	840	ECH	C9-C10-C11-C12
26	B2	841	ECH	C9-C10-C11-C12
22	B	852	LHG	O9-C7-O7-C5
19	L1	206	CLA	C8-C10-C11-C12
19	B	823	CLA	C10-C11-C12-C13
19	B1	804	CLA	O1A-CGA-O2A-C1
19	B2	804	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
25	BB	844	LMG	C35-C36-C37-C38
23	A1	847	BCR	C35-C13-C14-C15
23	B1	838	BCR	C11-C10-C9-C34
23	B1	838	BCR	C35-C13-C14-C15
23	B1	842	BCR	C16-C17-C18-C36
23	K1	104	BCR	C11-C10-C9-C34
23	L1	201	BCR	C11-C10-C9-C34
23	A2	848	BCR	C35-C13-C14-C15
23	B2	843	BCR	C35-C13-C14-C15
23	A	848	BCR	C20-C21-C22-C37
23	B	840	BCR	C20-C21-C22-C37
23	B	842	BCR	C20-C21-C22-C37
23	B	848	BCR	C20-C21-C22-C37
23	F	304	BCR	C11-C10-C9-C34
23	BB	838	BCR	C11-C10-C9-C34
23	FF	306	BCR	C20-C21-C22-C37
23	II	101	BCR	C35-C13-C14-C15
23	II	104	BCR	C35-C13-C14-C15
23	JJ	104	BCR	C20-C21-C22-C37
19	A	835	CLA	CBA-CGA-O2A-C1
19	AA	830	CLA	C4C-C3C-CAC-CBC
19	B2	813	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A1	826	CLA	C5-C6-C7-C8
19	B1	801	CLA	C8-C10-C11-C12
19	B	804	CLA	O1A-CGA-O2A-C1
19	BB	804	CLA	O1A-CGA-O2A-C1
19	B2	825	CLA	CBD-CGD-O2D-CED
19	A	830	CLA	C4C-C3C-CAC-CBC
25	B	845	LMG	C16-C17-C18-C19
19	A1	806	CLA	CAD-CBD-CGD-O2D
19	A1	816	CLA	CAD-CBD-CGD-O2D
19	A1	818	CLA	CAD-CBD-CGD-O2D
19	A1	824	CLA	CAD-CBD-CGD-O2D
19	A1	852	CLA	CAD-CBD-CGD-O2D
19	B1	809	CLA	CAD-CBD-CGD-O2D
19	B1	825	CLA	CAD-CBD-CGD-O2D
19	K1	102	CLA	CAD-CBD-CGD-O2D
19	A2	802	CLA	CAD-CBD-CGD-O2D
19	A2	807	CLA	CAD-CBD-CGD-O2D
19	A2	819	CLA	CAD-CBD-CGD-O2D
19	B2	809	CLA	CAD-CBD-CGD-O2D
19	B2	819	CLA	CAD-CBD-CGD-O2D
19	B2	825	CLA	CAD-CBD-CGD-O2D
19	B2	828	CLA	CAD-CBD-CGD-O2D
19	A	814	CLA	CAD-CBD-CGD-O2D
19	A	816	CLA	CAD-CBD-CGD-O2D
19	A	819	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O2D
19	A	827	CLA	CAD-CBD-CGD-O2D
19	B	809	CLA	CAD-CBD-CGD-O2D
19	B	828	CLA	CAD-CBD-CGD-O2D
19	B	833	CLA	CAD-CBD-CGD-O2D
19	AA	814	CLA	CAD-CBD-CGD-O2D
19	AA	819	CLA	CAD-CBD-CGD-O2D
19	AA	823	CLA	CAD-CBD-CGD-O2D
19	AA	824	CLA	CAD-CBD-CGD-O2D
19	BB	812	CLA	CAD-CBD-CGD-O2D
19	BB	817	CLA	CAD-CBD-CGD-O2D
19	BB	828	CLA	CAD-CBD-CGD-O2D
19	BB	832	CLA	CAD-CBD-CGD-O2D
22	L	207	LHG	C6-C5-O7-C7
22	LL	205	LHG	C6-C5-O7-C7
19	A2	830	CLA	C3-C5-C6-C7
19	B	815	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	BB	811	CLA	C8-C10-C11-C12
19	B	808	CLA	O1D-CGD-O2D-CED
19	BB	833	CLA	O1D-CGD-O2D-CED
23	L1	209	BCR	C6-C7-C8-C9
23	F	303	BCR	C6-C7-C8-C9
23	BB	838	BCR	C6-C7-C8-C9
23	BB	841	BCR	C22-C23-C24-C25
23	MM	101	BCR	C22-C23-C24-C25
19	B1	825	CLA	CBA-CGA-O2A-C1
19	B1	848	CLA	C4-C3-C5-C6
19	L1	205	CLA	C4-C3-C5-C6
20	A	803	CL0	C5-C6-C7-C8
22	X1	103	LHG	C2-C3-O3-P
22	X2	102	LHG	C4-C5-C6-O8
22	L	207	LHG	C4-C5-C6-O8
22	X	102	LHG	C4-C5-C6-O8
22	LL	205	LHG	C4-C5-C6-O8
22	XX	102	LHG	C4-C5-C6-O8
25	B2	845	LMG	O1-C7-C8-C9
25	B	845	LMG	O1-C7-C8-C9
25	II	105	LMG	O1-C7-C8-C9
19	BB	835	CLA	CBD-CGD-O2D-CED
22	L1	211	LHG	O6-C4-C5-O7
19	A2	827	CLA	C5-C6-C7-C8
19	A2	852	CLA	C5-C6-C7-C8
19	A1	829	CLA	C3-C5-C6-C7
19	L	204	CLA	C2C-C3C-CAC-CBC
22	X2	102	LHG	C27-C28-C29-C30
19	A1	818	CLA	C2A-CAA-CBA-CGA
19	A2	842	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C2A-CAA-CBA-CGA
19	AA	826	CLA	C2A-CAA-CBA-CGA
19	KK	102	CLA	C2A-CAA-CBA-CGA
23	F2	305	BCR	C14-C15-C16-C17
23	A	847	BCR	C14-C15-C16-C17
23	AA	848	BCR	C14-C15-C16-C17
19	A2	816	CLA	O1A-CGA-O2A-C1
19	B	801	CLA	C16-C17-C18-C19
19	A1	815	CLA	CHA-CBD-CGD-O1D
19	A1	815	CLA	CHA-CBD-CGD-O2D
19	A1	822	CLA	CHA-CBD-CGD-O1D
19	A1	830	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A1	830	CLA	CHA-CBD-CGD-O2D
19	A1	832	CLA	CHA-CBD-CGD-O1D
19	A1	832	CLA	CHA-CBD-CGD-O2D
19	A1	835	CLA	CHA-CBD-CGD-O1D
19	A1	835	CLA	CHA-CBD-CGD-O2D
19	A1	837	CLA	CHA-CBD-CGD-O1D
19	A1	837	CLA	CHA-CBD-CGD-O2D
19	A1	838	CLA	CHA-CBD-CGD-O1D
19	A1	838	CLA	CHA-CBD-CGD-O2D
19	B1	805	CLA	CHA-CBD-CGD-O1D
19	B1	805	CLA	CHA-CBD-CGD-O2D
19	B1	817	CLA	CHA-CBD-CGD-O1D
19	B1	817	CLA	CHA-CBD-CGD-O2D
19	B1	820	CLA	CHA-CBD-CGD-O1D
19	B1	820	CLA	CHA-CBD-CGD-O2D
19	B1	826	CLA	CHA-CBD-CGD-O1D
19	B1	826	CLA	CHA-CBD-CGD-O2D
19	B1	833	CLA	CHA-CBD-CGD-O1D
19	B1	833	CLA	CHA-CBD-CGD-O2D
19	B1	836	CLA	CHA-CBD-CGD-O1D
19	B1	836	CLA	CHA-CBD-CGD-O2D
19	B1	848	CLA	CHA-CBD-CGD-O2D
19	F1	301	CLA	CHA-CBD-CGD-O1D
19	F1	301	CLA	CHA-CBD-CGD-O2D
19	K1	103	CLA	CHA-CBD-CGD-O1D
19	K1	103	CLA	CHA-CBD-CGD-O2D
19	A2	838	CLA	CHA-CBD-CGD-O1D
19	A2	838	CLA	CHA-CBD-CGD-O2D
19	A2	839	CLA	CHA-CBD-CGD-O1D
19	A2	839	CLA	CHA-CBD-CGD-O2D
19	A2	852	CLA	CHA-CBD-CGD-O1D
19	A2	852	CLA	CHA-CBD-CGD-O2D
19	B2	803	CLA	CHA-CBD-CGD-O2D
19	B2	805	CLA	CHA-CBD-CGD-O1D
19	B2	805	CLA	CHA-CBD-CGD-O2D
19	B2	813	CLA	CHA-CBD-CGD-O1D
19	B2	813	CLA	CHA-CBD-CGD-O2D
19	B2	815	CLA	CHA-CBD-CGD-O1D
19	B2	815	CLA	CHA-CBD-CGD-O2D
19	B2	817	CLA	CHA-CBD-CGD-O1D
19	B2	817	CLA	CHA-CBD-CGD-O2D
19	B2	820	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B2	820	CLA	CHA-CBD-CGD-O2D
19	B2	821	CLA	CHA-CBD-CGD-O1D
19	B2	821	CLA	CHA-CBD-CGD-O2D
19	B2	826	CLA	CHA-CBD-CGD-O1D
19	B2	826	CLA	CHA-CBD-CGD-O2D
19	B2	833	CLA	CHA-CBD-CGD-O1D
19	B2	834	CLA	CHA-CBD-CGD-O1D
19	B2	834	CLA	CHA-CBD-CGD-O2D
19	B2	837	CLA	CHA-CBD-CGD-O1D
19	B2	837	CLA	CHA-CBD-CGD-O2D
19	B2	851	CLA	CHA-CBD-CGD-O1D
19	L2	204	CLA	CHA-CBD-CGD-O1D
19	L2	204	CLA	CHA-CBD-CGD-O2D
19	A	805	CLA	CHA-CBD-CGD-O1D
19	A	826	CLA	CHA-CBD-CGD-O1D
19	A	826	CLA	CHA-CBD-CGD-O2D
19	A	836	CLA	CHA-CBD-CGD-O1D
19	A	836	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	A	852	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O2D
19	B	803	CLA	CHA-CBD-CGD-O2D
19	B	813	CLA	CHA-CBD-CGD-O1D
19	B	817	CLA	CHA-CBD-CGD-O1D
19	B	817	CLA	CHA-CBD-CGD-O2D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O2D
19	B	826	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	CHA-CBD-CGD-O2D
19	F	301	CLA	CHA-CBD-CGD-O1D
19	AA	816	CLA	CHA-CBD-CGD-O1D
19	AA	822	CLA	CHA-CBD-CGD-O1D
19	AA	832	CLA	CHA-CBD-CGD-O1D
19	AA	832	CLA	CHA-CBD-CGD-O2D
19	AA	836	CLA	CHA-CBD-CGD-O1D
19	AA	836	CLA	CHA-CBD-CGD-O2D
19	AA	838	CLA	CHA-CBD-CGD-O1D
19	AA	838	CLA	CHA-CBD-CGD-O2D
19	AA	839	CLA	CHA-CBD-CGD-O1D
19	BB	805	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	BB	821	CLA	CHA-CBD-CGD-O1D
19	BB	826	CLA	CHA-CBD-CGD-O1D
19	BB	836	CLA	CHA-CBD-CGD-O1D
19	BB	836	CLA	CHA-CBD-CGD-O2D
19	BB	852	CLA	CHA-CBD-CGD-O1D
19	BB	852	CLA	CHA-CBD-CGD-O2D
19	LL	201	CLA	CHA-CBD-CGD-O1D
19	LL	201	CLA	CHA-CBD-CGD-O2D
19	LL	203	CLA	CHA-CBD-CGD-O1D
20	A1	802	CL0	CHA-CBD-CGD-O2D
20	A2	803	CL0	CHA-CBD-CGD-O2D
22	A1	845	LHG	C15-C16-C17-C18
19	A	808	CLA	C3-C5-C6-C7
19	A1	805	CLA	O1A-CGA-O2A-C1
19	A2	833	CLA	O1A-CGA-O2A-C1
19	B2	849	CLA	O1A-CGA-O2A-C1
19	BB	814	CLA	O1A-CGA-O2A-C1
23	B1	839	BCR	C20-C21-C22-C23
23	I1	101	BCR	C20-C21-C22-C23
23	L1	208	BCR	C16-C17-C18-C19
23	M1	101	BCR	C16-C17-C18-C19
23	F2	303	BCR	C20-C21-C22-C23
23	I2	101	BCR	C20-C21-C22-C23
23	I2	103	BCR	C16-C17-C18-C19
23	A	848	BCR	C16-C17-C18-C19
23	BB	839	BCR	C12-C13-C14-C15
23	BB	839	BCR	C16-C17-C18-C19
23	BB	841	BCR	C12-C13-C14-C15
22	A1	845	LHG	O7-C5-C6-O8
22	B1	847	LHG	O7-C5-C6-O8
22	X1	102	LHG	O7-C5-C6-O8
22	B2	848	LHG	O7-C5-C6-O8
22	X2	102	LHG	O7-C5-C6-O8
22	X	102	LHG	O7-C5-C6-O8
22	XX	102	LHG	O7-C5-C6-O8
25	B2	845	LMG	O1-C7-C8-O7
25	B	845	LMG	O1-C7-C8-O7
22	X2	103	LHG	C10-C11-C12-C13
19	B1	826	CLA	C15-C16-C17-C18
19	B	859	CLA	C8-C10-C11-C12
19	A1	815	CLA	O1A-CGA-O2A-C1
19	B1	825	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	AA	816	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	C32-C33-C34-C35
19	AA	843	CLA	C16-C17-C18-C19
19	BB	801	CLA	C16-C17-C18-C20
19	B1	835	CLA	C3-C5-C6-C7
19	B2	834	CLA	C15-C16-C17-C18
19	A2	828	CLA	C4-C3-C5-C6
22	X1	102	LHG	C27-C28-C29-C30
19	BB	852	CLA	O1A-CGA-O2A-C1
19	A2	828	CLA	C2-C3-C5-C6
25	II	105	LMG	C13-C14-C15-C16
19	A2	842	CLA	C5-C6-C7-C8
19	L	202	CLA	C10-C11-C12-C13
19	BB	810	CLA	C5-C6-C7-C8
19	B1	803	CLA	C6-C7-C8-C9
19	B1	806	CLA	C14-C13-C15-C16
19	A2	835	CLA	C14-C13-C15-C16
19	B2	803	CLA	C6-C7-C8-C9
19	B2	806	CLA	C14-C13-C15-C16
19	B2	825	CLA	C11-C10-C8-C9
19	B2	826	CLA	C14-C13-C15-C16
19	A	808	CLA	C6-C7-C8-C9
19	B	803	CLA	C6-C7-C8-C9
19	AA	807	CLA	C14-C13-C15-C16
19	AA	835	CLA	C14-C13-C15-C16
19	BB	835	CLA	C14-C13-C15-C16
20	A2	803	CL0	C11-C12-C13-C14
21	BB	837	PQN	C21-C22-C23-C24
19	B2	823	CLA	C15-C16-C17-C18
19	AA	806	CLA	C2A-CAA-CBA-CGA
23	B1	843	BCR	C7-C8-C9-C34
23	B2	844	BCR	C7-C8-C9-C34
23	F2	303	BCR	C37-C22-C23-C24
23	F2	304	BCR	C36-C18-C19-C20
23	F	303	BCR	C11-C12-C13-C35
23	I	102	BCR	C37-C22-C23-C24
26	B1	840	ECH	C36-C18-C19-C20
26	B	841	ECH	C36-C18-C19-C20
26	BB	840	ECH	C36-C18-C19-C20
22	A	845	LHG	C15-C16-C17-C18
25	B2	845	LMG	C39-C40-C41-C42
23	B1	838	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	B1	841	BCR	C17-C18-C19-C20
23	I1	101	BCR	C17-C18-C19-C20
23	B2	839	BCR	C11-C12-C13-C14
23	A	850	BCR	C21-C22-C23-C24
23	AA	850	BCR	C21-C22-C23-C24
23	II	101	BCR	C11-C12-C13-C14
23	JJ	104	BCR	C11-C12-C13-C14
26	B1	840	ECH	C17-C18-C19-C20
26	B	841	ECH	C17-C18-C19-C20
26	BB	840	ECH	C17-C18-C19-C20
22	X	102	LHG	C29-C30-C31-C32
19	B1	802	CLA	C1A-C2A-CAA-CBA
19	F1	305	CLA	C1A-C2A-CAA-CBA
19	B2	801	CLA	C1A-C2A-CAA-CBA
19	B2	829	CLA	C1A-C2A-CAA-CBA
19	B2	833	CLA	C1A-C2A-CAA-CBA
19	L2	205	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C1A-C2A-CAA-CBA
19	AA	823	CLA	C1A-C2A-CAA-CBA
19	BB	821	CLA	C1A-C2A-CAA-CBA
19	BB	834	CLA	C1A-C2A-CAA-CBA
19	FF	305	CLA	C1A-C2A-CAA-CBA
19	B1	815	CLA	C13-C15-C16-C17
19	B	801	CLA	C15-C16-C17-C18
23	I2	103	BCR	C15-C16-C17-C18
23	J2	102	BCR	C15-C16-C17-C18
23	K	103	BCR	C9-C10-C11-C12
23	BB	843	BCR	C9-C10-C11-C12
23	JJ	102	BCR	C15-C16-C17-C18
26	B	841	ECH	C9-C10-C11-C12
19	B2	815	CLA	C13-C15-C16-C17
19	BB	801	CLA	C13-C15-C16-C17
21	B	838	PQN	C18-C20-C21-C22
25	L1	210	LMG	C42-C43-C44-C45
19	A1	832	CLA	O1D-CGD-O2D-CED
19	B	814	CLA	C10-C11-C12-C13
22	AA	846	LHG	C32-C33-C34-C35
19	L2	204	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	821	CLA	C4-C3-C5-C6
22	L2	208	LHG	C2-C3-O3-P
22	BB	851	LHG	C2-C3-O3-P
19	A	812	CLA	O1A-CGA-O2A-C1
22	L1	211	LHG	C3-O3-P-O5
22	L2	208	LHG	C4-O6-P-O5
22	X2	102	LHG	C4-O6-P-O5
22	X	102	LHG	C4-O6-P-O4
22	X	102	LHG	C4-O6-P-O5
19	A1	842	CLA	C16-C17-C18-C19
19	L	204	CLA	C16-C17-C18-C20
19	BB	808	CLA	C11-C12-C13-C15
19	B	858	CLA	C5-C6-C7-C8
19	L2	206	CLA	CBA-CGA-O2A-C1
22	B	852	LHG	O6-C4-C5-C6
22	B	853	LHG	C10-C11-C12-C13
25	B	851	LMG	C34-C35-C36-C37
19	BB	826	CLA	O1D-CGD-O2D-CED
25	B	851	LMG	C42-C43-C44-C45
19	A1	841	CLA	C2A-CAA-CBA-CGA
19	A2	819	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	C2A-CAA-CBA-CGA
19	BB	825	CLA	C3-C5-C6-C7
20	A2	803	CL0	C3-C5-C6-C7
19	A	835	CLA	O1A-CGA-O2A-C1
19	A1	806	CLA	C16-C17-C18-C19
19	B1	808	CLA	C11-C12-C13-C15
19	B2	808	CLA	C11-C12-C13-C15
19	B	808	CLA	C11-C12-C13-C15
22	AA	846	LHG	C16-C17-C18-C19
19	A1	815	CLA	CAD-CBD-CGD-O1D
19	A1	823	CLA	CAD-CBD-CGD-O1D
19	A1	844	CLA	CAD-CBD-CGD-O1D
19	B1	802	CLA	CAD-CBD-CGD-O1D
19	B1	810	CLA	CAD-CBD-CGD-O1D
19	B1	811	CLA	CAD-CBD-CGD-O1D
19	B1	830	CLA	CAD-CBD-CGD-O1D
19	K1	103	CLA	CAD-CBD-CGD-O1D
19	A2	824	CLA	CAD-CBD-CGD-O1D
19	A2	844	CLA	CAD-CBD-CGD-O1D
19	A2	852	CLA	CAD-CBD-CGD-O1D
19	B2	810	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	L2	204	CLA	CAD-CBD-CGD-O1D
19	A	807	CLA	CAD-CBD-CGD-O1D
19	B	802	CLA	CAD-CBD-CGD-O1D
19	B	810	CLA	CAD-CBD-CGD-O1D
19	B	831	CLA	CAD-CBD-CGD-O1D
19	AA	806	CLA	CAD-CBD-CGD-O1D
19	AA	816	CLA	CAD-CBD-CGD-O1D
19	AA	845	CLA	CAD-CBD-CGD-O1D
19	BB	810	CLA	CAD-CBD-CGD-O1D
19	BB	830	CLA	CAD-CBD-CGD-O1D
19	KK	102	CLA	CAD-CBD-CGD-O1D
19	LL	201	CLA	CAD-CBD-CGD-O1D
19	A1	841	CLA	C5-C6-C7-C8
19	A2	820	CLA	C8-C10-C11-C12
22	XX	102	LHG	C29-C30-C31-C32
19	L2	206	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	C16-C17-C18-C19
19	B2	823	CLA	C16-C17-C18-C20
19	B	824	CLA	C4-C3-C5-C6
19	A1	805	CLA	C6-C7-C8-C10
19	A1	812	CLA	C11-C12-C13-C15
19	A1	852	CLA	C11-C12-C13-C15
19	B1	825	CLA	C6-C7-C8-C10
19	B1	832	CLA	C11-C12-C13-C15
19	B1	835	CLA	C12-C13-C15-C16
19	B1	836	CLA	C6-C7-C8-C10
19	A2	806	CLA	C6-C7-C8-C10
19	A2	819	CLA	C11-C10-C8-C7
19	A2	829	CLA	C11-C10-C8-C7
19	A2	836	CLA	C12-C13-C15-C16
19	A2	852	CLA	C11-C10-C8-C7
19	B2	803	CLA	C6-C7-C8-C10
19	B2	804	CLA	C3A-C2A-CAA-CBA
19	B2	807	CLA	C6-C7-C8-C10
19	B2	825	CLA	C6-C7-C8-C10
19	B2	825	CLA	C12-C13-C15-C16
19	B2	833	CLA	C11-C12-C13-C15
19	B2	834	CLA	C11-C10-C8-C7
19	B2	837	CLA	C6-C7-C8-C10
19	A	829	CLA	C11-C10-C8-C7
19	A	836	CLA	C12-C13-C15-C16
19	A	852	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	806	CLA	C12-C13-C15-C16
19	B	810	CLA	C11-C10-C8-C7
19	B	811	CLA	C11-C10-C8-C7
19	B	815	CLA	C6-C7-C8-C10
19	B	825	CLA	C6-C7-C8-C10
19	B	826	CLA	C12-C13-C15-C16
19	B	833	CLA	C11-C12-C13-C15
19	B	836	CLA	C12-C13-C15-C16
19	AA	806	CLA	C6-C7-C8-C10
19	AA	807	CLA	C12-C13-C15-C16
19	AA	853	CLA	C11-C10-C8-C7
19	BB	811	CLA	C11-C10-C8-C7
19	BB	814	CLA	C2-C3-C5-C6
19	BB	815	CLA	C6-C7-C8-C10
19	BB	825	CLA	C6-C7-C8-C10
19	BB	832	CLA	C11-C12-C13-C15
19	BB	836	CLA	C6-C7-C8-C10
20	A2	803	CL0	C11-C12-C13-C15
21	B1	837	PQN	C21-C22-C23-C25
22	BB	851	LHG	C10-C11-C12-C13
23	A2	853	BCR	C9-C10-C11-C12
19	B	834	CLA	C15-C16-C17-C18
25	II	105	LMG	C37-C38-C39-C40
19	A1	829	CLA	C13-C15-C16-C17
19	A	835	CLA	C15-C16-C17-C18
19	A1	839	CLA	CBD-CGD-O2D-CED
19	A	806	CLA	C2A-CAA-CBA-CGA
19	AA	843	CLA	C16-C17-C18-C20
20	A1	802	CL0	C16-C17-C18-C19
22	L1	211	LHG	C24-C25-C26-C27
22	X2	103	LHG	C23-C24-C25-C26
25	B1	844	LMG	O1-C7-C8-C9
25	BB	844	LMG	O1-C7-C8-C9
22	XX	102	LHG	O9-C7-O7-C5
22	L1	211	LHG	O7-C5-C6-O8
22	L2	208	LHG	O7-C5-C6-O8
25	B1	846	LMG	O1-C7-C8-O7
25	B2	847	LMG	O1-C7-C8-O7
25	BB	844	LMG	O1-C7-C8-O7
28	BB	854	DGD	O2G-C2G-C3G-O3G
19	A2	836	CLA	C5-C6-C7-C8
19	B	830	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	B1	814	CLA	O1A-CGA-O2A-C1
19	AA	840	CLA	C5-C6-C7-C8
19	BB	829	CLA	C3-C5-C6-C7
19	B1	814	CLA	C10-C11-C12-C13
22	L1	211	LHG	C2-C3-O3-P
19	A1	842	CLA	C15-C16-C17-C18
19	B	810	CLA	C5-C6-C7-C8
19	BB	824	CLA	C4-C3-C5-C6
19	B1	814	CLA	CBA-CGA-O2A-C1
19	L1	207	CLA	CBA-CGA-O2A-C1
19	L1	205	CLA	C2-C3-C5-C6
19	AA	807	CLA	C10-C11-C12-C13
19	A1	807	CLA	C6-C7-C8-C9
19	A1	828	CLA	C11-C12-C13-C14
19	A1	834	CLA	C14-C13-C15-C16
19	B1	826	CLA	C14-C13-C15-C16
19	A2	808	CLA	C6-C7-C8-C9
19	A2	810	CLA	C14-C13-C15-C16
19	A	813	CLA	C6-C7-C8-C9
19	B	816	CLA	C6-C7-C8-C9
19	B	825	CLA	C11-C10-C8-C9
19	AA	808	CLA	C6-C7-C8-C9
19	AA	827	CLA	C14-C13-C15-C16
19	BB	806	CLA	C14-C13-C15-C16
19	BB	810	CLA	C11-C10-C8-C9
19	BB	825	CLA	C11-C10-C8-C9
19	BB	826	CLA	C14-C13-C15-C16
21	A1	843	PQN	C16-C17-C18-C19
21	B1	837	PQN	C21-C22-C23-C24
21	B2	838	PQN	C21-C22-C23-C24
21	B	838	PQN	C21-C22-C23-C24
22	AA	846	LHG	C7-C8-C9-C10
19	L1	207	CLA	O1A-CGA-O2A-C1
19	BB	825	CLA	O1A-CGA-O2A-C1
25	B1	844	LMG	C19-C20-C21-C22
25	BB	844	LMG	C19-C20-C21-C22
19	B1	823	CLA	C10-C11-C12-C13
22	BB	851	LHG	C25-C26-C27-C28
19	AA	819	CLA	CBD-CGD-O2D-CED
19	B2	825	CLA	O1A-CGA-O2A-C1
23	M	101	BCR	C13-C14-C15-C16
23	B2	840	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
23	A	851	BCR	C36-C18-C19-C20
23	F	303	BCR	C36-C18-C19-C20
23	FF	303	BCR	C36-C18-C19-C20
19	A	832	CLA	C3-C5-C6-C7
19	B2	801	CLA	C15-C16-C17-C18
20	AA	803	CL0	C8-C10-C11-C12
22	A2	845	LHG	C7-C8-C9-C10
19	B	860	CLA	C16-C17-C18-C19
25	B1	844	LMG	C33-C34-C35-C36
23	J1	104	BCR	C17-C18-C19-C20
23	AA	855	BCR	C21-C22-C23-C24
23	BB	839	BCR	C21-C22-C23-C24
23	BB	842	BCR	C17-C18-C19-C20
26	B	841	ECH	C11-C12-C13-C14
19	A2	827	CLA	C10-C11-C12-C13
23	A2	847	BCR	C35-C13-C14-C15
23	JJ	102	BCR	C20-C21-C22-C37
19	LL	202	CLA	C3-C5-C6-C7
19	A2	830	CLA	C13-C15-C16-C17
19	L2	204	CLA	C2-C3-C5-C6
19	B	824	CLA	C2-C3-C5-C6
19	BB	856	CLA	C8-C10-C11-C12
19	BB	801	CLA	C16-C17-C18-C19
25	M	102	LMG	C30-C31-C32-C33
19	AA	835	CLA	CBA-CGA-O2A-C1
19	B1	825	CLA	CBD-CGD-O2D-CED
19	AA	853	CLA	C5-C6-C7-C8
22	A2	845	LHG	C26-C27-C28-C29
19	B	825	CLA	C3-C5-C6-C7
22	BB	850	LHG	O6-C4-C5-C6
19	L	204	CLA	C2A-CAA-CBA-CGA
19	AA	842	CLA	C2A-CAA-CBA-CGA
19	B2	814	CLA	C11-C12-C13-C14
22	X1	102	LHG	O9-C7-O7-C5
19	A1	834	CLA	CBA-CGA-O2A-C1
19	A2	835	CLA	CBA-CGA-O2A-C1
19	BB	824	CLA	C2-C1-O2A-CGA
22	AA	846	LHG	C15-C16-C17-C18
19	A1	806	CLA	C16-C17-C18-C20
19	A1	842	CLA	C16-C17-C18-C20
23	A2	847	BCR	C14-C15-C16-C17
25	B	845	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	BB	821	CLA	O1D-CGD-O2D-CED
22	A1	845	LHG	C9-C10-C11-C12
22	X1	103	LHG	C25-C26-C27-C28
22	A1	845	LHG	C29-C30-C31-C32
23	J1	102	BCR	C15-C16-C17-C18
19	A2	835	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	O1A-CGA-O2A-C1
19	B1	814	CLA	C11-C12-C13-C14
25	B2	845	LMG	C19-C20-C21-C22
23	A1	851	BCR	C1-C6-C7-C8
23	B1	842	BCR	C23-C24-C25-C26
23	F1	303	BCR	C5-C6-C7-C8
23	F1	306	BCR	C23-C24-C25-C30
23	J1	102	BCR	C1-C6-C7-C8
23	L1	208	BCR	C5-C6-C7-C8
23	A2	850	BCR	C1-C6-C7-C8
23	A2	851	BCR	C1-C6-C7-C8
23	I2	103	BCR	C5-C6-C7-C8
23	J2	102	BCR	C1-C6-C7-C8
23	J2	102	BCR	C5-C6-C7-C8
23	K2	105	BCR	C23-C24-C25-C26
23	A	848	BCR	C1-C6-C7-C8
23	A	850	BCR	C1-C6-C7-C8
23	A	851	BCR	C1-C6-C7-C8
23	L	205	BCR	C1-C6-C7-C8
23	M	101	BCR	C5-C6-C7-C8
23	AA	849	BCR	C1-C6-C7-C8
23	AA	851	BCR	C1-C6-C7-C8
23	AA	852	BCR	C1-C6-C7-C8
23	II	104	BCR	C1-C6-C7-C8
19	B2	821	CLA	C2-C3-C5-C6
19	A1	834	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	O1A-CGA-O2A-C1
20	AA	803	CL0	C4C-C3C-CAC-CBC
19	AA	819	CLA	O1D-CGD-O2D-CED
19	BB	835	CLA	O1D-CGD-O2D-CED
19	AA	853	CLA	C8-C10-C11-C12
19	B1	801	CLA	C16-C17-C18-C20
22	X1	102	LHG	C8-C7-O7-C5
22	XX	102	LHG	C8-C7-O7-C5
19	B	805	CLA	C16-C17-C18-C19
19	LL	201	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	A	831	CLA	C2A-CAA-CBA-CGA
23	B2	843	BCR	C20-C21-C22-C23
23	J2	102	BCR	C11-C10-C9-C8
23	B	840	BCR	C12-C13-C14-C15
23	B	842	BCR	C11-C10-C9-C8
23	B	844	BCR	C16-C17-C18-C19
23	I	102	BCR	C20-C21-C22-C23
23	K	103	BCR	C11-C10-C9-C8
23	BB	841	BCR	C11-C10-C9-C8
23	FF	303	BCR	C20-C21-C22-C23
25	B1	844	LMG	O1-C7-C8-O7
25	II	105	LMG	O1-C7-C8-O7
22	A1	845	LHG	C4-O6-P-O3
22	A1	846	LHG	C3-O3-P-O6
22	B1	847	LHG	C3-O3-P-O6
22	X1	102	LHG	C3-O3-P-O6
22	A2	845	LHG	C4-O6-P-O3
22	A2	846	LHG	C3-O3-P-O6
22	X2	102	LHG	C3-O3-P-O6
22	A	845	LHG	C4-O6-P-O3
22	A	846	LHG	C3-O3-P-O6
22	B	852	LHG	C4-O6-P-O3
22	L	207	LHG	C3-O3-P-O6
22	X	102	LHG	C3-O3-P-O6
22	AA	846	LHG	C4-O6-P-O3
22	AA	847	LHG	C3-O3-P-O6
22	BB	850	LHG	C4-O6-P-O3
22	LL	205	LHG	C3-O3-P-O6
22	XX	102	LHG	C3-O3-P-O6
19	B1	823	CLA	C16-C17-C18-C20
19	B2	826	CLA	C15-C16-C17-C18
19	B1	824	CLA	C4-C3-C5-C6
19	B2	824	CLA	C4-C3-C5-C6
19	AA	836	CLA	C4-C3-C5-C6
22	X1	103	LHG	C34-C35-C36-C37
22	AA	846	LHG	C18-C19-C20-C21
19	B1	810	CLA	C6-C7-C8-C10
19	B2	805	CLA	C11-C12-C13-C15
19	B	805	CLA	C11-C12-C13-C15
19	L	204	CLA	C6-C7-C8-C10
19	AA	819	CLA	C6-C7-C8-C10
19	AA	827	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	BB	805	CLA	C11-C12-C13-C15
22	B2	848	LHG	C12-C13-C14-C15
19	AA	835	CLA	O1A-CGA-O2A-C1
19	A1	805	CLA	C6-C7-C8-C9
19	A1	829	CLA	C11-C10-C8-C9
19	A1	835	CLA	C14-C13-C15-C16
19	B1	805	CLA	C6-C7-C8-C9
19	B1	811	CLA	C11-C10-C8-C9
19	B1	835	CLA	C14-C13-C15-C16
19	A2	806	CLA	C6-C7-C8-C9
19	A2	830	CLA	C11-C10-C8-C9
19	B2	805	CLA	C6-C7-C8-C9
19	B2	811	CLA	C11-C10-C8-C9
19	A	830	CLA	C11-C10-C8-C9
19	B	805	CLA	C6-C7-C8-C9
19	B	810	CLA	C11-C10-C8-C9
19	B	811	CLA	C11-C10-C8-C9
19	B	826	CLA	C14-C13-C15-C16
19	AA	830	CLA	C11-C10-C8-C9
19	BB	805	CLA	C6-C7-C8-C9
19	BB	811	CLA	C11-C10-C8-C9
20	A	803	CL0	C14-C13-C15-C16
19	LL	202	CLA	C8-C10-C11-C12
23	A1	848	BCR	C9-C10-C11-C12
23	A1	853	BCR	C9-C10-C11-C12
23	B1	838	BCR	C9-C10-C11-C12
23	B1	838	BCR	C13-C14-C15-C16
23	J1	104	BCR	C15-C16-C17-C18
23	B2	839	BCR	C9-C10-C11-C12
23	B2	839	BCR	C13-C14-C15-C16
23	B2	842	BCR	C15-C16-C17-C18
23	B2	844	BCR	C9-C10-C11-C12
23	F2	305	BCR	C19-C20-C21-C22
23	AA	849	BCR	C9-C10-C11-C12
19	B2	801	CLA	C16-C17-C18-C20
19	B2	825	CLA	CBA-CGA-O2A-C1
19	BB	825	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	C5-C6-C7-C8
19	B	801	CLA	C13-C15-C16-C17
19	A1	829	CLA	C4C-C3C-CAC-CBC
25	II	105	LMG	C32-C33-C34-C35
23	F2	303	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
19	L	204	CLA	C10-C11-C12-C13
19	B2	823	CLA	C16-C17-C18-C19
19	B	808	CLA	C11-C12-C13-C14
19	BB	808	CLA	C11-C12-C13-C14
20	A1	802	CL0	C16-C17-C18-C20
25	M	102	LMG	C37-C38-C39-C40
19	A	809	CLA	CBA-CGA-O2A-C1
22	L	207	LHG	C5-C4-O6-P
22	LL	205	LHG	C5-C4-O6-P
23	A	849	BCR	C21-C22-C23-C24
23	A	851	BCR	C7-C8-C9-C10
23	J	104	BCR	C11-C12-C13-C14
23	AA	850	BCR	C7-C8-C9-C10
22	B	853	LHG	C18-C19-C20-C21
19	A1	820	CLA	C16-C17-C18-C20
19	B	860	CLA	C16-C17-C18-C20
19	B	825	CLA	CBA-CGA-O2A-C1
22	A1	845	LHG	C24-C23-O8-C6
22	A1	845	LHG	O10-C23-O8-C6
19	BB	821	CLA	CBD-CGD-O2D-CED
19	LL	201	CLA	C5-C6-C7-C8
23	B1	838	BCR	C6-C7-C8-C9
23	BB	847	BCR	C22-C23-C24-C25
23	F1	304	BCR	C19-C20-C21-C22
23	L1	208	BCR	C15-C16-C17-C18
23	A2	848	BCR	C9-C10-C11-C12
23	B2	843	BCR	C19-C20-C21-C22
23	J2	104	BCR	C15-C16-C17-C18
23	B	839	BCR	C9-C10-C11-C12
23	F	304	BCR	C19-C20-C21-C22
23	I	101	BCR	C13-C14-C15-C16
23	J	104	BCR	C15-C16-C17-C18
23	BB	838	BCR	C9-C10-C11-C12
23	BB	842	BCR	C9-C10-C11-C12
22	XX	102	LHG	C25-C26-C27-C28
19	B2	801	CLA	C8-C10-C11-C12
22	L2	208	LHG	C10-C11-C12-C13
22	X	102	LHG	C25-C26-C27-C28
22	BB	851	LHG	C18-C19-C20-C21
23	F1	303	BCR	C18-C19-C20-C21
23	I2	101	BCR	C18-C19-C20-C21
23	I	101	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	I	102	BCR	C18-C19-C20-C21
19	A1	801	CLA	C16-C17-C18-C19
19	A2	801	CLA	C16-C17-C18-C19
19	A2	804	CLA	C16-C17-C18-C19
19	AA	842	CLA	C16-C17-C18-C20
19	BB	805	CLA	C16-C17-C18-C19
25	II	105	LMG	C31-C32-C33-C34
23	J	102	BCR	C14-C15-C16-C17
19	A	842	CLA	C5-C6-C7-C8
20	A	803	CL0	O1D-CGD-O2D-CED
19	B	859	CLA	C10-C11-C12-C13
22	X2	103	LHG	O2-C2-C3-O3
19	A2	818	CLA	CAA-CBA-CGA-O1A
19	B1	801	CLA	C2-C1-O2A-CGA
19	B1	824	CLA	C2-C1-O2A-CGA
19	B2	808	CLA	C2-C1-O2A-CGA
19	B2	805	CLA	C16-C17-C18-C19
19	B	829	CLA	C2C-C3C-CAC-CBC
19	B1	808	CLA	C11-C12-C13-C14
19	B2	808	CLA	C11-C12-C13-C14
19	L	204	CLA	C16-C17-C18-C19
19	B2	815	CLA	C5-C6-C7-C8
19	B	802	CLA	C15-C16-C17-C18
19	A1	819	CLA	C2A-CAA-CBA-CGA
19	B	824	CLA	C2A-CAA-CBA-CGA
19	AA	819	CLA	C2A-CAA-CBA-CGA
19	AA	824	CLA	C2A-CAA-CBA-CGA
19	J	103	CLA	C2C-C3C-CAC-CBC
22	A2	846	LHG	C11-C12-C13-C14
22	X2	103	LHG	C28-C29-C30-C31
22	A1	846	LHG	C11-C12-C13-C14
19	B1	810	CLA	C3A-C2A-CAA-CBA
19	B2	801	CLA	C3A-C2A-CAA-CBA
19	B2	807	CLA	C3A-C2A-CAA-CBA
19	L2	204	CLA	C3A-C2A-CAA-CBA
19	A	810	CLA	C3A-C2A-CAA-CBA
19	AA	836	CLA	C3A-C2A-CAA-CBA
19	BB	801	CLA	C3A-C2A-CAA-CBA
19	BB	802	CLA	C3A-C2A-CAA-CBA
19	A1	839	CLA	O1D-CGD-O2D-CED
19	AA	827	CLA	C10-C11-C12-C13
19	A	807	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	A	842	CLA	C16-C17-C18-C20
28	BB	854	DGD	O6D-C5D-C6D-O5D
22	X2	103	LHG	C25-C26-C27-C28
25	I1	102	LMG	C19-C20-C21-C22
23	B2	842	BCR	C13-C14-C15-C16
23	A	847	BCR	C13-C14-C15-C16
23	B	843	BCR	C9-C10-C11-C12
19	A1	819	CLA	C8-C10-C11-C12
22	A	845	LHG	C18-C19-C20-C21
19	AA	826	CLA	CAA-CBA-CGA-O1A
19	A	836	CLA	C4-C3-C5-C6
19	B	814	CLA	C4-C3-C5-C6
19	BB	825	CLA	O1D-CGD-O2D-CED
19	A1	818	CLA	CBD-CGD-O2D-CED
19	B	814	CLA	C2-C3-C5-C6
22	X2	102	LHG	C31-C32-C33-C34
19	A1	809	CLA	C14-C13-C15-C16
19	A1	812	CLA	C6-C7-C8-C9
19	B1	810	CLA	C6-C7-C8-C9
19	B1	825	CLA	C6-C7-C8-C9
19	B1	826	CLA	C11-C12-C13-C14
19	A2	836	CLA	C11-C10-C8-C9
19	B2	826	CLA	C11-C12-C13-C14
19	B2	834	CLA	C14-C13-C15-C16
19	B2	837	CLA	C6-C7-C8-C9
19	A	830	CLA	C11-C12-C13-C14
19	B	825	CLA	C6-C7-C8-C9
19	AA	821	CLA	C11-C10-C8-C9
19	BB	801	CLA	C6-C7-C8-C9
20	AA	803	CL0	C11-C10-C8-C9
21	A	843	PQN	C16-C17-C18-C19
19	B1	823	CLA	C16-C17-C18-C19
19	A2	842	CLA	C16-C17-C18-C20
19	B1	848	CLA	CBA-CGA-O2A-C1
19	BB	814	CLA	C10-C11-C12-C13
19	AA	842	CLA	C5-C6-C7-C8
22	A1	845	LHG	C4-C5-C6-O8
23	F1	303	BCR	C35-C13-C14-C15
23	L1	201	BCR	C20-C21-C22-C37
23	A2	851	BCR	C16-C17-C18-C36
23	B2	839	BCR	C11-C10-C9-C34
23	B2	842	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	F2	303	BCR	C35-C13-C14-C15
23	I	102	BCR	C20-C21-C22-C37
23	II	102	BCR	C20-C21-C22-C37
26	B1	840	ECH	C11-C10-C9-C34
26	B2	841	ECH	C11-C10-C9-C34
26	B	841	ECH	C11-C10-C9-C34
26	BB	840	ECH	C11-C10-C9-C34
19	A	818	CLA	CAA-CBA-CGA-O2A
19	X	101	CLA	C2A-CAA-CBA-CGA
19	A1	801	CLA	C16-C17-C18-C20
19	A2	801	CLA	C16-C17-C18-C20
19	A	827	CLA	O2A-C1-C2-C3
19	AA	827	CLA	O2A-C1-C2-C3
19	BB	821	CLA	O2A-C1-C2-C3
19	B	854	CLA	CBA-CGA-O2A-C1
19	BB	807	CLA	C2C-C3C-CAC-CBC
19	A2	818	CLA	CAA-CBA-CGA-O2A
19	A2	826	CLA	CAA-CBA-CGA-O1A
19	K2	104	CLA	CAA-CBA-CGA-O1A
23	A2	847	BCR	C7-C8-C9-C34
19	BB	802	CLA	O1D-CGD-O2D-CED
19	B2	823	CLA	C10-C11-C12-C13
19	B	806	CLA	C10-C11-C12-C13
19	B	834	CLA	CBD-CGD-O2D-CED
22	X1	103	LHG	C18-C19-C20-C21
25	I1	102	LMG	C17-C18-C19-C20
19	A	826	CLA	CAA-CBA-CGA-O1A
19	AA	818	CLA	CAA-CBA-CGA-O2A
19	BB	820	CLA	CAA-CBA-CGA-O1A
25	I1	102	LMG	C7-C8-O7-C10
19	B1	806	CLA	C10-C11-C12-C13
19	B2	810	CLA	C4-C3-C5-C6
19	A1	814	CLA	C1A-C2A-CAA-CBA
19	A1	852	CLA	C1A-C2A-CAA-CBA
19	B1	801	CLA	C1A-C2A-CAA-CBA
19	B1	810	CLA	C1A-C2A-CAA-CBA
19	B1	811	CLA	C1A-C2A-CAA-CBA
19	B1	821	CLA	C1A-C2A-CAA-CBA
19	B1	832	CLA	C1A-C2A-CAA-CBA
19	A2	810	CLA	C1A-C2A-CAA-CBA
19	A2	815	CLA	C1A-C2A-CAA-CBA
19	B2	810	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	815	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	B	801	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C1A-C2A-CAA-CBA
19	AA	810	CLA	C1A-C2A-CAA-CBA
19	AA	815	CLA	C1A-C2A-CAA-CBA
19	BB	802	CLA	C1A-C2A-CAA-CBA
19	BB	820	CLA	C1A-C2A-CAA-CBA
19	BB	831	CLA	C1A-C2A-CAA-CBA
19	LL	201	CLA	C1A-C2A-CAA-CBA
20	AA	803	CL0	C1A-C2A-CAA-CBA
19	B1	801	CLA	C16-C17-C18-C19
19	A1	818	CLA	C11-C10-C8-C7
19	A1	841	CLA	C6-C7-C8-C10
19	B1	803	CLA	C11-C12-C13-C15
19	B1	804	CLA	C11-C10-C8-C7
19	B1	805	CLA	C11-C12-C13-C15
19	B1	807	CLA	C11-C12-C13-C15
19	B1	815	CLA	C6-C7-C8-C10
19	B2	803	CLA	C11-C12-C13-C15
19	B2	804	CLA	C11-C10-C8-C7
19	B2	807	CLA	C11-C12-C13-C15
19	B2	815	CLA	C6-C7-C8-C10
19	B2	825	CLA	C11-C10-C8-C7
19	A	806	CLA	C6-C7-C8-C10
19	A	819	CLA	C11-C10-C8-C7
19	BB	803	CLA	C11-C12-C13-C15
19	BB	808	CLA	C6-C7-C8-C10
19	BB	815	CLA	C11-C10-C8-C7
19	BB	825	CLA	C11-C10-C8-C7
19	A1	818	CLA	O1D-CGD-O2D-CED
19	B1	805	CLA	C16-C17-C18-C19
19	B2	806	CLA	C10-C11-C12-C13
19	A1	817	CLA	CAA-CBA-CGA-O1A
19	K2	104	CLA	CAA-CBA-CGA-O2A
23	F	304	BCR	C15-C16-C17-C18
23	AA	848	BCR	C13-C14-C15-C16
22	B	853	LHG	C12-C13-C14-C15
28	BB	854	DGD	C4D-C5D-C6D-O5D
19	A	818	CLA	CAA-CBA-CGA-O1A
19	AA	818	CLA	CAA-CBA-CGA-O1A
21	BB	837	PQN	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	L2	206	CLA	C2A-CAA-CBA-CGA
19	BB	824	CLA	C2A-CAA-CBA-CGA
22	X2	103	LHG	O1-C1-C2-O2
19	A1	828	CLA	C13-C15-C16-C17
19	BB	806	CLA	C10-C11-C12-C13
22	B1	847	LHG	O6-C4-C5-O7
25	B1	846	LMG	O7-C10-C11-C12
19	A1	817	CLA	CAA-CBA-CGA-O2A
19	B2	807	CLA	C13-C15-C16-C17
19	BB	804	CLA	C10-C11-C12-C13
19	B2	801	CLA	C16-C17-C18-C19
19	A2	805	CLA	C8-C10-C11-C12
19	B	854	CLA	C13-C15-C16-C17
19	XX	101	CLA	CAA-CBA-CGA-O2A
19	B1	802	CLA	C4-C3-C5-C6
19	A2	808	CLA	C4-C3-C5-C6
19	BB	802	CLA	C4-C3-C5-C6
19	B2	837	CLA	C2C-C3C-CAC-CBC
25	II	105	LMG	C29-C30-C31-C32
19	BB	825	CLA	C5-C6-C7-C8
19	BB	824	CLA	C2-C3-C5-C6
19	B	827	CLA	CAA-CBA-CGA-O2A
19	B1	825	CLA	C5-C6-C7-C8
19	BB	802	CLA	CBD-CGD-O2D-CED
23	L1	201	BCR	C20-C21-C22-C23
23	B2	842	BCR	C16-C17-C18-C19
23	A	850	BCR	C20-C21-C22-C23
26	B1	840	ECH	C11-C10-C9-C8
26	B2	841	ECH	C11-C10-C9-C8
26	B	841	ECH	C11-C10-C9-C8
26	BB	840	ECH	C11-C10-C9-C8
19	B	820	CLA	CAA-CBA-CGA-O1A
19	B	820	CLA	CAA-CBA-CGA-O2A
22	AA	846	LHG	C33-C34-C35-C36
19	A	829	CLA	C13-C15-C16-C17
22	X1	102	LHG	C31-C32-C33-C34
23	B1	842	BCR	C9-C10-C11-C12
23	F2	304	BCR	C19-C20-C21-C22
23	J2	104	BCR	C9-C10-C11-C12
23	FF	304	BCR	C19-C20-C21-C22
23	II	104	BCR	C15-C16-C17-C18
19	X1	101	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	A2	848	BCR	C22-C23-C24-C25
23	B2	839	BCR	C6-C7-C8-C9
19	B	834	CLA	O1D-CGD-O2D-CED
19	BB	845	CLA	C2A-CAA-CBA-CGA
19	A	807	CLA	C16-C17-C18-C20
19	BB	822	CLA	C16-C17-C18-C19
22	B	853	LHG	C28-C29-C30-C31
20	A2	803	CL0	C10-C11-C12-C13
19	X2	101	CLA	CAA-CBA-CGA-O1A
19	XX	101	CLA	CAA-CBA-CGA-O1A
19	AA	808	CLA	C4-C3-C5-C6
19	AA	836	CLA	C2-C3-C5-C6
19	B2	825	CLA	C5-C6-C7-C8
19	AA	829	CLA	C13-C15-C16-C17
19	A2	826	CLA	CAA-CBA-CGA-O2A
19	B2	814	CLA	C10-C11-C12-C13
22	X	102	LHG	C31-C32-C33-C34
19	B1	802	CLA	C6-C7-C8-C9
19	B1	848	CLA	C6-C7-C8-C9
19	A2	821	CLA	C11-C10-C8-C9
19	A2	829	CLA	C11-C12-C13-C14
19	A	819	CLA	C6-C7-C8-C9
19	AA	819	CLA	C6-C7-C8-C9
19	BB	802	CLA	C6-C7-C8-C9
19	B1	848	CLA	O1A-CGA-O2A-C1
19	A2	830	CLA	O1A-CGA-O2A-C1
28	B	856	DGD	O6D-C5D-C6D-O5D
19	A	826	CLA	CAA-CBA-CGA-O2A
19	AA	826	CLA	CAA-CBA-CGA-O2A
19	BB	820	CLA	CAA-CBA-CGA-O2A
22	X2	103	LHG	C31-C32-C33-C34
19	A1	806	CLA	C10-C11-C12-C13
19	B2	849	CLA	C8-C10-C11-C12
19	A1	810	CLA	C2A-CAA-CBA-CGA
19	L1	207	CLA	C2A-CAA-CBA-CGA
19	A2	806	CLA	C2A-CAA-CBA-CGA
19	B	802	CLA	C2A-CAA-CBA-CGA
19	AA	831	CLA	C2A-CAA-CBA-CGA
19	XX	101	CLA	C2A-CAA-CBA-CGA
19	B2	825	CLA	O1D-CGD-O2D-CED
19	A1	820	CLA	C16-C17-C18-C19
19	AA	801	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	827	CLA	CAA-CBA-CGA-O1A
19	B	854	CLA	O1A-CGA-O2A-C1
19	AA	809	CLA	O1A-CGA-O2A-C1
23	A1	847	BCR	C1-C6-C7-C8
23	A1	848	BCR	C1-C6-C7-C8
23	A1	849	BCR	C1-C6-C7-C8
23	A1	850	BCR	C1-C6-C7-C8
23	B1	839	BCR	C1-C6-C7-C8
23	F1	306	BCR	C23-C24-C25-C26
23	K1	104	BCR	C1-C6-C7-C8
23	L1	208	BCR	C1-C6-C7-C8
23	A2	847	BCR	C1-C6-C7-C8
23	A2	848	BCR	C1-C6-C7-C8
23	A2	853	BCR	C1-C6-C7-C8
23	B2	840	BCR	C1-C6-C7-C8
23	I2	103	BCR	C1-C6-C7-C8
23	K2	103	BCR	C1-C6-C7-C8
23	K2	103	BCR	C23-C24-C25-C30
23	M2	102	BCR	C1-C6-C7-C8
23	A	847	BCR	C1-C6-C7-C8
23	A	847	BCR	C23-C24-C25-C30
23	A	848	BCR	C23-C24-C25-C30
23	A	849	BCR	C1-C6-C7-C8
23	A	853	BCR	C23-C24-C25-C30
23	A	854	BCR	C1-C6-C7-C8
23	B	848	BCR	C23-C24-C25-C30
23	K	103	BCR	C1-C6-C7-C8
23	L	206	BCR	C23-C24-C25-C30
23	AA	848	BCR	C1-C6-C7-C8
23	AA	848	BCR	C23-C24-C25-C30
23	AA	849	BCR	C23-C24-C25-C30
23	AA	850	BCR	C1-C6-C7-C8
23	AA	852	BCR	C23-C24-C25-C30
23	AA	854	BCR	C23-C24-C25-C30
23	AA	855	BCR	C1-C6-C7-C8
23	BB	839	BCR	C1-C6-C7-C8
23	BB	847	BCR	C23-C24-C25-C30
23	FF	306	BCR	C23-C24-C25-C30
23	KK	103	BCR	C1-C6-C7-C8
23	LL	204	BCR	C23-C24-C25-C30
28	B	856	DGD	C4D-C5D-C6D-O5D
19	X1	101	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	B	853	LHG	O1-C1-C2-C3
19	A2	809	CLA	O1A-CGA-O2A-C1
23	A1	847	BCR	C13-C14-C15-C16
23	J1	104	BCR	C9-C10-C11-C12
23	J1	104	BCR	C19-C20-C21-C22
23	LL	204	BCR	C13-C14-C15-C16
22	B	852	LHG	C11-C10-C9-C8
19	A2	840	CLA	C4-C3-C5-C6
19	B	807	CLA	C4-C3-C5-C6
19	BB	807	CLA	C4-C3-C5-C6
23	I1	101	BCR	C11-C12-C13-C14
23	A	849	BCR	C7-C8-C9-C10
23	I	101	BCR	C17-C18-C19-C20
23	BB	843	BCR	C7-C8-C9-C10
19	BB	856	CLA	C10-C11-C12-C13
19	B1	824	CLA	C2-C3-C5-C6
19	B2	824	CLA	C2-C3-C5-C6
19	BB	821	CLA	C2-C3-C5-C6
19	B	837	CLA	C3-C5-C6-C7
22	A2	845	LHG	C15-C16-C17-C18
22	LL	205	LHG	C10-C11-C12-C13
19	B1	833	CLA	C15-C16-C17-C18
21	AA	844	PQN	C23-C25-C26-C27
23	F1	303	BCR	C14-C15-C16-C17
22	X2	103	LHG	C18-C19-C20-C21
22	X	102	LHG	C30-C31-C32-C33
19	X2	101	CLA	CAA-CBA-CGA-O2A
19	X	101	CLA	CAA-CBA-CGA-O2A
19	B1	829	CLA	C3-C5-C6-C7
19	B2	807	CLA	C3-C5-C6-C7
22	BB	851	LHG	C12-C13-C14-C15
19	A2	837	CLA	CAA-CBA-CGA-O2A
19	A2	831	CLA	C2A-CAA-CBA-CGA
19	B1	848	CLA	C8-C10-C11-C12
19	B	807	CLA	C2C-C3C-CAC-CBC
19	AA	809	CLA	CBA-CGA-O2A-C1
19	A1	801	CLA	C3-C5-C6-C7
19	A2	801	CLA	C3-C5-C6-C7
19	A1	836	CLA	CAA-CBA-CGA-O2A
19	A1	841	CLA	C16-C17-C18-C20
19	B1	811	CLA	C8-C10-C11-C12
19	B2	811	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	BB	821	CLA	C5-C6-C7-C8
22	X2	103	LHG	C12-C13-C14-C15
19	B2	802	CLA	C4-C3-C5-C6
22	BB	850	LHG	C11-C10-C9-C8
19	A1	809	CLA	C12-C13-C15-C16
19	A1	828	CLA	C11-C12-C13-C15
19	B1	802	CLA	C6-C7-C8-C10
19	B1	826	CLA	C11-C12-C13-C15
19	A2	810	CLA	C12-C13-C15-C16
19	A	819	CLA	C6-C7-C8-C10
19	A	836	CLA	C2-C3-C5-C6
19	B	825	CLA	C11-C10-C8-C7
19	AA	808	CLA	C2-C3-C5-C6
19	A2	829	CLA	C13-C15-C16-C17
19	B	825	CLA	C5-C6-C7-C8
19	BB	833	CLA	C15-C16-C17-C18
23	B	840	BCR	C13-C14-C15-C16
19	A	816	CLA	O1A-CGA-O2A-C1
19	A1	838	CLA	CAA-CBA-CGA-O2A
19	AA	822	CLA	CAA-CBA-CGA-O2A
19	AA	831	CLA	CAA-CBA-CGA-O2A
25	B	851	LMG	O7-C10-C11-C12
22	XX	102	LHG	C30-C31-C32-C33
22	XX	102	LHG	C31-C32-C33-C34
19	A1	830	CLA	C2A-CAA-CBA-CGA
19	B2	852	CLA	C16-C17-C18-C19
19	BB	822	CLA	C16-C17-C18-C20
19	A1	825	CLA	CAA-CBA-CGA-O2A
19	F1	305	CLA	CAA-CBA-CGA-O2A
19	X	101	CLA	CAA-CBA-CGA-O1A
19	A	816	CLA	CBA-CGA-O2A-C1
23	B1	843	BCR	C11-C10-C9-C34
23	B2	839	BCR	C35-C13-C14-C15
23	B2	844	BCR	C11-C10-C9-C34
23	I2	102	BCR	C20-C21-C22-C37
23	AA	851	BCR	C35-C13-C14-C15
25	B	845	LMG	C39-C40-C41-C42
19	A	839	CLA	CAA-CBA-CGA-O2A
19	B	854	CLA	CAA-CBA-CGA-O2A
19	A2	804	CLA	C4-C3-C5-C6
19	B	846	CLA	C2A-CAA-CBA-CGA
22	L2	208	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
19	B1	848	CLA	C2-C3-C5-C6
19	B2	810	CLA	C2-C3-C5-C6
19	B1	815	CLA	C5-C6-C7-C8
19	A2	809	CLA	CBA-CGA-O2A-C1
19	A1	830	CLA	CAA-CBA-CGA-O2A
19	B1	848	CLA	CAA-CBA-CGA-O2A
19	A2	830	CLA	CAA-CBA-CGA-O2A
19	A1	818	CLA	C6-C7-C8-C9
19	A1	829	CLA	C11-C12-C13-C14
19	A1	852	CLA	C11-C12-C13-C14
19	B1	804	CLA	C11-C10-C8-C9
19	B1	832	CLA	C11-C12-C13-C14
19	B1	836	CLA	C6-C7-C8-C9
19	A2	819	CLA	C11-C10-C8-C9
19	A2	836	CLA	C14-C13-C15-C16
19	B2	825	CLA	C6-C7-C8-C9
19	B2	833	CLA	C11-C12-C13-C14
19	L2	206	CLA	C11-C12-C13-C14
19	B	802	CLA	C6-C7-C8-C9
19	B	815	CLA	C6-C7-C8-C9
19	B	826	CLA	C11-C12-C13-C14
19	B	833	CLA	C11-C12-C13-C14
19	B	836	CLA	C14-C13-C15-C16
19	AA	806	CLA	C6-C7-C8-C9
19	BB	815	CLA	C6-C7-C8-C9
19	BB	825	CLA	C6-C7-C8-C9
19	BB	826	CLA	C11-C12-C13-C14
19	BB	832	CLA	C11-C12-C13-C14
19	BB	836	CLA	C6-C7-C8-C9
19	B2	825	CLA	C3-C5-C6-C7
19	A1	832	CLA	C3A-C2A-CAA-CBA
19	A1	852	CLA	C3A-C2A-CAA-CBA
19	B1	801	CLA	C3A-C2A-CAA-CBA
19	B1	807	CLA	C3A-C2A-CAA-CBA
19	B1	833	CLA	C3A-C2A-CAA-CBA
19	A2	833	CLA	C3A-C2A-CAA-CBA
19	A2	836	CLA	C3A-C2A-CAA-CBA
19	B2	810	CLA	C3A-C2A-CAA-CBA
19	A	836	CLA	C3A-C2A-CAA-CBA
19	B	834	CLA	C3A-C2A-CAA-CBA
19	F	301	CLA	C3A-C2A-CAA-CBA
19	AA	833	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	BB	831	CLA	C3A-C2A-CAA-CBA
19	A1	827	CLA	CAA-CBA-CGA-O2A
19	A2	839	CLA	CAA-CBA-CGA-O2A
20	A2	803	CL0	CAA-CBA-CGA-O2A
19	B2	820	CLA	CAA-CBA-CGA-O2A
19	A1	808	CLA	CAD-CBD-CGD-O2D
19	A1	822	CLA	CAD-CBD-CGD-O2D
19	B1	819	CLA	CAD-CBD-CGD-O2D
19	B1	832	CLA	CAD-CBD-CGD-O2D
19	B1	850	CLA	CAD-CBD-CGD-O2D
19	F1	305	CLA	CAD-CBD-CGD-O2D
19	A2	804	CLA	CAD-CBD-CGD-O2D
19	A2	806	CLA	CAD-CBD-CGD-O2D
19	A2	817	CLA	CAD-CBD-CGD-O2D
19	B2	802	CLA	CAD-CBD-CGD-O2D
19	J2	101	CLA	CAD-CBD-CGD-O2D
19	K2	102	CLA	CAD-CBD-CGD-O2D
19	X2	101	CLA	CAD-CBD-CGD-O2D
19	A	817	CLA	CAD-CBD-CGD-O2D
19	A	844	CLA	CAD-CBD-CGD-O2D
19	B	811	CLA	CAD-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O2D
19	B	829	CLA	CAD-CBD-CGD-O2D
19	B	859	CLA	CAD-CBD-CGD-O2D
19	J	101	CLA	CAD-CBD-CGD-O2D
19	K	101	CLA	CAD-CBD-CGD-O2D
19	K	102	CLA	CAD-CBD-CGD-O2D
19	AA	822	CLA	CAD-CBD-CGD-O2D
19	AA	827	CLA	CAD-CBD-CGD-O2D
19	BB	811	CLA	CAD-CBD-CGD-O2D
19	BB	816	CLA	CAD-CBD-CGD-O2D
19	BB	822	CLA	CAD-CBD-CGD-O2D
19	BB	825	CLA	CAD-CBD-CGD-O2D
19	BB	829	CLA	CAD-CBD-CGD-O2D
19	BB	856	CLA	CAD-CBD-CGD-O2D
19	KK	101	CLA	CAD-CBD-CGD-O2D
19	XX	101	CLA	CAD-CBD-CGD-O2D
25	I1	102	LMG	C9-C8-O7-C10
19	A	830	CLA	C13-C15-C16-C17
19	A	801	CLA	C3-C5-C6-C7
19	AA	801	CLA	C3-C5-C6-C7
22	L	207	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B2	824	CLA	C2-C1-O2A-CGA
19	B1	831	CLA	CAA-CBA-CGA-O2A
19	A1	828	CLA	CAA-CBA-CGA-O2A
19	A1	852	CLA	CAA-CBA-CGA-O2A
19	B1	810	CLA	CAA-CBA-CGA-O2A
19	A	842	CLA	CAA-CBA-CGA-O2A
19	L	202	CLA	CAA-CBA-CGA-O2A
23	A2	849	BCR	C6-C7-C8-C9
23	A	850	BCR	C22-C23-C24-C25
19	A	804	CLA	C4-C3-C5-C6
20	A2	803	CL0	C4-C3-C5-C6
19	A1	828	CLA	C16-C17-C18-C20
19	B1	802	CLA	C2-C3-C5-C6
19	A2	804	CLA	C2-C3-C5-C6
19	A2	808	CLA	C2-C3-C5-C6
19	BB	802	CLA	C2-C3-C5-C6
19	B1	801	CLA	CAA-CBA-CGA-O2A
19	A2	842	CLA	CAA-CBA-CGA-O2A
19	BB	852	CLA	CAA-CBA-CGA-O2A
23	A1	847	BCR	C11-C12-C13-C14
23	A1	851	BCR	C7-C8-C9-C10
23	K1	104	BCR	C11-C12-C13-C14
23	A2	847	BCR	C11-C12-C13-C14
23	F2	303	BCR	C7-C8-C9-C10
23	J2	104	BCR	C11-C12-C13-C14
23	J2	104	BCR	C17-C18-C19-C20
23	B	840	BCR	C21-C22-C23-C24
23	F	303	BCR	C7-C8-C9-C10
25	I2	105	LMG	O1-C7-C8-C9
25	I2	105	LMG	C7-C8-C9-O8
28	BB	854	DGD	O1G-C1G-C2G-C3G
19	A1	836	CLA	CAA-CBA-CGA-O1A
19	B2	832	CLA	CAA-CBA-CGA-O2A
19	B	828	CLA	CAA-CBA-CGA-O2A
19	A1	821	CLA	CAA-CBA-CGA-O2A
19	A1	829	CLA	CAA-CBA-CGA-O2A
19	A1	841	CLA	CAA-CBA-CGA-O2A
19	A2	852	CLA	CAA-CBA-CGA-O2A
19	A	822	CLA	CAA-CBA-CGA-O2A
19	A	852	CLA	CAA-CBA-CGA-O2A
19	AA	839	CLA	CAA-CBA-CGA-O2A
19	AA	843	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	A	803	CL0	CAA-CBA-CGA-O2A
19	AA	801	CLA	C16-C17-C18-C20
23	LL	204	BCR	C18-C19-C20-C21
19	A1	825	CLA	CAA-CBA-CGA-O1A
22	A2	845	LHG	C33-C34-C35-C36
25	I2	105	LMG	C13-C14-C15-C16
19	A1	826	CLA	O2A-C1-C2-C3
19	A1	832	CLA	O2A-C1-C2-C3
19	B1	821	CLA	O2A-C1-C2-C3
19	A2	827	CLA	O2A-C1-C2-C3
19	A2	833	CLA	O2A-C1-C2-C3
19	A	833	CLA	O2A-C1-C2-C3
19	B	821	CLA	O2A-C1-C2-C3
19	L	204	CLA	C4C-C3C-CAC-CBC
22	X1	103	LHG	C28-C29-C30-C31
22	A2	845	LHG	C11-C12-C13-C14
23	I2	103	BCR	C14-C15-C16-C17
23	II	104	BCR	C14-C15-C16-C17
19	A1	806	CLA	C15-C16-C17-C18
19	L	204	CLA	C13-C15-C16-C17
19	AA	807	CLA	C15-C16-C17-C18
19	B1	801	CLA	C3-C5-C6-C7
19	B1	820	CLA	CAA-CBA-CGA-O2A
19	A2	837	CLA	CAA-CBA-CGA-O1A
19	A1	804	CLA	C11-C12-C13-C15
19	AA	821	CLA	C16-C17-C18-C19
19	A2	829	CLA	C2C-C3C-CAC-CBC
19	B	817	CLA	CBD-CGD-O2D-CED
19	FF	301	CLA	C2C-C3C-CAC-CBC
22	XX	102	LHG	C27-C28-C29-C30
19	A1	816	CLA	CHA-CBD-CGD-O2D
19	A1	822	CLA	CHA-CBD-CGD-O2D
19	A1	829	CLA	CHA-CBD-CGD-O1D
19	A1	829	CLA	CHA-CBD-CGD-O2D
19	A1	831	CLA	CHA-CBD-CGD-O1D
19	A1	831	CLA	CHA-CBD-CGD-O2D
19	B1	801	CLA	CHA-CBD-CGD-O1D
19	B1	807	CLA	CHA-CBD-CGD-O2D
19	B1	812	CLA	CHA-CBD-CGD-O1D
19	B1	812	CLA	CHA-CBD-CGD-O2D
19	B1	815	CLA	CHA-CBD-CGD-O2D
19	B1	816	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B1	827	CLA	CHA-CBD-CGD-O1D
19	B1	827	CLA	CHA-CBD-CGD-O2D
19	A2	820	CLA	CHA-CBD-CGD-O1D
19	A2	820	CLA	CHA-CBD-CGD-O2D
19	A2	830	CLA	CHA-CBD-CGD-O1D
19	A2	830	CLA	CHA-CBD-CGD-O2D
19	A2	836	CLA	CHA-CBD-CGD-O1D
19	A2	836	CLA	CHA-CBD-CGD-O2D
19	A2	837	CLA	CHA-CBD-CGD-O1D
19	A2	837	CLA	CHA-CBD-CGD-O2D
19	B2	801	CLA	CHA-CBD-CGD-O1D
19	B2	807	CLA	CHA-CBD-CGD-O1D
19	B2	807	CLA	CHA-CBD-CGD-O2D
19	B2	822	CLA	CHA-CBD-CGD-O2D
19	B2	835	CLA	CHA-CBD-CGD-O2D
19	B2	851	CLA	CHA-CBD-CGD-O2D
19	A	820	CLA	CHA-CBD-CGD-O1D
19	A	820	CLA	CHA-CBD-CGD-O2D
19	A	830	CLA	CHA-CBD-CGD-O1D
19	A	830	CLA	CHA-CBD-CGD-O2D
19	A	832	CLA	CHA-CBD-CGD-O1D
19	A	832	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A	852	CLA	CHA-CBD-CGD-O2D
19	B	801	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	CHA-CBD-CGD-O1D
19	B	814	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O2D
19	B	837	CLA	CHA-CBD-CGD-O1D
19	B	837	CLA	CHA-CBD-CGD-O2D
19	B	859	CLA	CHA-CBD-CGD-O1D
19	F	301	CLA	CHA-CBD-CGD-O2D
19	AA	816	CLA	CHA-CBD-CGD-O2D
19	AA	820	CLA	CHA-CBD-CGD-O1D
19	AA	820	CLA	CHA-CBD-CGD-O2D
19	AA	853	CLA	CHA-CBD-CGD-O1D
19	BB	801	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	BB	801	CLA	CHA-CBD-CGD-O2D
19	BB	807	CLA	CHA-CBD-CGD-O1D
19	BB	807	CLA	CHA-CBD-CGD-O2D
19	BB	808	CLA	CHA-CBD-CGD-O1D
19	BB	808	CLA	CHA-CBD-CGD-O2D
19	BB	814	CLA	CHA-CBD-CGD-O1D
19	BB	814	CLA	CHA-CBD-CGD-O2D
19	BB	856	CLA	CHA-CBD-CGD-O1D
19	LL	203	CLA	CHA-CBD-CGD-O2D
23	B2	843	BCR	C9-C10-C11-C12
23	BB	839	BCR	C13-C14-C15-C16
19	B1	820	CLA	CAA-CBA-CGA-O1A
19	F1	305	CLA	CAA-CBA-CGA-O1A
19	B2	820	CLA	CAA-CBA-CGA-O1A
19	AA	842	CLA	CAA-CBA-CGA-O2A
20	A2	803	CL0	C2-C3-C5-C6
25	I2	105	LMG	C20-C21-C22-C23
19	BB	803	CLA	C3-C5-C6-C7
23	A1	850	BCR	C20-C21-C22-C23
23	I1	101	BCR	C11-C10-C9-C8
23	A2	851	BCR	C16-C17-C18-C19
23	BB	841	BCR	C20-C21-C22-C23
23	II	102	BCR	C20-C21-C22-C23
19	B	828	CLA	CAA-CBA-CGA-O1A
19	AA	842	CLA	C16-C17-C18-C19
19	B2	801	CLA	CAA-CBA-CGA-O2A
19	B2	852	CLA	CAA-CBA-CGA-O2A
19	A	829	CLA	CAA-CBA-CGA-O2A
19	A	831	CLA	CAA-CBA-CGA-O2A
19	A	840	CLA	CAA-CBA-CGA-O2A
19	B	860	CLA	CAA-CBA-CGA-O2A
22	B	852	LHG	O8-C23-C24-C25
22	BB	850	LHG	O8-C23-C24-C25
22	B1	847	LHG	C24-C25-C26-C27
22	A	845	LHG	O7-C5-C6-O8
22	A1	846	LHG	C14-C15-C16-C17
19	A1	842	CLA	CAA-CBA-CGA-O2A
19	B1	821	CLA	CAA-CBA-CGA-O2A
19	A2	822	CLA	CAA-CBA-CGA-O2A
19	A2	831	CLA	CAA-CBA-CGA-O2A
19	B2	810	CLA	CAA-CBA-CGA-O2A
19	AA	840	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A1	807	CLA	C2A-CAA-CBA-CGA
19	A	827	CLA	C2A-CAA-CBA-CGA
19	B2	836	CLA	C16-C17-C18-C19
19	B2	837	CLA	C11-C12-C13-C15
19	B2	852	CLA	C16-C17-C18-C20
22	B	852	LHG	O1-C1-C2-O2
22	BB	850	LHG	O1-C1-C2-O2
19	A	820	CLA	C5-C6-C7-C8
19	A2	830	CLA	CBA-CGA-O2A-C1
22	B1	847	LHG	C25-C26-C27-C28
19	A2	813	CLA	C3-C5-C6-C7
19	A2	828	CLA	CAA-CBA-CGA-O2A
19	AA	830	CLA	CAA-CBA-CGA-O2A
22	X	102	LHG	C27-C28-C29-C30
19	B1	821	CLA	C5-C6-C7-C8
19	A2	842	CLA	C6-C7-C8-C10
19	A2	852	CLA	C11-C12-C13-C15
19	A	852	CLA	C11-C12-C13-C15
19	B	802	CLA	C6-C7-C8-C10
19	B	808	CLA	C6-C7-C8-C10
19	B	821	CLA	C2-C3-C5-C6
19	B	837	CLA	C6-C7-C8-C10
19	AA	810	CLA	C11-C12-C13-C15
19	AA	819	CLA	C11-C10-C8-C7
19	BB	802	CLA	C6-C7-C8-C10
19	BB	825	CLA	C12-C13-C15-C16
19	A	842	CLA	C16-C17-C18-C19
19	AA	821	CLA	C16-C17-C18-C20
22	X2	102	LHG	O9-C7-O7-C5
19	L1	205	CLA	C8-C10-C11-C12
19	L2	204	CLA	C8-C10-C11-C12
19	A2	829	CLA	C4C-C3C-CAC-CBC
19	A1	818	CLA	C11-C10-C8-C9
19	B1	808	CLA	C6-C7-C8-C9
19	B2	804	CLA	C11-C10-C8-C9
19	B2	834	CLA	C11-C10-C8-C9
19	A	806	CLA	C6-C7-C8-C9
19	A	810	CLA	C14-C13-C15-C16
19	A	819	CLA	C11-C10-C8-C9
19	A	821	CLA	C11-C10-C8-C9
19	B	806	CLA	C14-C13-C15-C16
19	B	837	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	BB	808	CLA	C6-C7-C8-C9
23	I2	101	BCR	C15-C16-C17-C18
23	JJ	104	BCR	C15-C16-C17-C18
19	A	852	CLA	C5-C6-C7-C8
22	X2	103	LHG	C34-C35-C36-C37
19	B2	821	CLA	CAA-CBA-CGA-O2A
19	A	828	CLA	CAA-CBA-CGA-O2A
19	L	204	CLA	CAA-CBA-CGA-O2A
19	A1	828	CLA	C16-C17-C18-C19
19	B2	822	CLA	C16-C17-C18-C19
19	B1	824	CLA	C2A-CAA-CBA-CGA
19	B2	810	CLA	C2A-CAA-CBA-CGA
19	AA	827	CLA	C2A-CAA-CBA-CGA
19	B	854	CLA	CAA-CBA-CGA-O1A
19	AA	828	CLA	CAA-CBA-CGA-O2A
25	L1	210	LMG	O7-C10-C11-C12
22	X1	103	LHG	C31-C32-C33-C34
22	B	853	LHG	C25-C26-C27-C28
19	B1	831	CLA	CAA-CBA-CGA-O1A
19	A1	830	CLA	CAA-CBA-CGA-O1A
19	B1	810	CLA	CAA-CBA-CGA-O1A
19	A	821	CLA	C16-C17-C18-C19
19	A1	803	CLA	C4-C3-C5-C6
19	L	203	CLA	CAA-CBA-CGA-O2A
19	B2	832	CLA	CAA-CBA-CGA-O1A
19	BB	809	CLA	CAA-CBA-CGA-O1A
19	A1	828	CLA	CAA-CBA-CGA-O1A
19	B1	848	CLA	CAA-CBA-CGA-O1A
19	A2	842	CLA	CAA-CBA-CGA-O1A
23	K1	104	BCR	C17-C18-C19-C20
23	A2	853	BCR	C17-C18-C19-C20
22	L	207	LHG	C13-C14-C15-C16
19	A1	830	CLA	C8-C10-C11-C12
19	L	203	CLA	C8-C10-C11-C12
19	A1	831	CLA	C1A-C2A-CAA-CBA
19	A1	832	CLA	C1A-C2A-CAA-CBA
19	B1	807	CLA	C1A-C2A-CAA-CBA
19	L1	207	CLA	C1A-C2A-CAA-CBA
19	X1	101	CLA	C1A-C2A-CAA-CBA
19	A2	832	CLA	C1A-C2A-CAA-CBA
19	A2	833	CLA	C1A-C2A-CAA-CBA
19	A2	836	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A2	852	CLA	C1A-C2A-CAA-CBA
19	B2	807	CLA	C1A-C2A-CAA-CBA
19	B2	811	CLA	C1A-C2A-CAA-CBA
19	L2	204	CLA	C1A-C2A-CAA-CBA
19	L2	206	CLA	C1A-C2A-CAA-CBA
19	X2	101	CLA	C1A-C2A-CAA-CBA
19	A	832	CLA	C1A-C2A-CAA-CBA
19	A	836	CLA	C1A-C2A-CAA-CBA
19	B	810	CLA	C1A-C2A-CAA-CBA
19	AA	833	CLA	C1A-C2A-CAA-CBA
19	AA	836	CLA	C1A-C2A-CAA-CBA
19	BB	810	CLA	C1A-C2A-CAA-CBA
19	BB	811	CLA	C1A-C2A-CAA-CBA
19	BB	830	CLA	C1A-C2A-CAA-CBA
19	BB	832	CLA	C1A-C2A-CAA-CBA
19	XX	101	CLA	C1A-C2A-CAA-CBA
20	A1	802	CL0	C1A-C2A-CAA-CBA
19	A2	839	CLA	CAA-CBA-CGA-O1A
19	B2	821	CLA	CAA-CBA-CGA-O1A
19	A	839	CLA	CAA-CBA-CGA-O1A
19	AA	822	CLA	CAA-CBA-CGA-O1A
19	AA	828	CLA	CAA-CBA-CGA-O1A
19	AA	831	CLA	CAA-CBA-CGA-O1A
22	A2	846	LHG	C14-C15-C16-C17
19	A1	829	CLA	O1A-CGA-O2A-C1
19	BB	811	CLA	O1D-CGD-O2D-CED
19	B1	808	CLA	C2-C1-O2A-CGA
22	A2	845	LHG	C18-C19-C20-C21
19	A1	852	CLA	CAA-CBA-CGA-O1A
19	AA	842	CLA	CAA-CBA-CGA-O1A
28	B	856	DGD	O1B-C1B-C2B-C3B
28	BB	854	DGD	O1B-C1B-C2B-C3B
19	B2	809	CLA	CAA-CBA-CGA-O2A
28	B	856	DGD	O1G-C1G-C2G-C3G
28	BB	854	DGD	C4E-C5E-C6E-O5E
19	A	825	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	CAA-CBA-CGA-O2A
19	BB	821	CLA	CAA-CBA-CGA-O2A
19	B1	804	CLA	C10-C11-C12-C13
19	B2	824	CLA	C2A-CAA-CBA-CGA
22	BB	851	LHG	C28-C29-C30-C31
19	B1	836	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	F	301	CLA	C11-C12-C13-C15
19	A1	838	CLA	CAA-CBA-CGA-O1A
19	B1	801	CLA	CAA-CBA-CGA-O1A
19	A	828	CLA	CAA-CBA-CGA-O1A
19	A	852	CLA	CAA-CBA-CGA-O1A
19	AA	830	CLA	CAA-CBA-CGA-O1A
19	BB	852	CLA	CAA-CBA-CGA-O1A
19	A	807	CLA	C15-C16-C17-C18
22	A	845	LHG	C33-C34-C35-C36
19	B1	809	CLA	CAA-CBA-CGA-O2A
19	A1	839	CLA	CAA-CBA-CGA-O2A
19	B	860	CLA	C5-C6-C7-C8
19	B1	836	CLA	C2C-C3C-CAC-CBC
19	A1	841	CLA	CAA-CBA-CGA-O1A
19	A2	822	CLA	CAA-CBA-CGA-O1A
19	A2	828	CLA	CAA-CBA-CGA-O1A
19	B	860	CLA	CAA-CBA-CGA-O1A
19	L	202	CLA	CAA-CBA-CGA-O1A
23	A1	848	BCR	C22-C23-C24-C25
23	AA	851	BCR	C22-C23-C24-C25
23	I	101	BCR	C14-C15-C16-C17
19	A1	819	CLA	C5-C6-C7-C8
22	A1	845	LHG	C4-O6-P-O5
22	A2	845	LHG	C4-O6-P-O5
22	L2	208	LHG	C3-O3-P-O5
22	A	845	LHG	C4-O6-P-O5
22	B	852	LHG	C4-O6-P-O5
22	AA	846	LHG	C4-O6-P-O5
22	BB	850	LHG	C3-O3-P-O5
22	XX	102	LHG	C3-O3-P-O5
19	AA	807	CLA	C16-C17-C18-C20
19	A1	821	CLA	CAA-CBA-CGA-O1A
19	A1	827	CLA	CAA-CBA-CGA-O1A
19	A1	829	CLA	CAA-CBA-CGA-O1A
19	A2	830	CLA	CAA-CBA-CGA-O1A
19	A2	852	CLA	CAA-CBA-CGA-O1A
19	B2	801	CLA	CAA-CBA-CGA-O1A
19	B2	852	CLA	CAA-CBA-CGA-O1A
22	B	852	LHG	O10-C23-C24-C25
22	BB	850	LHG	O10-C23-C24-C25
25	B	845	LMG	O10-C28-C29-C30
25	BB	844	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	II	105	LMG	O8-C28-C29-C30
19	B2	836	CLA	C3-C5-C6-C7
23	J1	102	BCR	C5-C6-C7-C8
23	K1	106	BCR	C1-C6-C7-C8
23	K2	103	BCR	C5-C6-C7-C8
23	A	848	BCR	C5-C6-C7-C8
23	A	848	BCR	C23-C24-C25-C26
23	A	853	BCR	C1-C6-C7-C8
23	AA	849	BCR	C5-C6-C7-C8
23	AA	849	BCR	C23-C24-C25-C26
23	AA	854	BCR	C1-C6-C7-C8
19	A2	821	CLA	O1D-CGD-O2D-CED
19	A1	842	CLA	CAA-CBA-CGA-O1A
19	B1	821	CLA	CAA-CBA-CGA-O1A
19	AA	839	CLA	CAA-CBA-CGA-O1A
19	AA	843	CLA	CAA-CBA-CGA-O1A
22	BB	850	LHG	O7-C7-C8-C9
28	BB	854	DGD	O2G-C1B-C2B-C3B
19	A2	829	CLA	C15-C16-C17-C18
19	A2	842	CLA	C16-C17-C18-C19
19	AA	836	CLA	C16-C17-C18-C20
23	F2	303	BCR	C18-C19-C20-C21
19	A	820	CLA	C2A-CAA-CBA-CGA
19	J	103	CLA	C4C-C3C-CAC-CBC
19	B	821	CLA	C5-C6-C7-C8
19	B	815	CLA	C5-C6-C7-C8
19	B2	822	CLA	C16-C17-C18-C20
19	A	837	CLA	CAA-CBA-CGA-O2A
19	B1	816	CLA	CAD-CBD-CGD-O1D
19	J1	101	CLA	CAD-CBD-CGD-O1D
19	A2	820	CLA	CAD-CBD-CGD-O1D
19	A2	822	CLA	CAD-CBD-CGD-O1D
19	A2	830	CLA	CAD-CBD-CGD-O1D
19	A	821	CLA	CAD-CBD-CGD-O1D
19	A	823	CLA	CAD-CBD-CGD-O1D
19	A	838	CLA	CAD-CBD-CGD-O1D
19	A	852	CLA	CAD-CBD-CGD-O1D
19	B	816	CLA	CAD-CBD-CGD-O1D
19	B	820	CLA	CAD-CBD-CGD-O1D
19	AA	820	CLA	CAD-CBD-CGD-O1D
19	AA	821	CLA	CAD-CBD-CGD-O1D
19	AA	822	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	AA	836	CLA	CAD-CBD-CGD-O1D
19	AA	853	CLA	CAD-CBD-CGD-O1D
19	BB	814	CLA	CAD-CBD-CGD-O1D
19	BB	820	CLA	CAD-CBD-CGD-O1D
19	JJ	101	CLA	CAD-CBD-CGD-O1D
19	A	822	CLA	CAA-CBA-CGA-O1A
19	A	829	CLA	CAA-CBA-CGA-O1A
19	A	830	CLA	CAA-CBA-CGA-O1A
19	A	842	CLA	CAA-CBA-CGA-O1A
22	X1	102	LHG	C29-C30-C31-C32
19	A2	807	CLA	C15-C16-C17-C18
19	B	804	CLA	C10-C11-C12-C13
22	L1	211	LHG	O2-C2-C3-O3
19	B1	807	CLA	C11-C12-C13-C14
19	B1	830	CLA	C6-C7-C8-C9
19	B2	807	CLA	C11-C12-C13-C14
19	B2	808	CLA	C6-C7-C8-C9
19	B2	831	CLA	C6-C7-C8-C9
19	A	842	CLA	C11-C10-C8-C9
19	B	801	CLA	C11-C10-C8-C9
19	B	808	CLA	C6-C7-C8-C9
19	AA	810	CLA	C11-C12-C13-C14
19	AA	810	CLA	C14-C13-C15-C16
19	AA	819	CLA	C11-C10-C8-C9
19	BB	821	CLA	C11-C10-C8-C9
20	A1	802	CL0	C11-C10-C8-C9
22	LL	205	LHG	C13-C14-C15-C16
22	AA	846	LHG	C25-C26-C27-C28
19	B1	809	CLA	CAA-CBA-CGA-O1A
19	A1	809	CLA	C5-C6-C7-C8
19	A2	831	CLA	CAA-CBA-CGA-O1A
19	B2	814	CLA	CBA-CGA-O2A-C1
19	AA	835	CLA	C16-C17-C18-C20
19	B1	802	CLA	CAA-CBA-CGA-O2A
19	A2	841	CLA	CAA-CBA-CGA-O2A
19	AA	820	CLA	CAA-CBA-CGA-O2A
19	FF	301	CLA	CAA-CBA-CGA-O2A
19	LL	202	CLA	CAA-CBA-CGA-O2A
22	LL	205	LHG	C12-C13-C14-C15
19	B2	852	CLA	C5-C6-C7-C8
19	L2	206	CLA	C8-C10-C11-C12
19	B2	809	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	B1	846	LMG	C14-C15-C16-C17
19	B2	810	CLA	CAA-CBA-CGA-O1A
22	A1	845	LHG	C16-C17-C18-C19
22	A	846	LHG	C11-C12-C13-C14
19	X1	101	CLA	C2A-CAA-CBA-CGA
19	A2	820	CLA	C2A-CAA-CBA-CGA
19	B1	824	CLA	CAA-CBA-CGA-O2A
19	L1	205	CLA	CAA-CBA-CGA-O2A
19	B	801	CLA	CAA-CBA-CGA-O2A
19	B	821	CLA	CAA-CBA-CGA-O2A
19	BB	802	CLA	CAA-CBA-CGA-O2A
19	BB	811	CLA	CAA-CBA-CGA-O2A
22	X	102	LHG	O7-C7-C8-C9
22	X1	103	LHG	C1-C2-C3-O3
22	B	852	LHG	C1-C2-C3-O3
19	A1	842	CLA	C5-C6-C7-C8
19	B	806	CLA	C13-C15-C16-C17
19	BB	809	CLA	CAA-CBA-CGA-O2A
19	A	840	CLA	CAA-CBA-CGA-O1A
19	AA	840	CLA	CAA-CBA-CGA-O1A
19	BB	821	CLA	CAA-CBA-CGA-O1A
19	B2	821	CLA	C13-C15-C16-C17
23	B1	839	BCR	C11-C12-C13-C35
22	AA	847	LHG	C11-C12-C13-C14
19	A1	818	CLA	C6-C7-C8-C10
19	B1	808	CLA	C6-C7-C8-C10
19	B1	848	CLA	C6-C7-C8-C10
19	A2	821	CLA	C11-C10-C8-C7
19	A2	829	CLA	C11-C12-C13-C15
19	B2	808	CLA	C6-C7-C8-C10
19	B2	816	CLA	C6-C7-C8-C10
19	B2	822	CLA	C11-C10-C8-C7
19	B2	826	CLA	C11-C12-C13-C15
19	A	810	CLA	C11-C12-C13-C15
19	A	810	CLA	C12-C13-C15-C16
19	B	803	CLA	C11-C12-C13-C15
19	B	807	CLA	C6-C7-C8-C10
19	L	204	CLA	C12-C13-C15-C16
19	AA	807	CLA	C11-C10-C8-C7
19	AA	821	CLA	C11-C10-C8-C7
19	BB	804	CLA	C11-C10-C8-C7
19	BB	807	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	BB	810	CLA	C3A-C2A-CAA-CBA
19	BB	822	CLA	C11-C10-C8-C7
19	BB	826	CLA	C11-C12-C13-C15
19	BB	833	CLA	C3A-C2A-CAA-CBA
22	L	207	LHG	C12-C13-C14-C15
19	A2	840	CLA	CAA-CBA-CGA-O2A
19	AA	829	CLA	CAA-CBA-CGA-O2A
25	I1	102	LMG	O7-C10-C11-C12
28	B	856	DGD	O2G-C1B-C2B-C3B
19	A2	810	CLA	C5-C6-C7-C8
23	A1	853	BCR	C17-C18-C19-C20
23	I2	101	BCR	C11-C12-C13-C14
23	B	844	BCR	C7-C8-C9-C10
23	II	104	BCR	C11-C12-C13-C14
19	A1	839	CLA	CAA-CBA-CGA-O1A
19	L	204	CLA	CAA-CBA-CGA-O1A
19	AA	829	CLA	CAA-CBA-CGA-O1A
25	B2	845	LMG	O10-C28-C29-C30
23	B1	841	BCR	C15-C16-C17-C18
23	K1	106	BCR	C9-C10-C11-C12
23	K2	105	BCR	C9-C10-C11-C12
23	M2	102	BCR	C13-C14-C15-C16
26	BB	840	ECH	C9-C10-C11-C12
22	A1	845	LHG	C18-C19-C20-C21
19	AA	807	CLA	C16-C17-C18-C19
19	B2	824	CLA	CAA-CBA-CGA-O2A
19	L2	204	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A
19	AA	853	CLA	CAA-CBA-CGA-O2A
19	B	817	CLA	O1D-CGD-O2D-CED
19	A2	808	CLA	C5-C6-C7-C8
19	AA	831	CLA	C8-C10-C11-C12
19	AA	843	CLA	C5-C6-C7-C8
19	B2	814	CLA	O1A-CGA-O2A-C1
19	A1	840	CLA	CAA-CBA-CGA-O1A
19	A2	840	CLA	CAA-CBA-CGA-O1A
19	A2	841	CLA	CAA-CBA-CGA-O1A
19	A	831	CLA	CAA-CBA-CGA-O1A
19	B	821	CLA	CAA-CBA-CGA-O1A
19	FF	301	CLA	CAA-CBA-CGA-O1A
19	LL	202	CLA	CAA-CBA-CGA-O1A
19	A	837	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	B2	821	CLA	C5-C6-C7-C8
25	B	845	LMG	C23-C24-C25-C26
19	A1	840	CLA	CAA-CBA-CGA-O2A
19	A	841	CLA	CAA-CBA-CGA-O2A
19	AA	841	CLA	CAA-CBA-CGA-O2A
19	BB	801	CLA	CAA-CBA-CGA-O2A
19	BB	829	CLA	CAA-CBA-CGA-O2A
22	B	852	LHG	O7-C7-C8-C9
25	B	845	LMG	O8-C28-C29-C30
19	B1	850	CLA	C8-C10-C11-C12
19	B2	826	CLA	C2A-CAA-CBA-CGA
19	B2	804	CLA	C10-C11-C12-C13
19	B2	810	CLA	C5-C6-C7-C8
19	B	829	CLA	C10-C11-C12-C13
19	AA	836	CLA	C5-C6-C7-C8
19	B	801	CLA	CAA-CBA-CGA-O1A
19	AA	853	CLA	CAA-CBA-CGA-O1A
19	BB	802	CLA	CAA-CBA-CGA-O1A
25	B1	844	LMG	O10-C28-C29-C30

There are no ring outliers.

346 monomers are involved in 565 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B1	824	CLA	1	0
19	B	821	CLA	1	0
23	B1	842	BCR	3	0
19	B1	826	CLA	1	0
19	A1	830	CLA	1	0
19	B	832	CLA	2	0
23	A	851	BCR	4	0
19	BB	813	CLA	1	0
19	B1	828	CLA	3	0
19	A	806	CLA	2	0
23	K2	103	BCR	1	0
23	M	101	BCR	2	0
19	B2	808	CLA	1	0
19	B2	806	CLA	2	0
23	B2	842	BCR	4	0
19	B	860	CLA	2	0
19	B1	802	CLA	1	0
19	B2	822	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	801	CLA	1	0
19	A2	840	CLA	1	0
19	B	835	CLA	8	0
19	B	837	CLA	2	0
19	A2	828	CLA	1	0
19	AA	842	CLA	2	0
19	BB	834	CLA	6	0
23	J1	104	BCR	1	0
23	LL	204	BCR	1	0
19	A	842	CLA	2	0
19	B1	833	CLA	14	0
19	BB	812	CLA	1	0
23	JJ	104	BCR	1	0
22	A	845	LHG	2	0
19	A2	807	CLA	2	0
19	AA	818	CLA	2	0
19	A2	802	CLA	1	0
19	B1	809	CLA	1	0
22	B1	847	LHG	1	0
19	A2	806	CLA	3	0
19	B1	813	CLA	1	0
19	B2	823	CLA	1	0
21	A1	843	PQN	1	0
19	A1	829	CLA	3	0
19	B	830	CLA	4	0
23	AA	848	BCR	1	0
23	AA	854	BCR	1	0
19	B1	845	CLA	1	0
23	J	102	BCR	1	0
23	J1	102	BCR	1	0
19	BB	826	CLA	2	0
19	A1	824	CLA	1	0
19	A1	833	CLA	2	0
19	BB	820	CLA	5	0
19	A	813	CLA	1	0
19	B1	815	CLA	3	0
19	LL	202	CLA	1	0
19	A2	818	CLA	2	0
19	B2	809	CLA	1	0
19	LL	203	CLA	1	0
19	F	301	CLA	3	0
19	A1	828	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	842	BCR	5	0
19	B	820	CLA	5	0
19	B1	836	CLA	1	0
19	A2	801	CLA	1	0
19	B2	811	CLA	2	0
19	A	824	CLA	1	0
19	B1	807	CLA	1	0
23	F	303	BCR	2	0
27	C	102	SF4	1	0
19	B1	806	CLA	1	0
19	AA	813	CLA	1	0
19	B2	827	CLA	1	0
23	F1	306	BCR	5	0
19	A1	827	CLA	1	0
19	A2	831	CLA	1	0
19	A1	819	CLA	2	0
19	K1	105	CLA	1	0
19	A2	816	CLA	1	0
19	AA	845	CLA	1	0
19	AA	826	CLA	4	0
19	AA	820	CLA	1	0
19	A2	835	CLA	1	0
19	B	834	CLA	14	0
28	B	856	DGD	1	0
20	AA	803	CL0	1	0
19	BB	802	CLA	1	0
19	B	813	CLA	1	0
19	B1	848	CLA	6	0
19	A	821	CLA	1	0
23	B2	839	BCR	1	0
19	B1	835	CLA	1	0
19	A1	806	CLA	4	0
19	A	837	CLA	2	0
19	A	841	CLA	1	0
19	A2	815	CLA	4	0
19	B1	831	CLA	3	0
19	BB	836	CLA	1	0
19	A	833	CLA	2	0
19	J1	103	CLA	1	0
19	L1	207	CLA	1	0
19	B	859	CLA	3	0
19	A1	814	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	828	CLA	1	0
19	A2	841	CLA	1	0
28	BB	854	DGD	1	0
19	K1	103	CLA	1	0
19	A2	825	CLA	1	0
19	A1	831	CLA	2	0
19	BB	852	CLA	6	0
19	F	302	CLA	1	0
23	B2	843	BCR	3	0
19	A1	807	CLA	1	0
23	F2	303	BCR	2	0
19	B2	821	CLA	3	0
19	BB	832	CLA	7	0
19	X2	101	CLA	1	0
19	AA	807	CLA	3	0
19	AA	843	CLA	1	0
23	B1	841	BCR	2	0
19	A	804	CLA	3	0
19	AA	805	CLA	2	0
23	A1	851	BCR	3	0
23	I2	103	BCR	1	0
20	A2	803	CL0	5	0
19	B	810	CLA	2	0
19	AA	836	CLA	1	0
19	AA	853	CLA	6	0
19	BB	823	CLA	2	0
19	A	836	CLA	1	0
19	BB	835	CLA	2	0
19	BB	821	CLA	2	0
19	A2	852	CLA	9	0
19	AA	830	CLA	5	0
19	B2	835	CLA	3	0
19	B1	849	CLA	1	0
19	A1	835	CLA	1	0
23	J2	102	BCR	1	0
19	A2	804	CLA	3	0
19	A2	844	CLA	1	0
23	A2	847	BCR	1	0
19	B1	820	CLA	1	0
19	B	828	CLA	3	0
19	B2	846	CLA	1	0
19	B1	834	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B1	810	CLA	3	0
23	FF	306	BCR	4	0
19	B1	804	CLA	2	0
19	B	829	CLA	3	0
23	MM	101	BCR	1	0
19	A1	815	CLA	2	0
23	AA	852	BCR	4	0
19	B2	813	CLA	1	0
19	A2	834	CLA	1	0
23	JJ	102	BCR	1	0
22	L2	208	LHG	2	0
19	BB	815	CLA	2	0
19	A	834	CLA	1	0
19	AA	821	CLA	3	0
19	A1	852	CLA	11	0
19	A1	841	CLA	3	0
19	B	836	CLA	2	0
19	A1	844	CLA	1	0
26	B	841	ECH	1	0
23	AA	851	BCR	1	0
19	AA	832	CLA	1	0
19	B1	850	CLA	2	0
19	B1	808	CLA	1	0
19	B2	849	CLA	5	0
19	A	832	CLA	3	0
19	B	811	CLA	2	0
19	A1	826	CLA	1	0
22	B	852	LHG	1	0
19	B1	822	CLA	1	0
19	A1	820	CLA	3	0
23	A2	850	BCR	1	0
23	A1	850	BCR	1	0
19	J2	103	CLA	2	0
23	FF	303	BCR	3	0
19	B2	834	CLA	4	0
21	AA	844	PQN	3	0
19	A1	834	CLA	2	0
19	A	812	CLA	1	0
19	BB	829	CLA	4	0
23	B	844	BCR	1	0
19	B2	828	CLA	1	0
19	AA	815	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	818	CLA	3	0
19	A	826	CLA	2	0
19	A	820	CLA	2	0
23	F2	305	BCR	5	0
19	A	840	CLA	1	0
19	A2	812	CLA	1	0
19	B2	826	CLA	2	0
23	AA	855	BCR	1	0
19	F2	301	CLA	3	0
19	A	818	CLA	1	0
23	A	854	BCR	2	0
19	B	804	CLA	2	0
19	B	833	CLA	7	0
22	AA	846	LHG	2	0
19	B1	823	CLA	1	0
19	B	809	CLA	1	0
19	B2	850	CLA	3	0
22	A	846	LHG	1	0
21	A	843	PQN	3	0
19	K2	104	CLA	1	0
19	A2	820	CLA	1	0
27	C1	102	SF4	1	0
19	A1	801	CLA	1	0
19	FF	305	CLA	3	0
19	BB	810	CLA	4	0
23	K2	105	BCR	2	0
19	B	815	CLA	1	0
19	B	827	CLA	1	0
19	A2	829	CLA	1	0
19	A	831	CLA	1	0
25	I2	105	LMG	1	0
19	A1	812	CLA	1	0
19	BB	806	CLA	2	0
19	A1	816	CLA	1	0
23	BB	838	BCR	2	0
23	F	305	BCR	6	0
19	A1	803	CLA	3	0
23	B	843	BCR	4	0
19	AA	828	CLA	3	0
19	BB	822	CLA	2	0
19	B2	802	CLA	1	0
19	B2	837	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	BB	828	CLA	3	0
19	BB	801	CLA	1	0
19	B2	833	CLA	3	0
22	A2	845	LHG	1	0
19	B	806	CLA	3	0
19	JJ	103	CLA	1	0
19	A2	805	CLA	3	0
20	A1	802	CL0	3	0
19	BB	831	CLA	1	0
23	J2	104	BCR	2	0
19	FF	301	CLA	3	0
19	B2	831	CLA	1	0
19	B1	829	CLA	2	0
19	A1	817	CLA	2	0
21	BB	837	PQN	2	0
19	AA	806	CLA	2	0
19	B	823	CLA	1	0
19	B	801	CLA	1	0
19	A	809	CLA	1	0
19	B	831	CLA	1	0
19	AA	822	CLA	2	0
23	J	104	BCR	1	0
19	B2	804	CLA	1	0
23	L	205	BCR	1	0
19	AA	801	CLA	1	0
19	A1	842	CLA	1	0
20	A	803	CL0	1	0
23	BB	842	BCR	2	0
19	BB	811	CLA	1	0
19	AA	816	CLA	1	0
19	A1	836	CLA	1	0
26	BB	840	ECH	1	0
19	A	816	CLA	1	0
19	B2	851	CLA	2	0
19	A	805	CLA	3	0
19	A1	805	CLA	2	0
19	A	810	CLA	1	0
19	A	852	CLA	11	0
19	BB	817	CLA	1	0
19	BB	833	CLA	14	0
19	AA	831	CLA	1	0
19	F2	302	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B2	810	CLA	3	0
19	B	822	CLA	2	0
23	A	847	BCR	1	0
19	F1	305	CLA	2	0
19	B2	852	CLA	2	0
23	B1	839	BCR	1	0
23	A1	847	BCR	2	0
19	L	202	CLA	4	0
23	BB	841	BCR	6	0
19	B2	832	CLA	3	0
19	B1	827	CLA	2	0
19	A2	821	CLA	4	0
19	B	858	CLA	3	0
19	A2	836	CLA	1	0
19	A2	832	CLA	2	0
23	K1	104	BCR	1	0
19	B1	814	CLA	1	0
19	B2	816	CLA	1	0
19	A	815	CLA	3	0
19	F1	301	CLA	3	0
19	B	824	CLA	1	0
22	A1	846	LHG	1	0
19	B	826	CLA	2	0
21	B	838	PQN	2	0
19	A2	830	CLA	2	0
23	F1	303	BCR	2	0
19	A1	804	CLA	2	0
19	B1	832	CLA	5	0
23	I1	101	BCR	1	0
19	B1	821	CLA	1	0
19	A1	822	CLA	1	0
19	LL	201	CLA	5	0
25	M	102	LMG	1	0
26	B1	840	ECH	1	0
19	A	807	CLA	3	0
19	BB	805	CLA	1	0
19	B	854	CLA	6	0
25	L1	210	LMG	1	0
19	B1	830	CLA	1	0
23	A2	851	BCR	5	0
23	K1	106	BCR	2	0
19	B2	820	CLA	1	0

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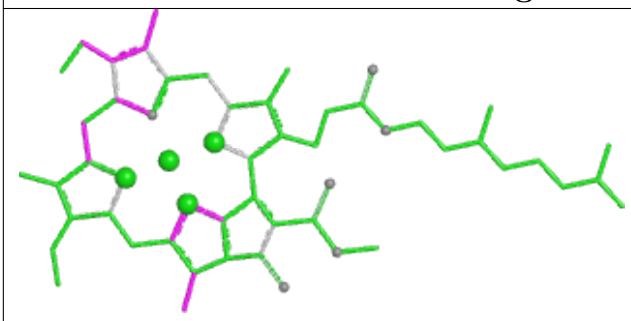
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	BB	804	CLA	2	0
19	J	103	CLA	4	0
19	L1	205	CLA	3	0
19	AA	810	CLA	1	0
19	A	830	CLA	4	0
19	A2	826	CLA	1	0
19	A1	839	CLA	2	0
19	A2	842	CLA	4	0
19	A2	813	CLA	1	0
19	B2	829	CLA	3	0
19	AA	833	CLA	1	0
19	B2	830	CLA	3	0
23	B2	840	BCR	1	0
19	B1	811	CLA	2	0
22	AA	847	LHG	1	0
19	B	802	CLA	2	0
23	B1	838	BCR	1	0
23	B	839	BCR	2	0
22	L1	211	LHG	3	0
19	A1	840	CLA	1	0
26	B2	841	ECH	1	0
19	BB	856	CLA	3	0
19	FF	302	CLA	1	0
21	A2	843	PQN	1	0
19	B2	836	CLA	1	0
19	AA	825	CLA	1	0
19	A1	832	CLA	1	0
19	A1	811	CLA	2	0
19	F1	302	CLA	1	0
19	A2	833	CLA	2	0
19	A	822	CLA	3	0
19	L1	206	CLA	1	0
19	AA	804	CLA	3	0
22	A2	846	LHG	1	0

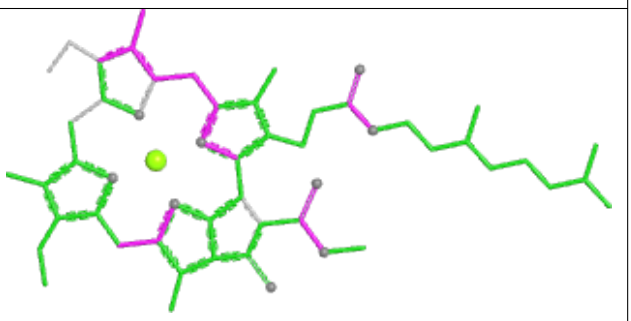
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

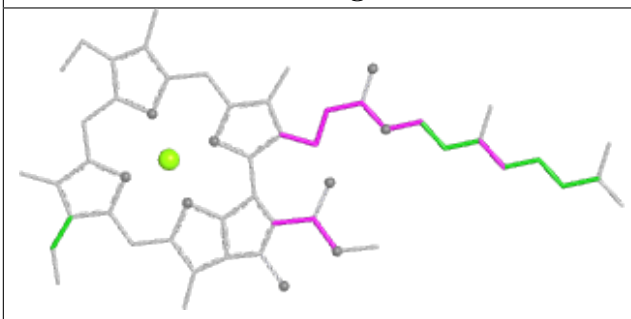
Ligand CLA B1 824



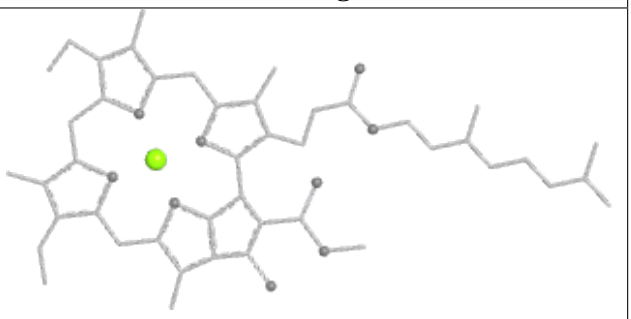
Bond lengths



Bond angles

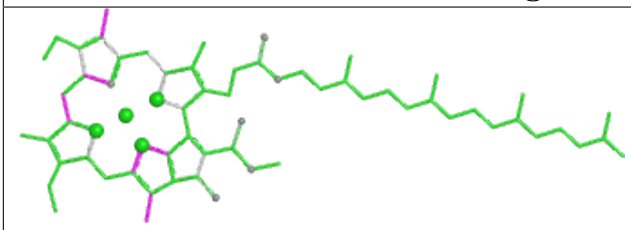


Torsions

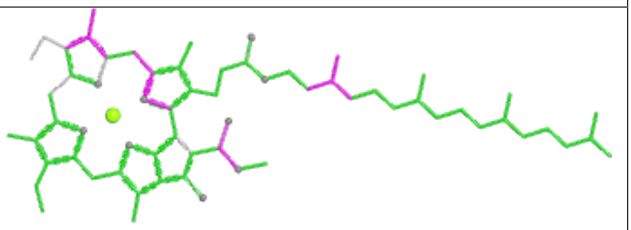


Rings

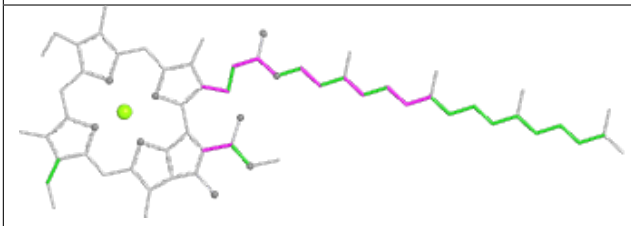
Ligand CLA B 821



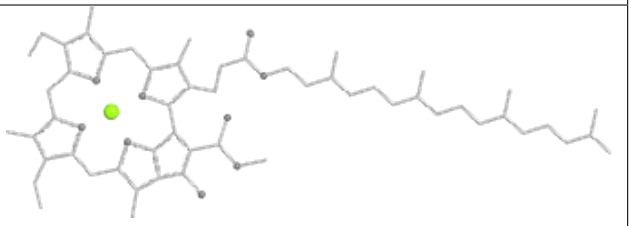
Bond lengths



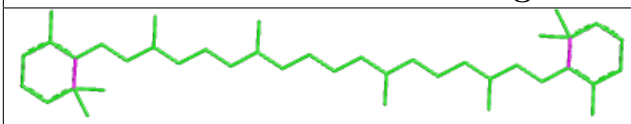
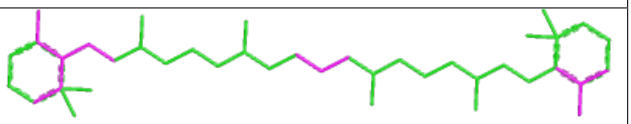
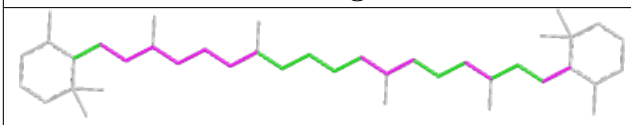
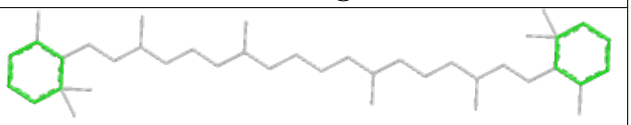
Bond angles

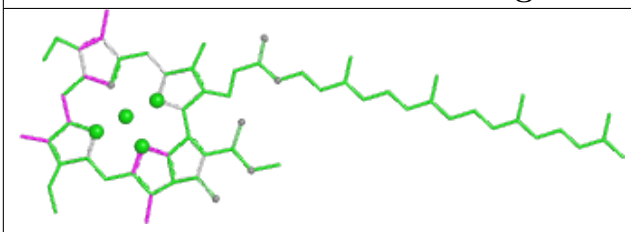
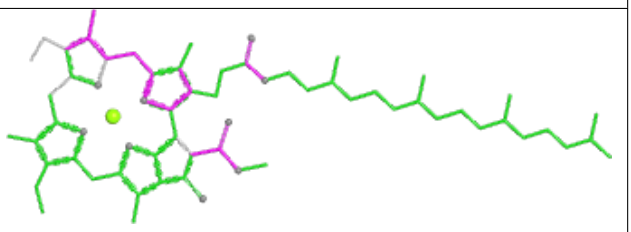
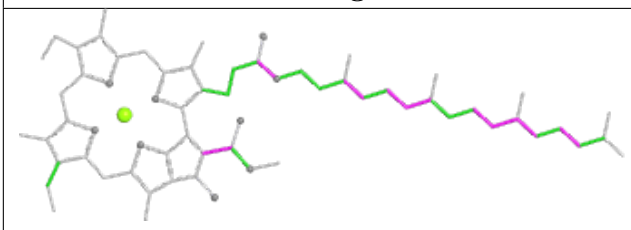
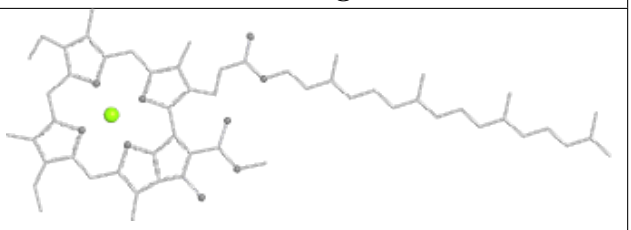


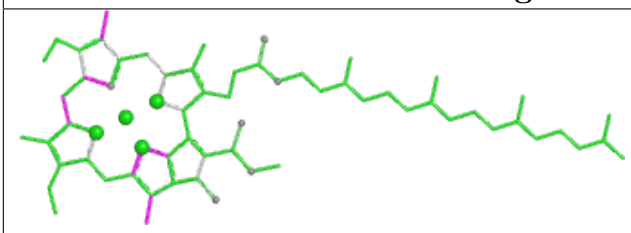
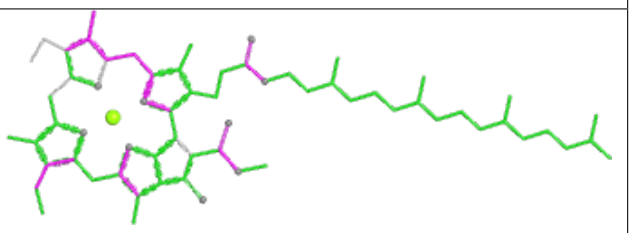
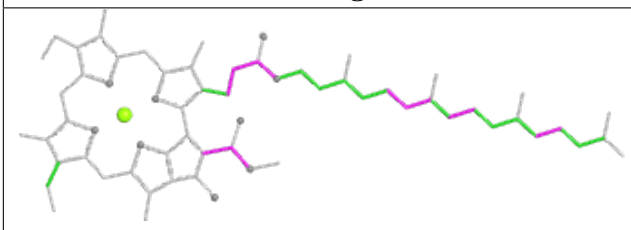
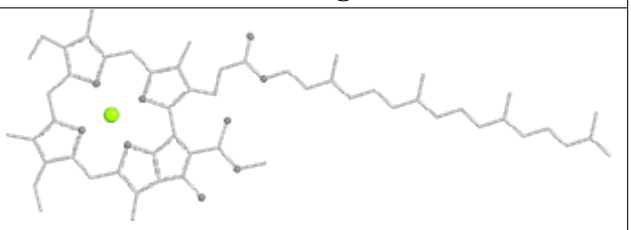
Torsions



Rings

Ligand BCR B1 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

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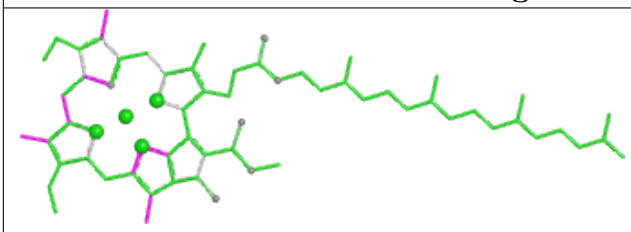
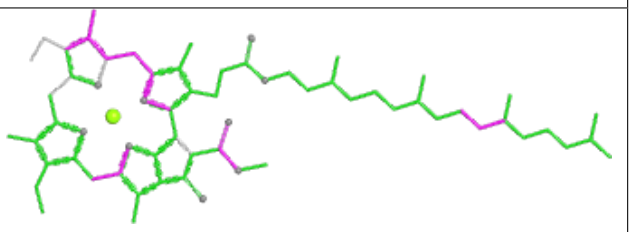
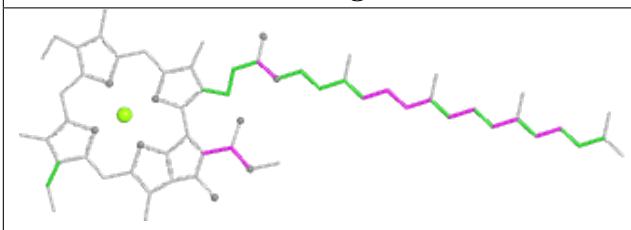
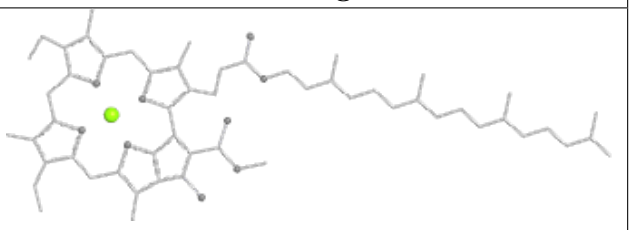
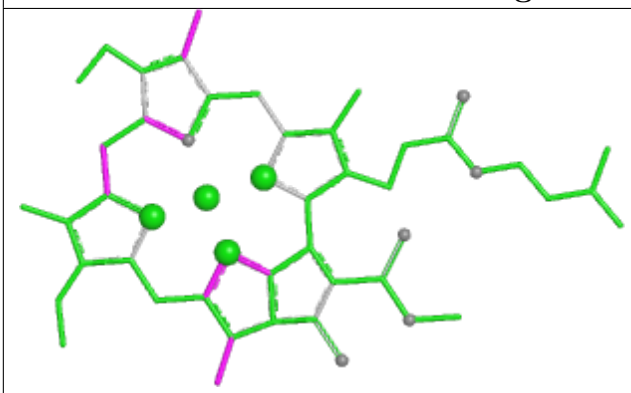
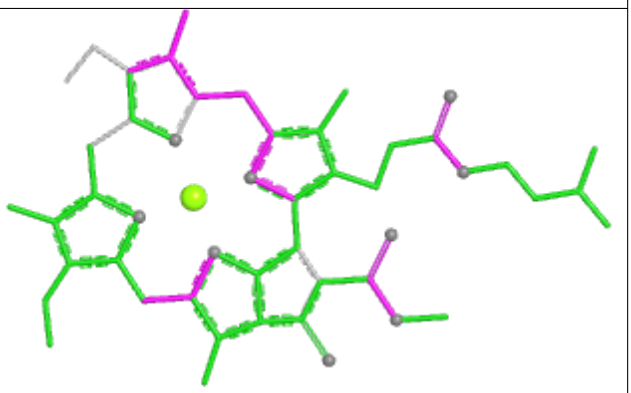
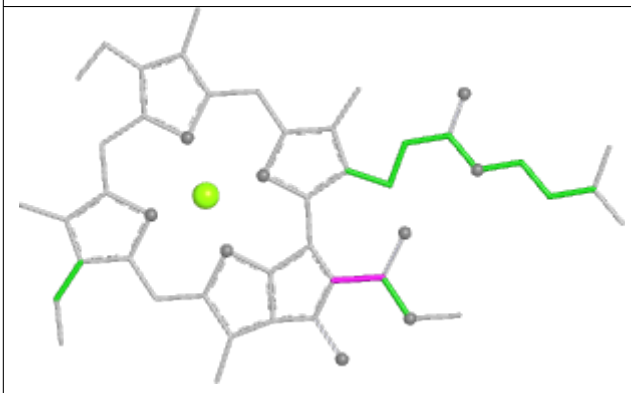
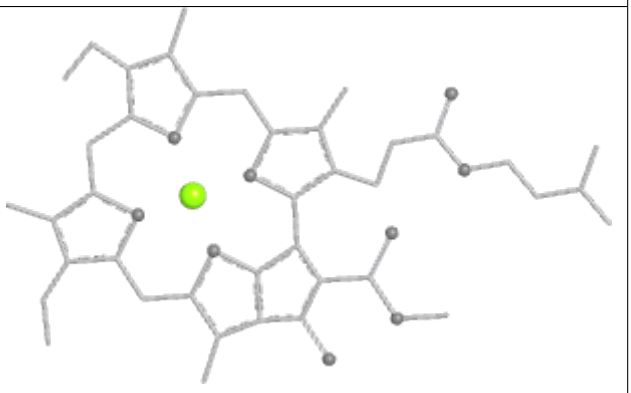
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

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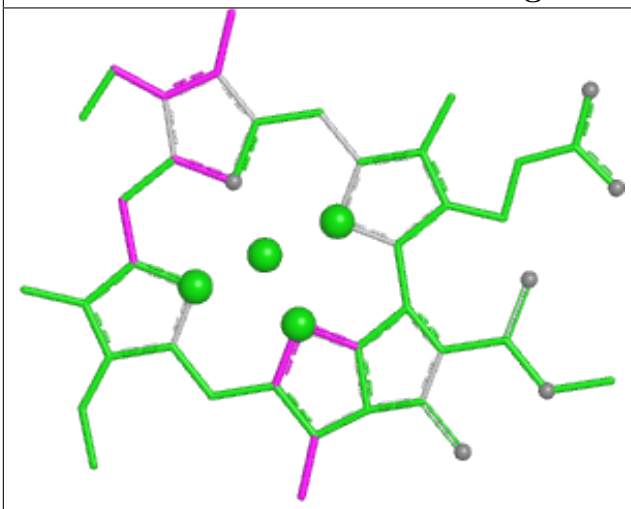
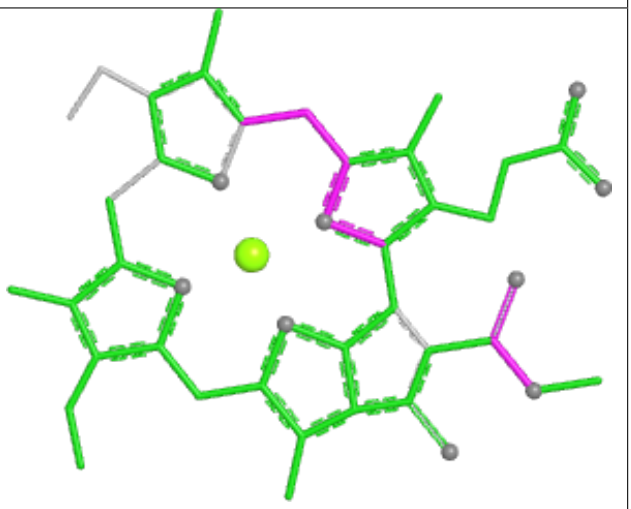
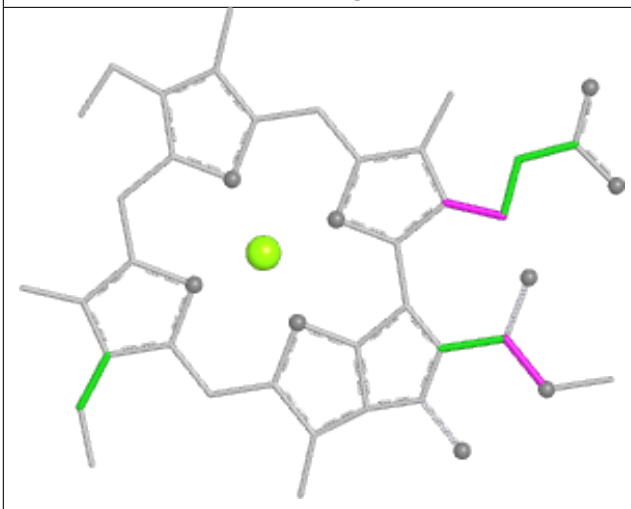
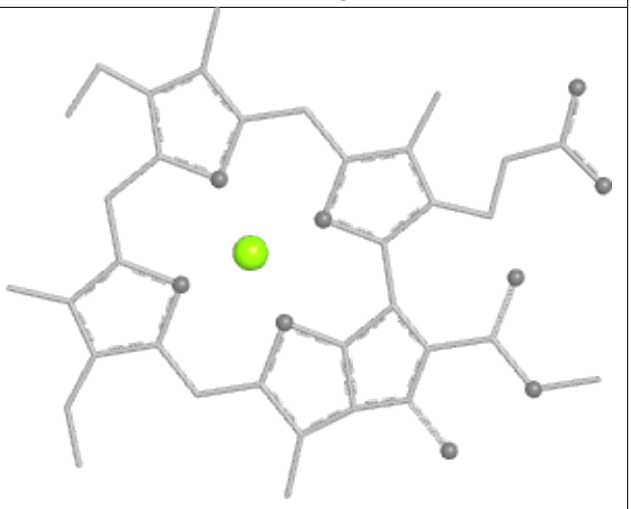
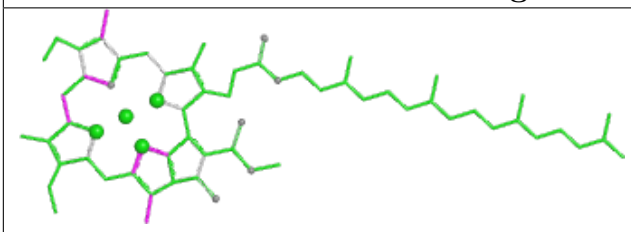
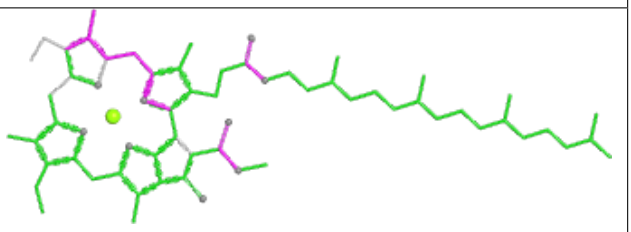
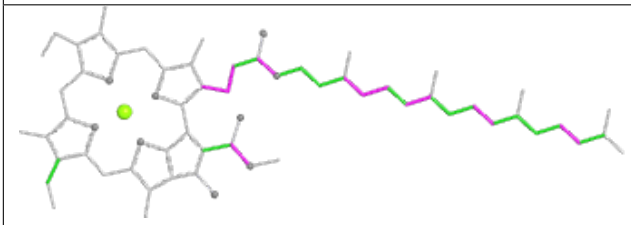
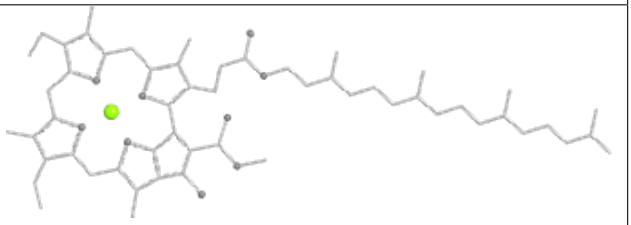
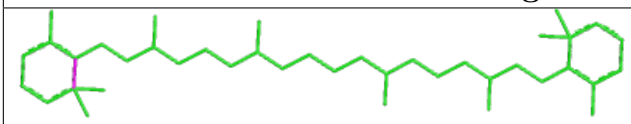
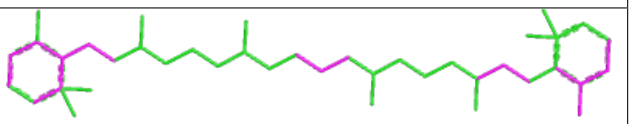
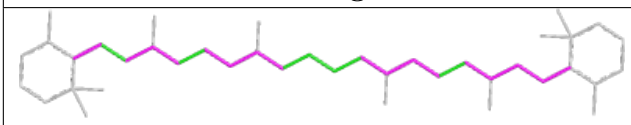
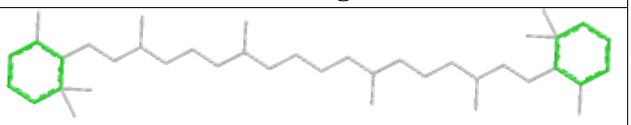
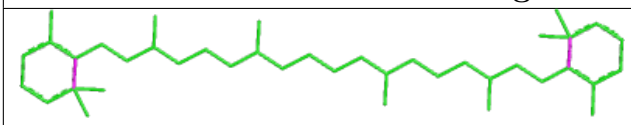
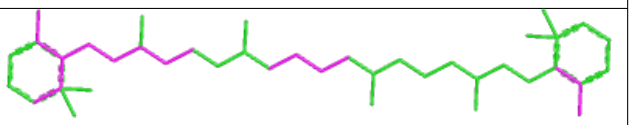
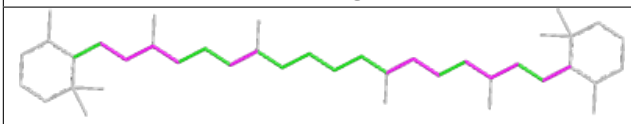
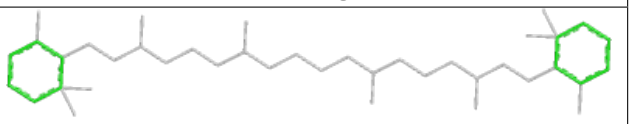
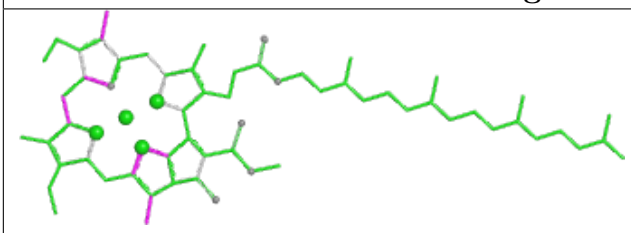
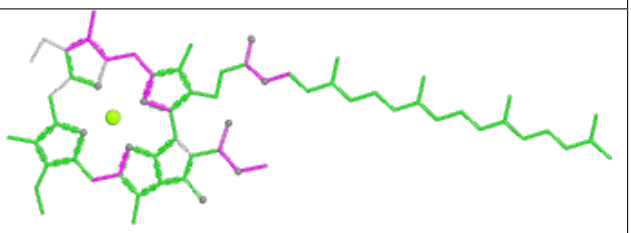
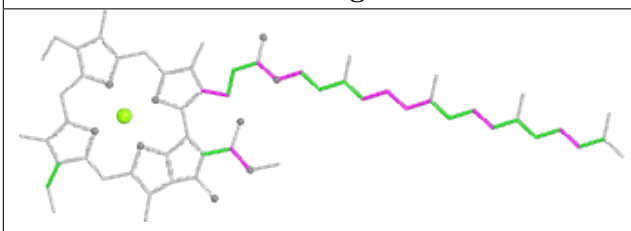
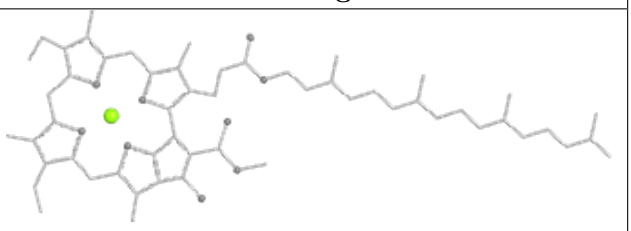
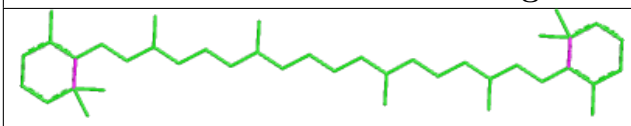
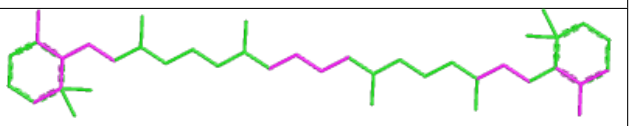
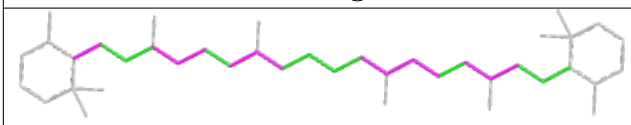
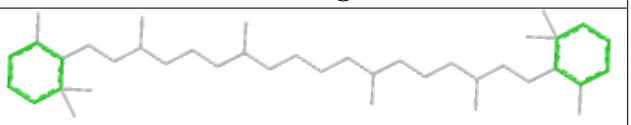
 Bond lengths	 Bond angles
 Torsions	 Rings

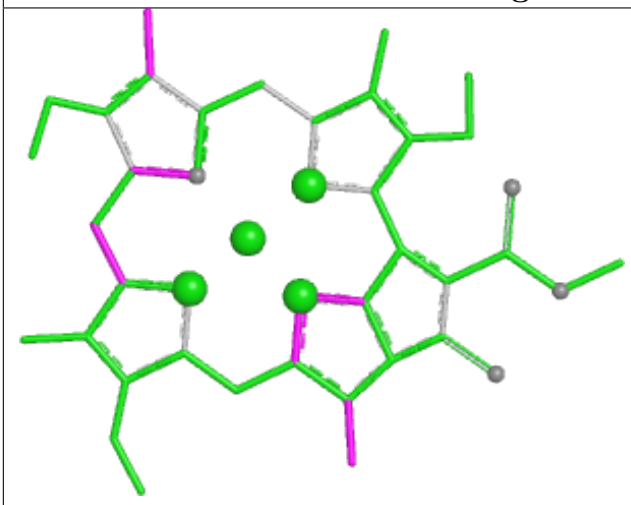
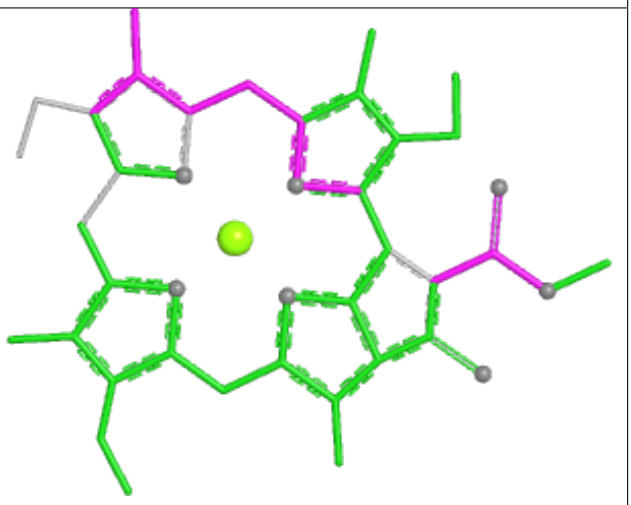
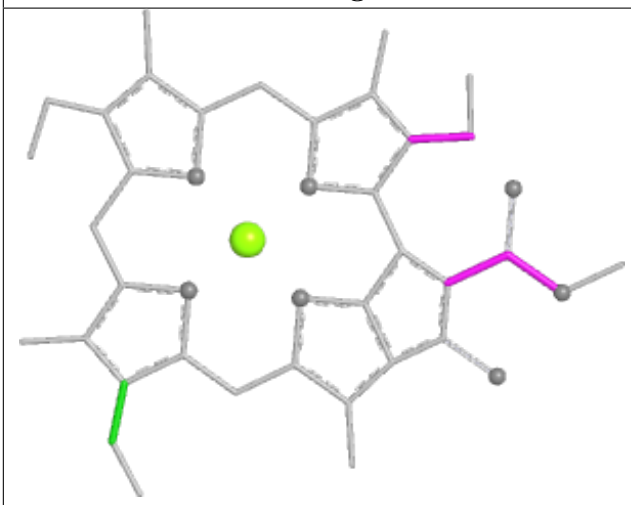
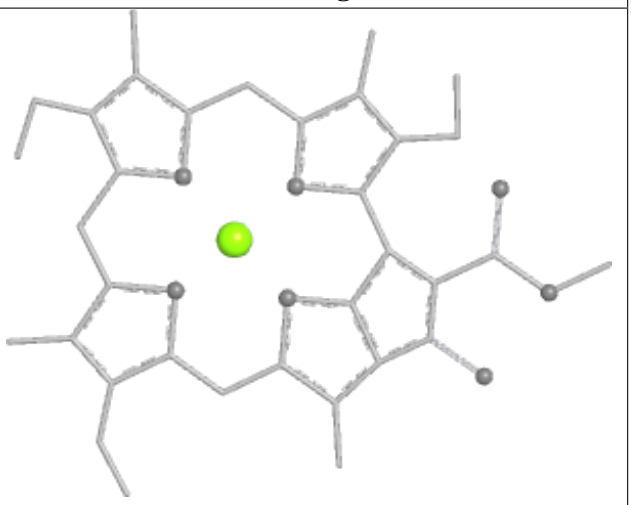
Ligand CLA AA 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

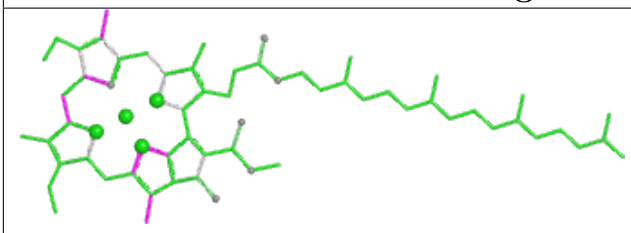
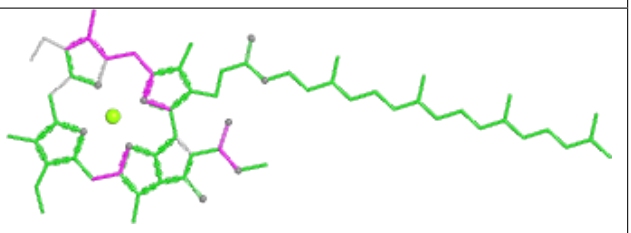
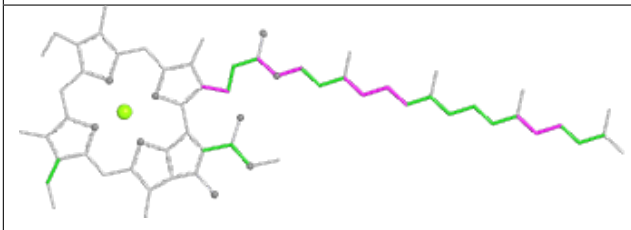
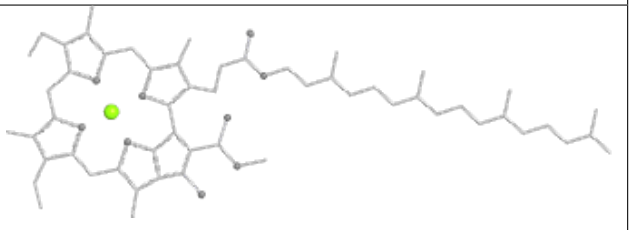
Ligand BCR A 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

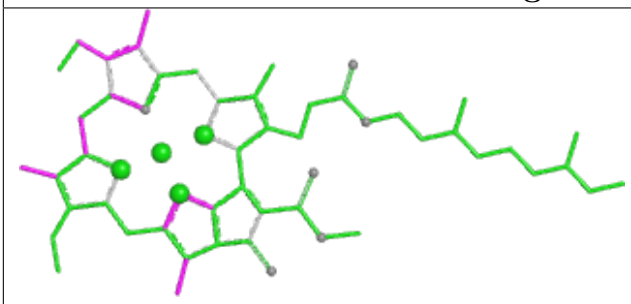
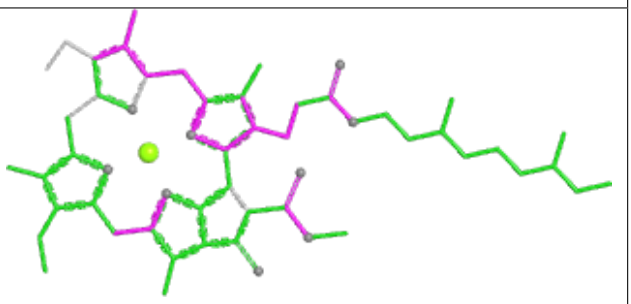
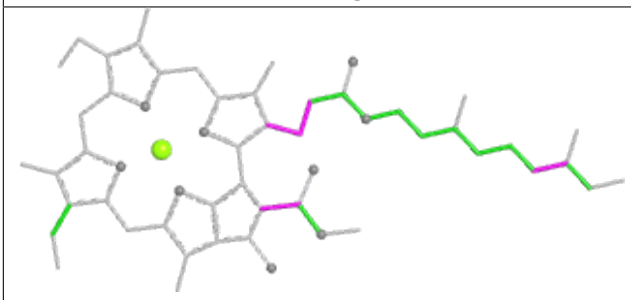
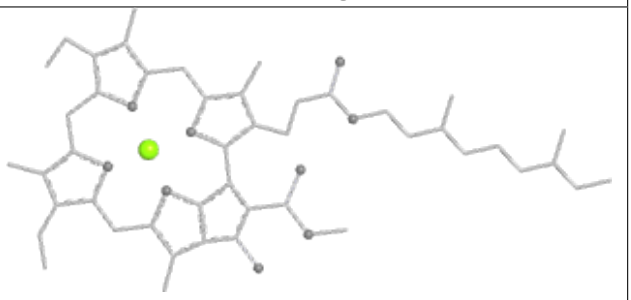
Ligand BCR A2 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

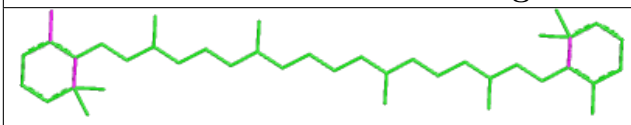
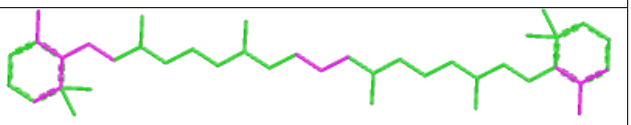
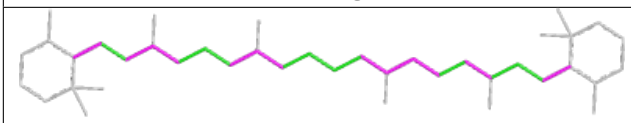
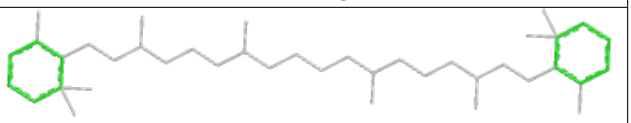
Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

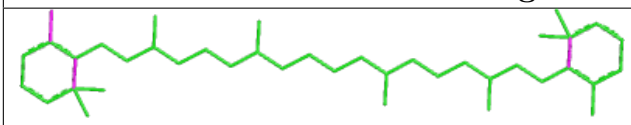
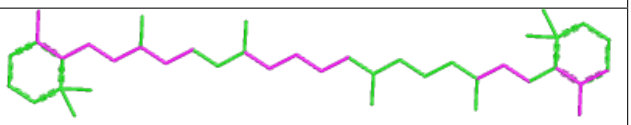
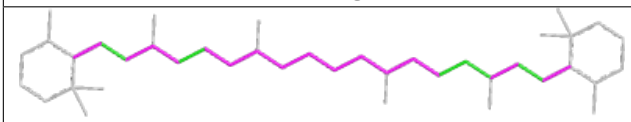
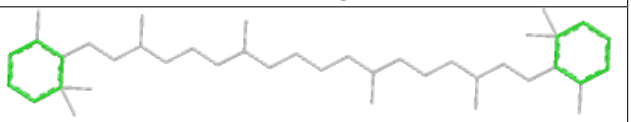
Ligand BCR II 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

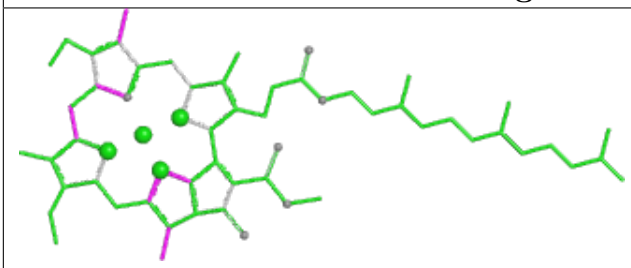
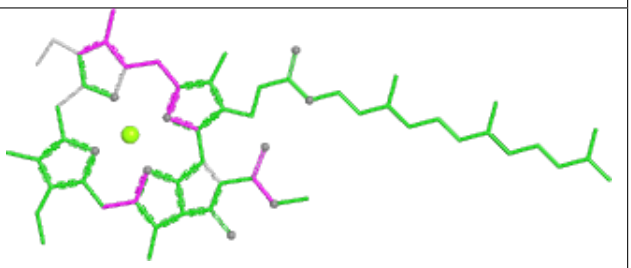
Ligand CLA BB 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B1 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K2 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 808	
	
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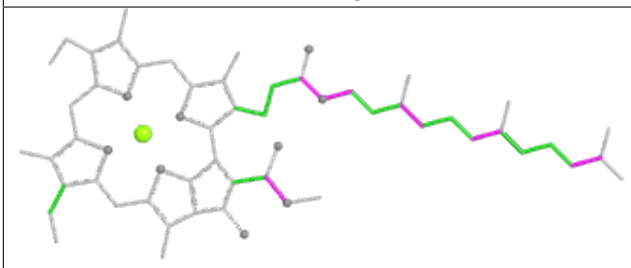
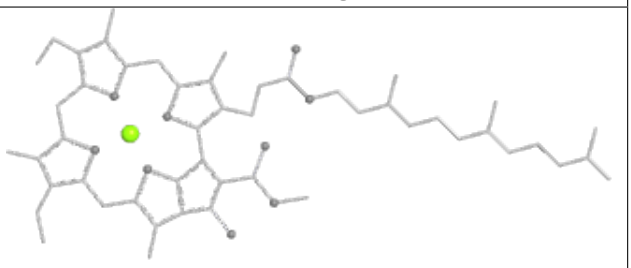
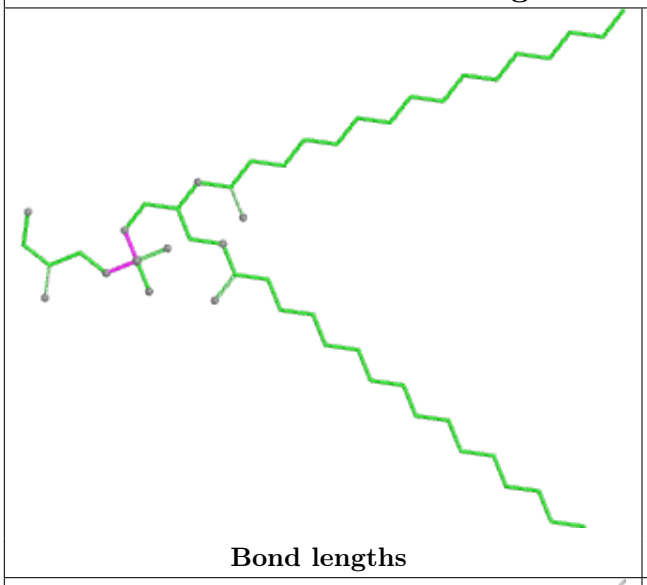
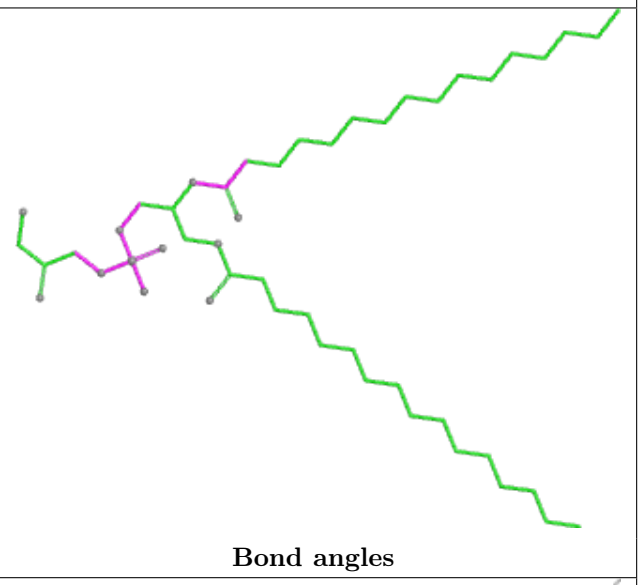
	
Torsions	**Rings**

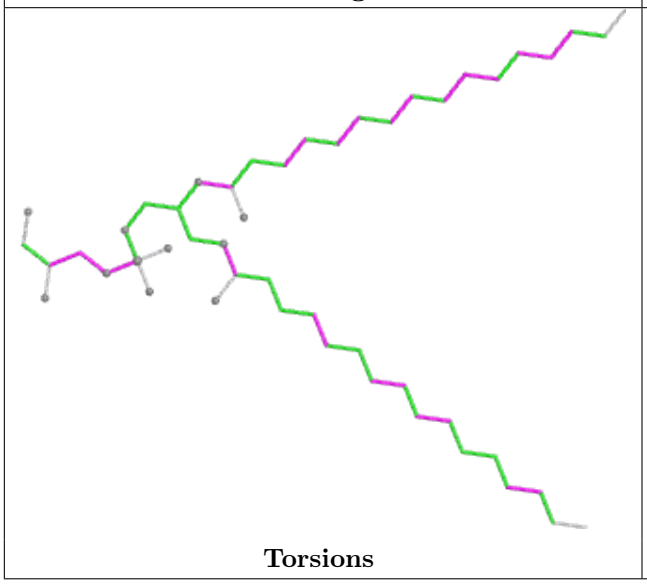
Ligand LHG BB 851



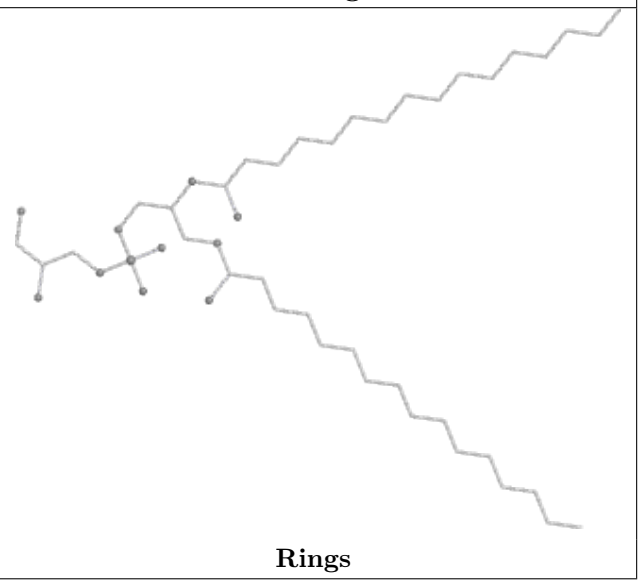
Bond lengths



Bond angles

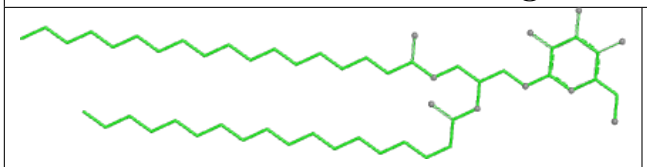


Torsions

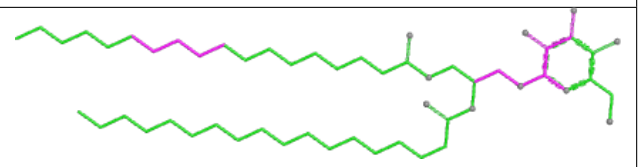


Rings

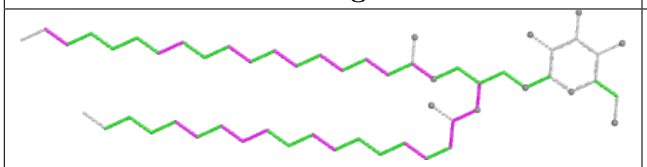
Ligand LMG B 851



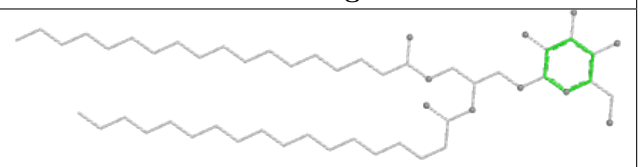
Bond lengths



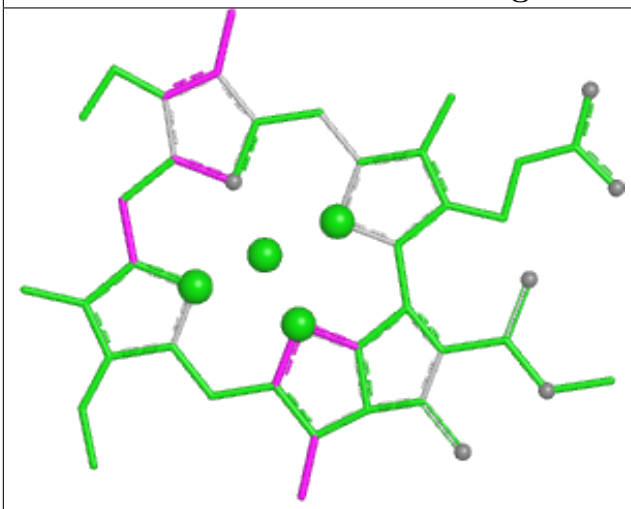
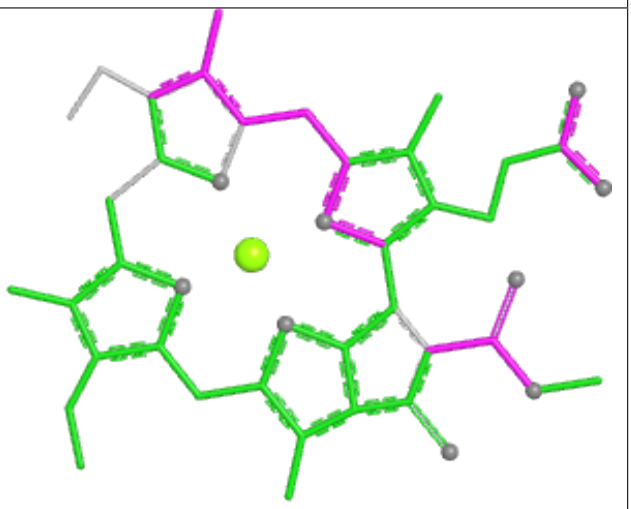
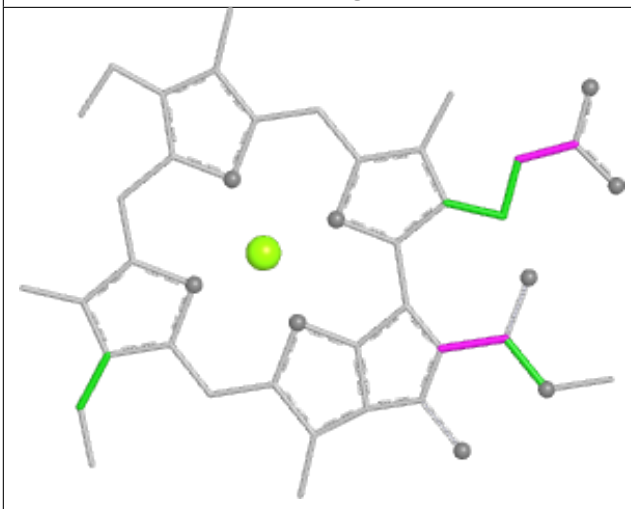
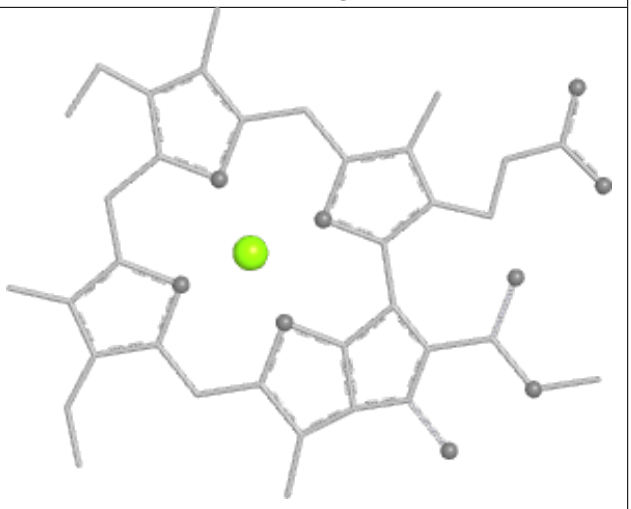
Bond angles

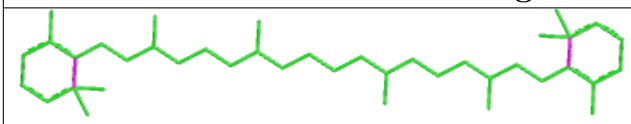
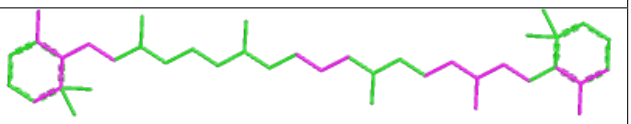
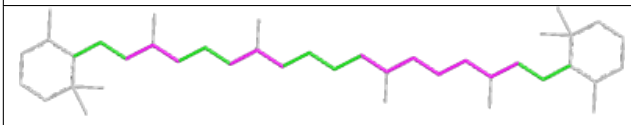
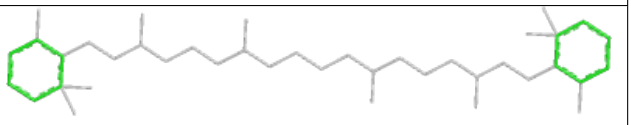


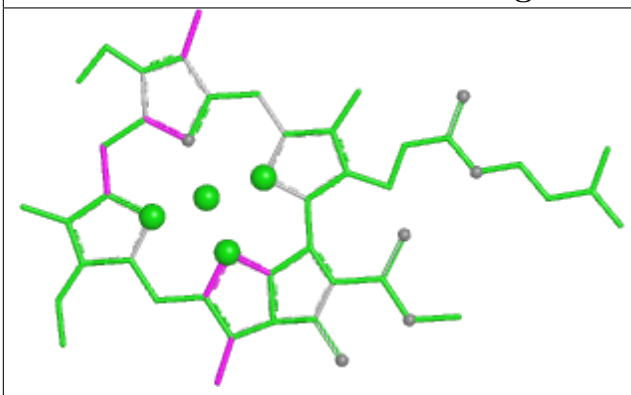
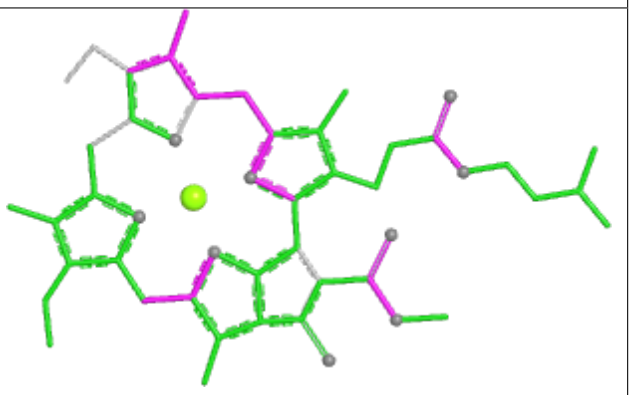
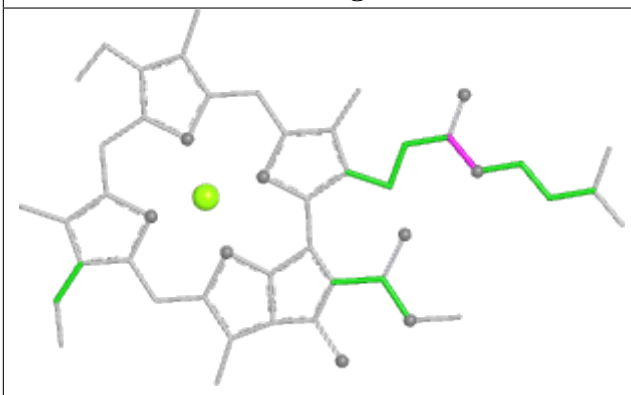
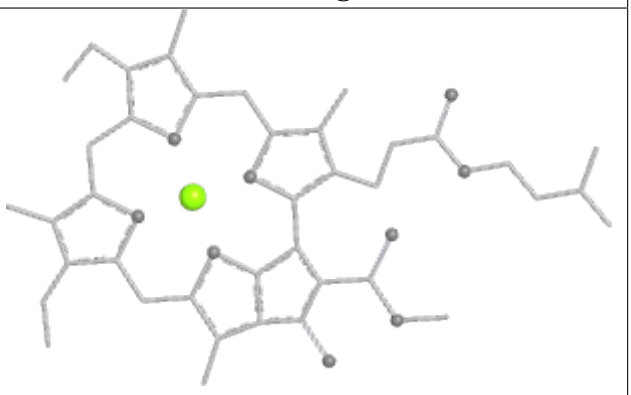
Torsions



Rings

Ligand CLA BB 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR F2 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

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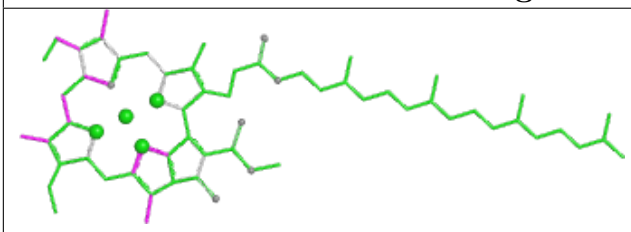
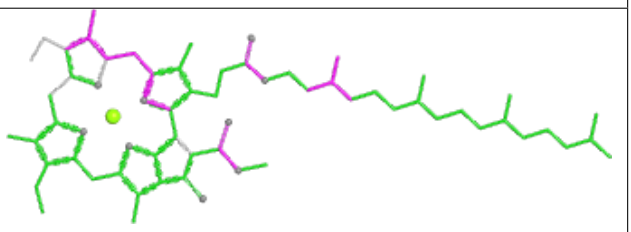
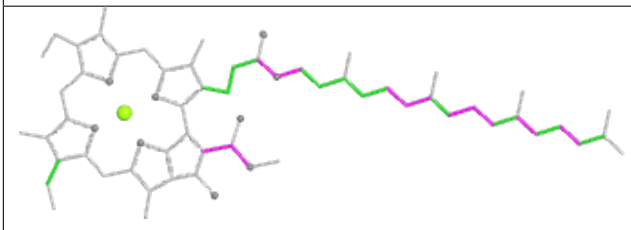
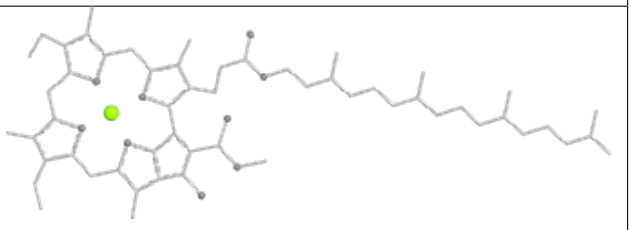
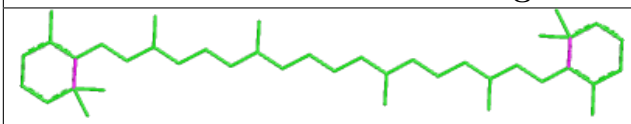
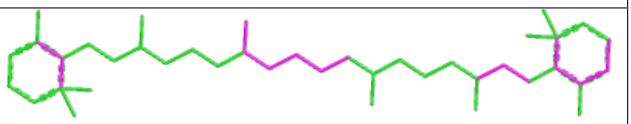
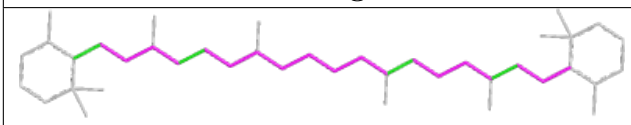
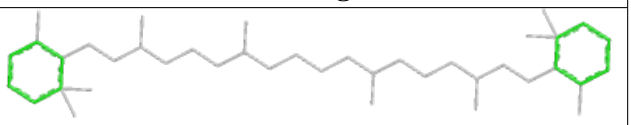
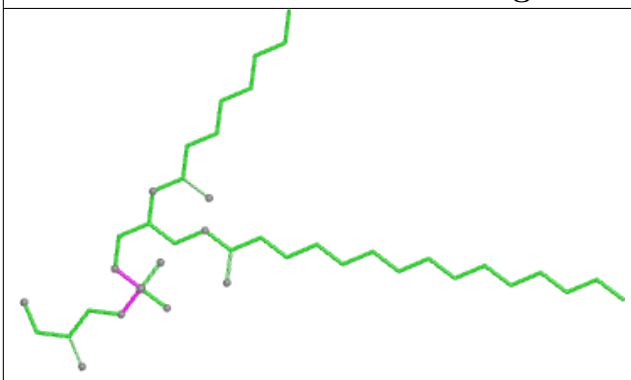
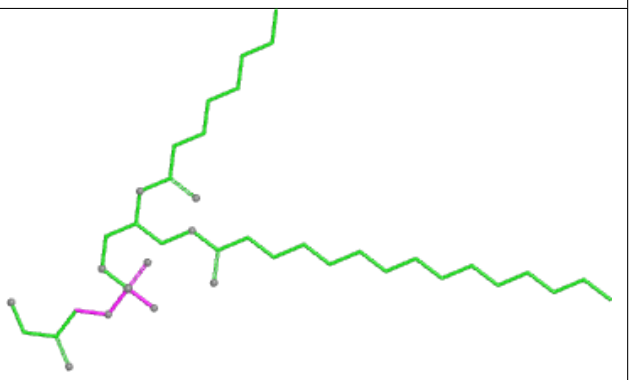
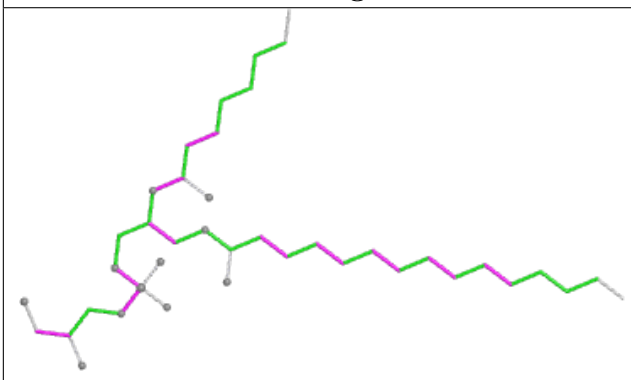
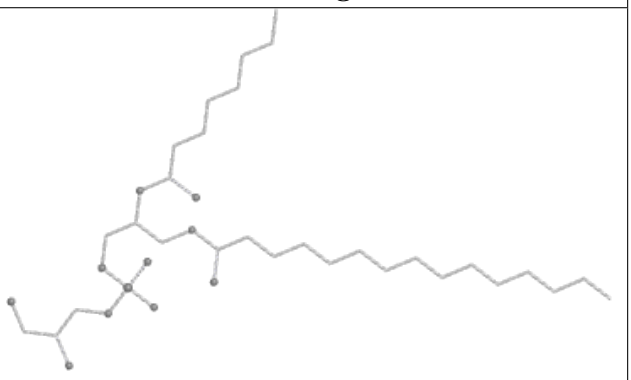
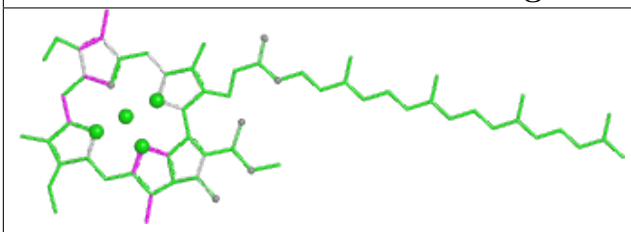
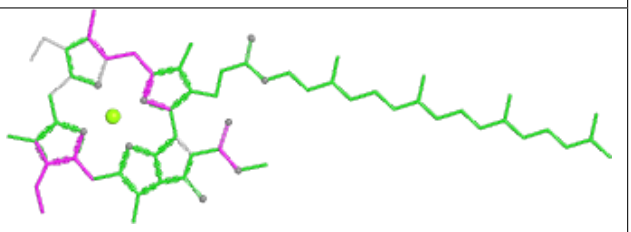
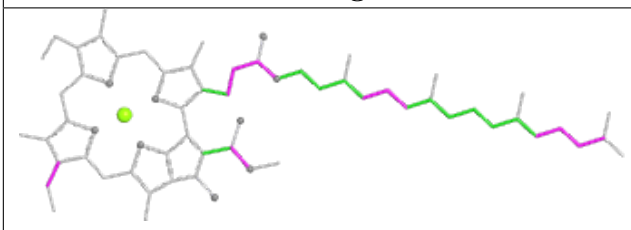
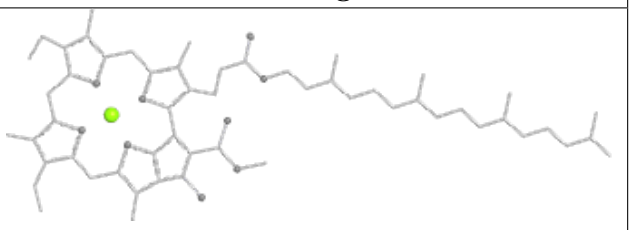
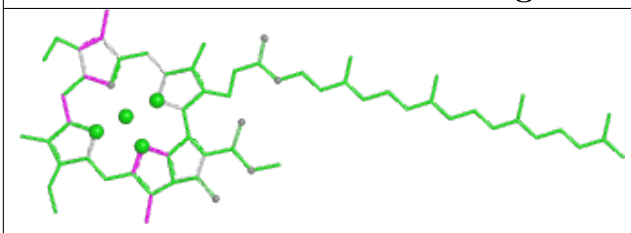
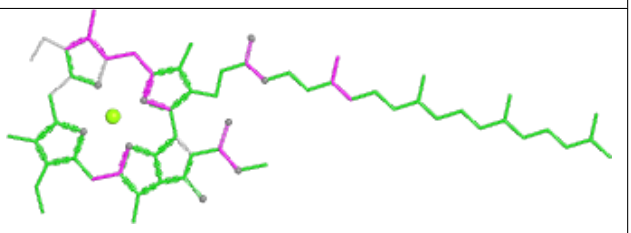
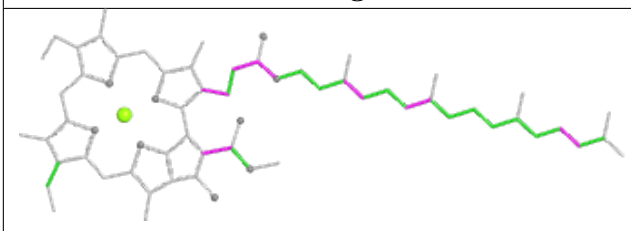
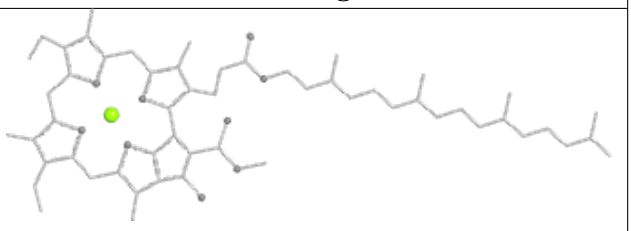
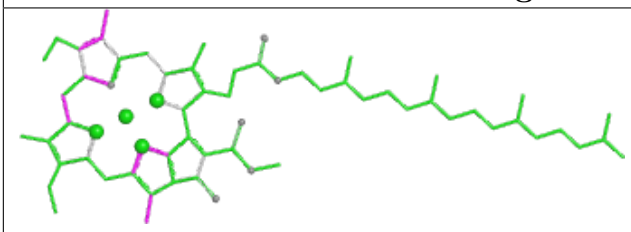
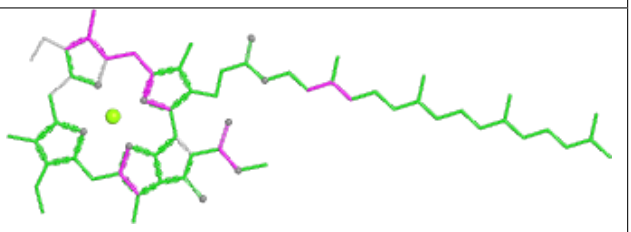
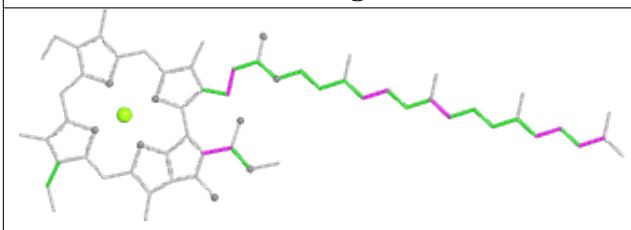
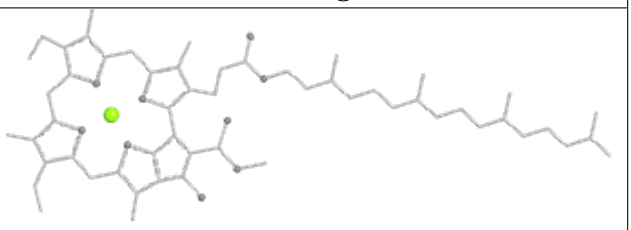
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B2 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG X1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 860	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

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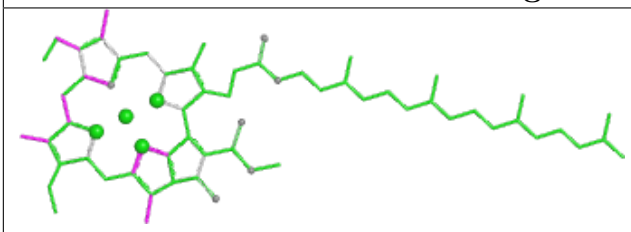
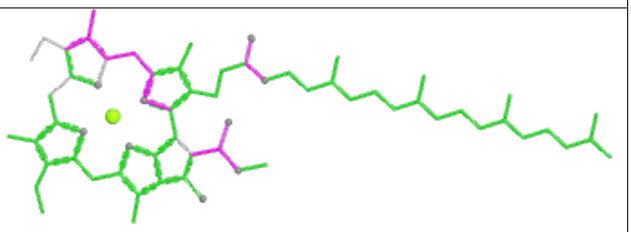
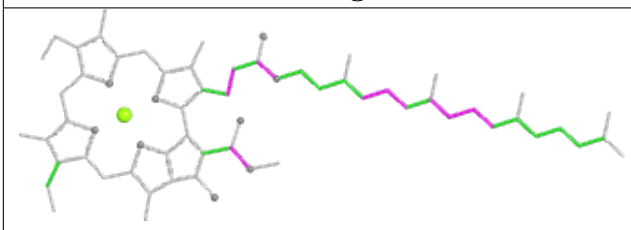
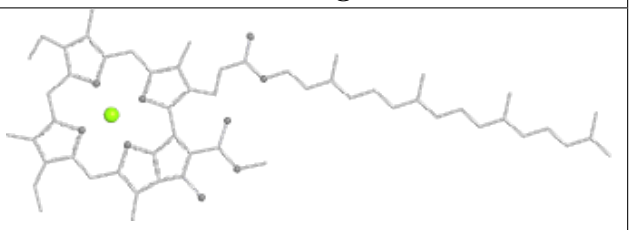
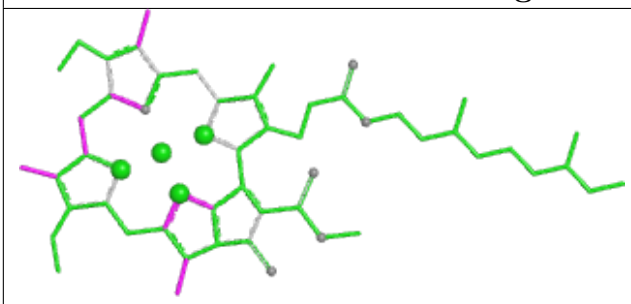
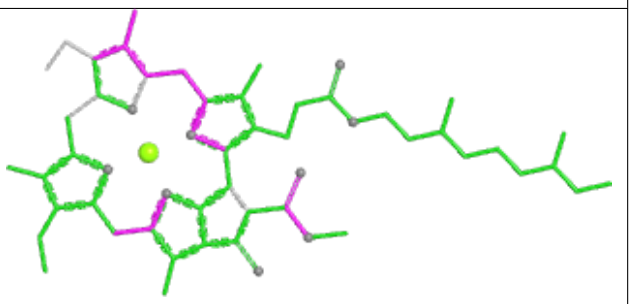
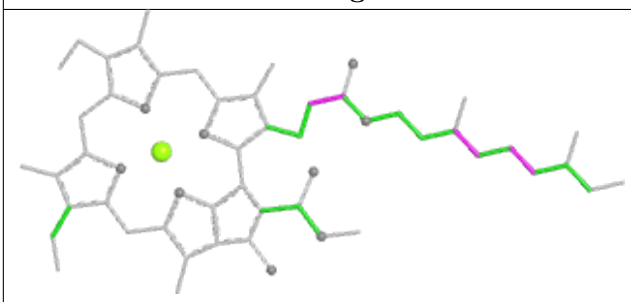
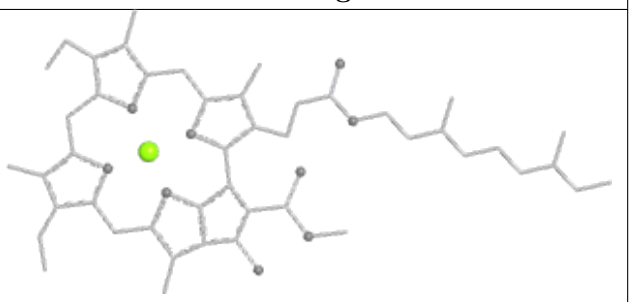
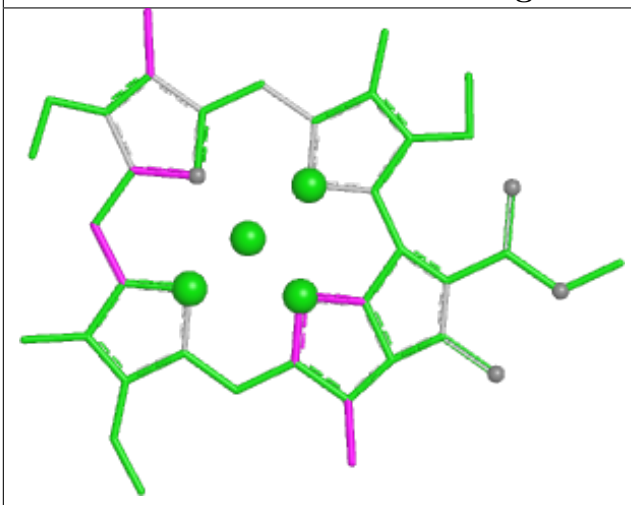
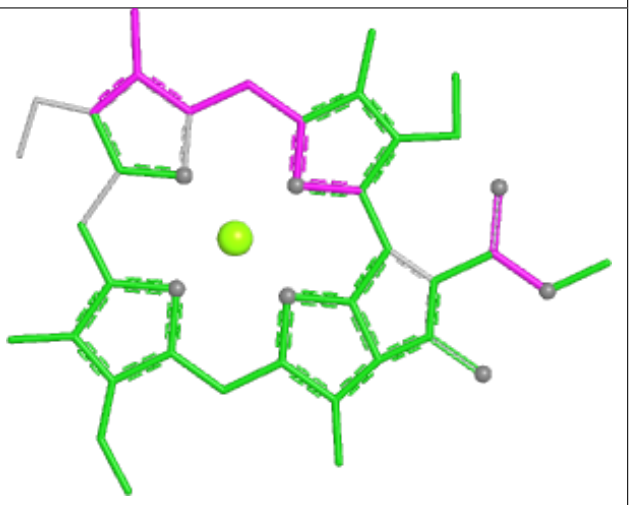
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

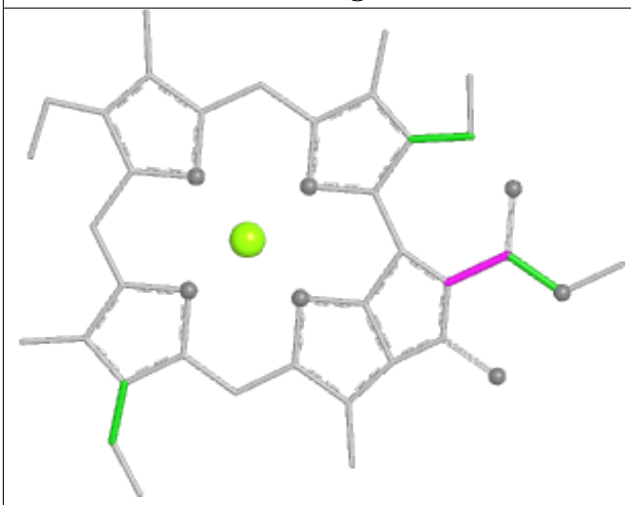
Ligand CLA B2 817



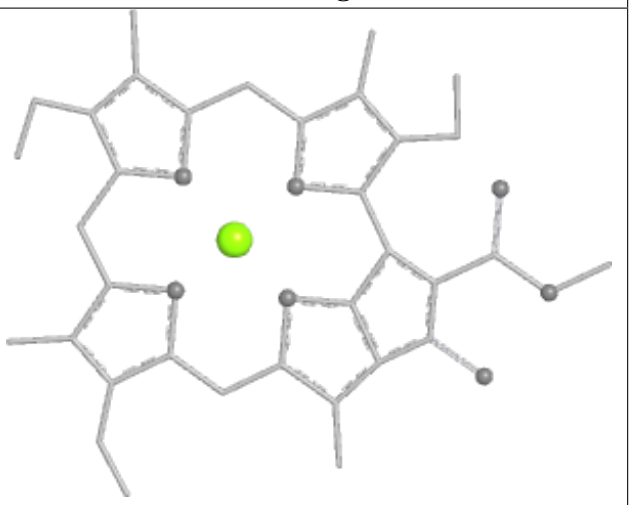
Bond lengths



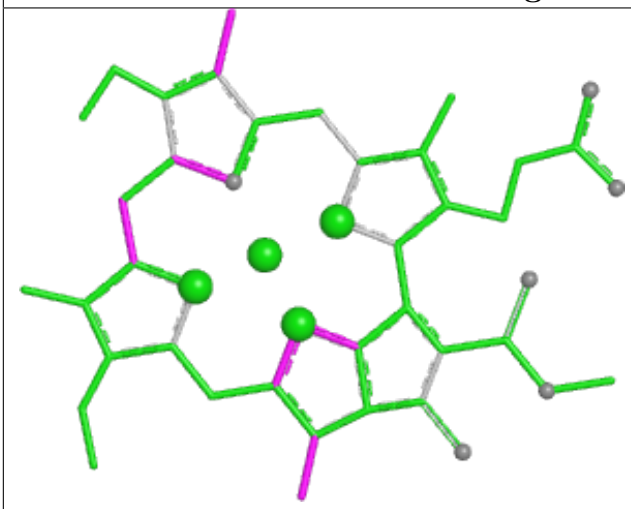
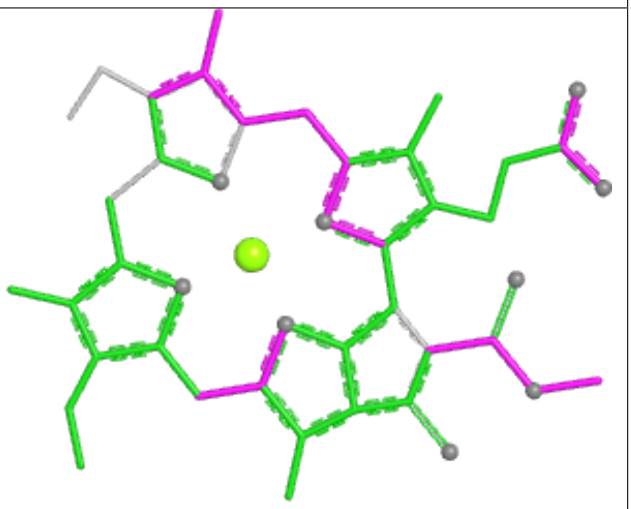
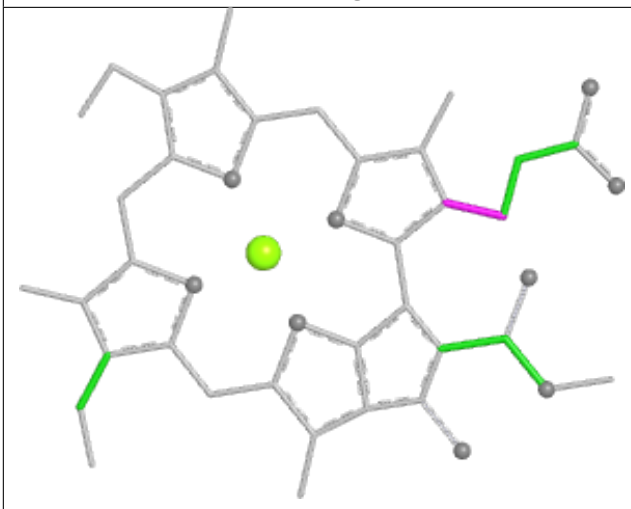
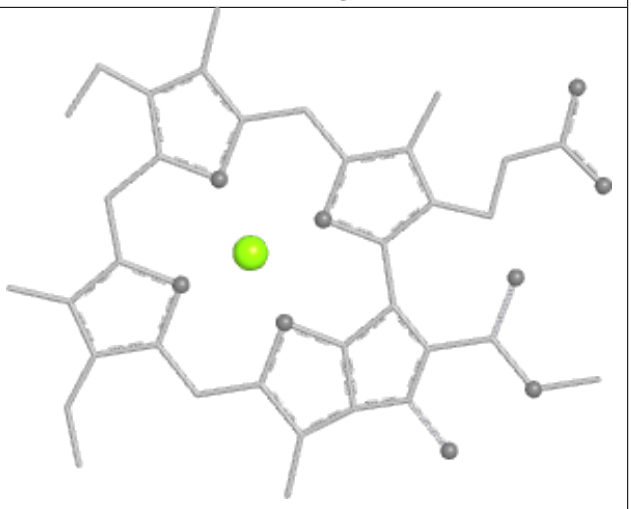
Bond angles

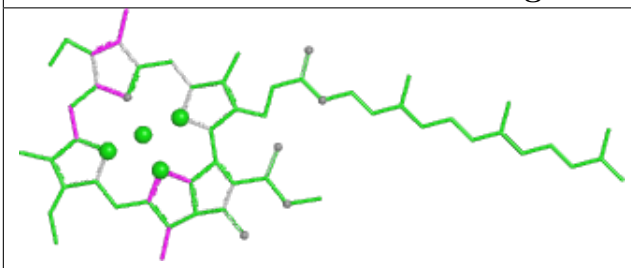
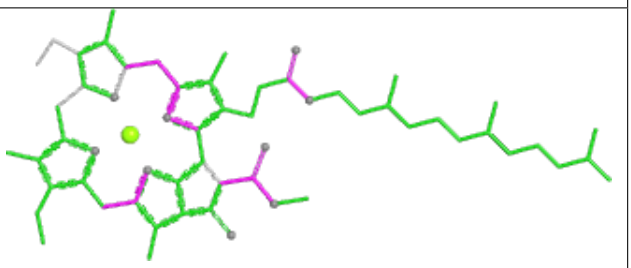
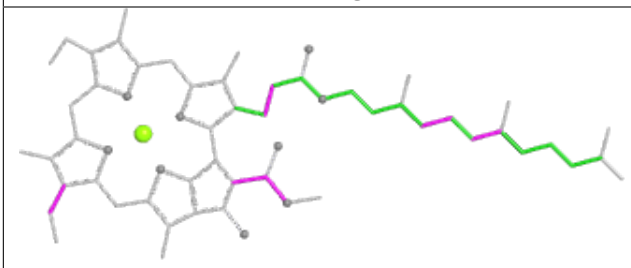
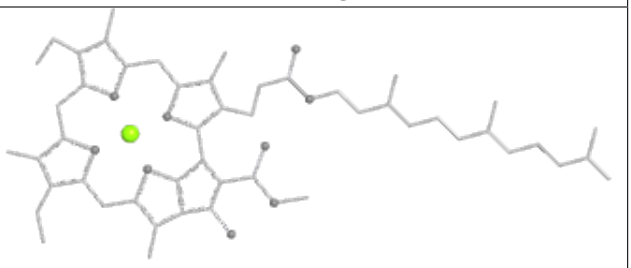


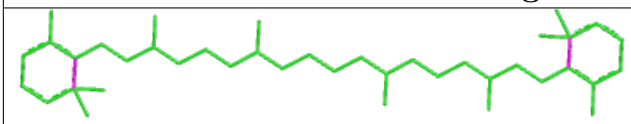
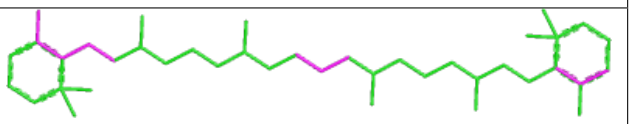
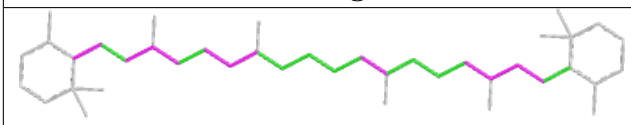
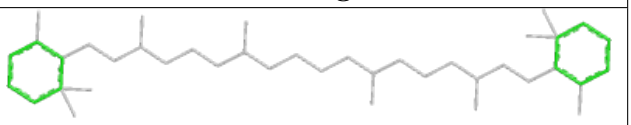
Torsions

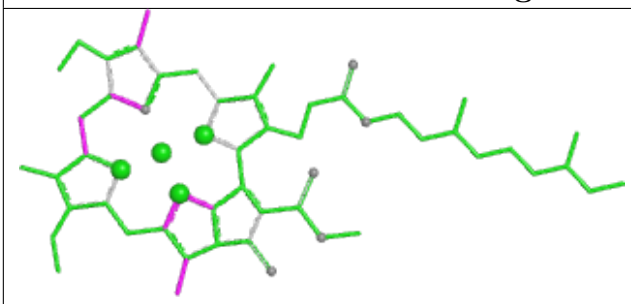
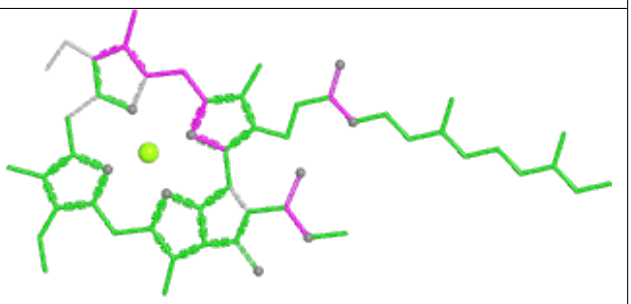
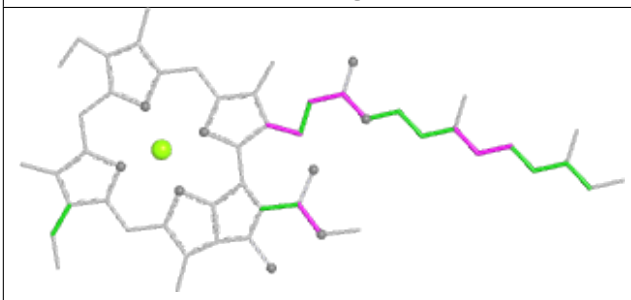
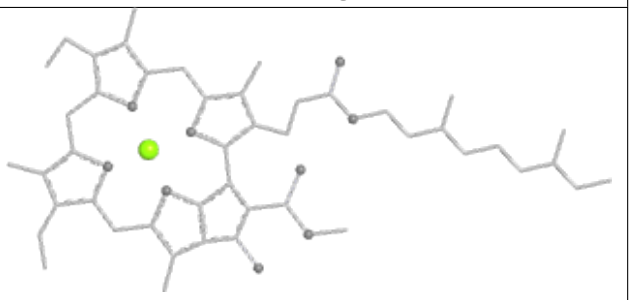


Rings

Ligand CLA B 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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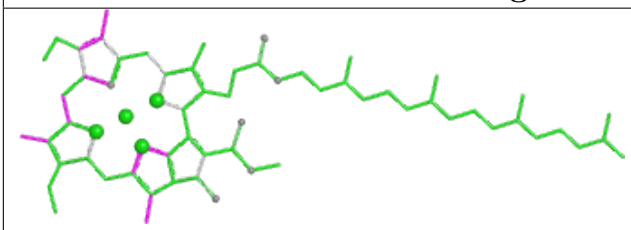
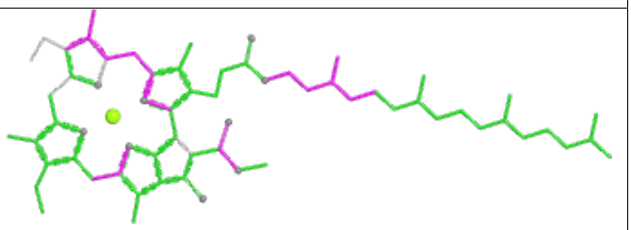
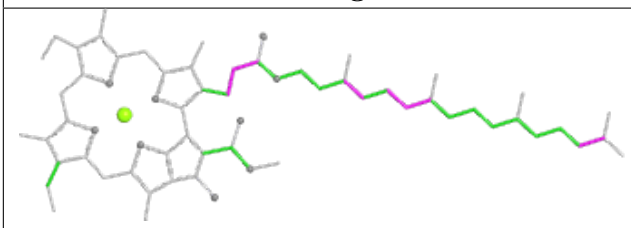
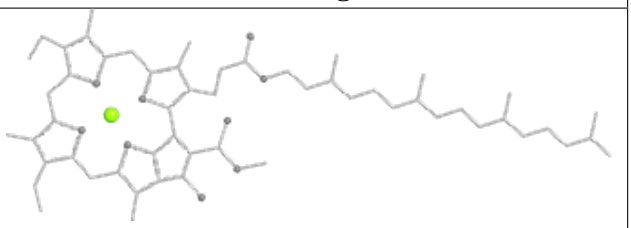
 Bond lengths	 Bond angles
 Torsions	 Rings

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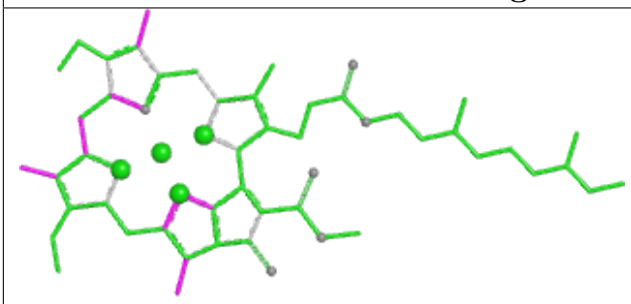
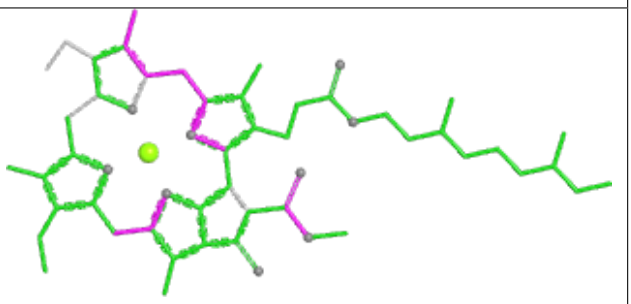
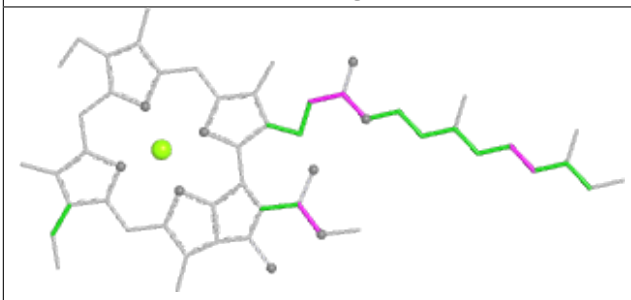
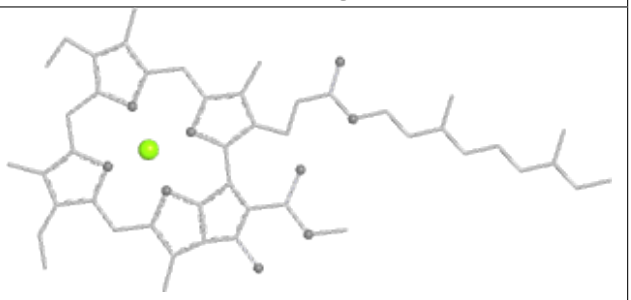
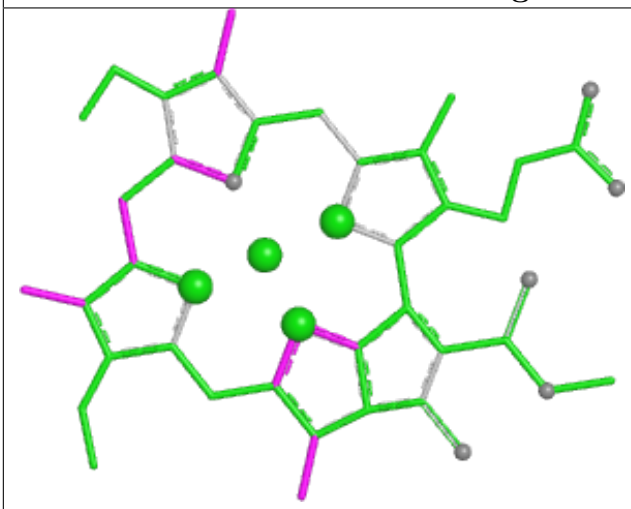
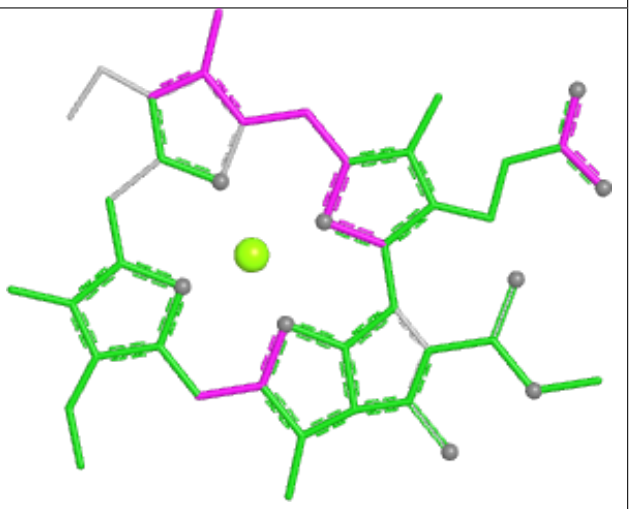
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

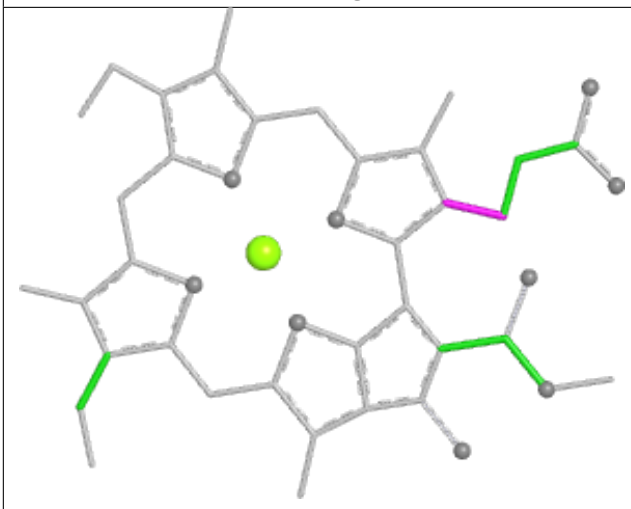
Ligand CLA BB 834



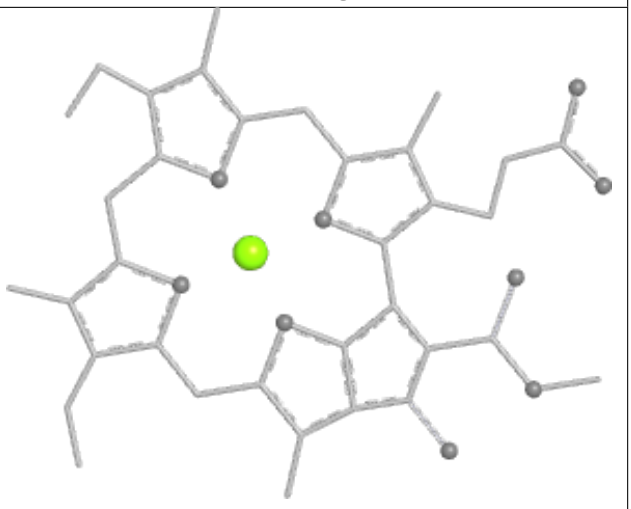
Bond lengths



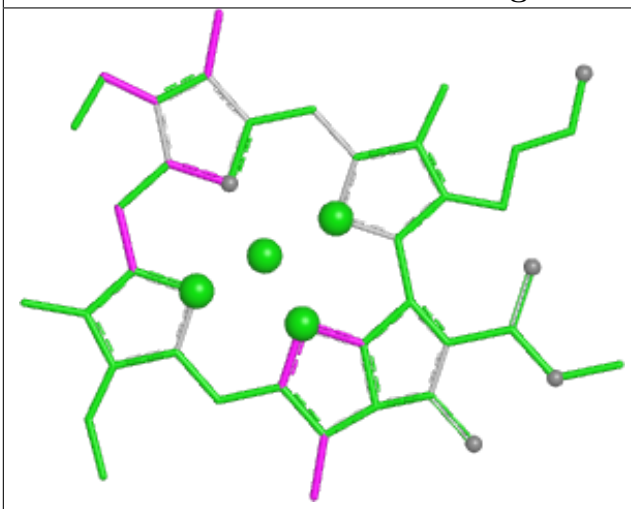
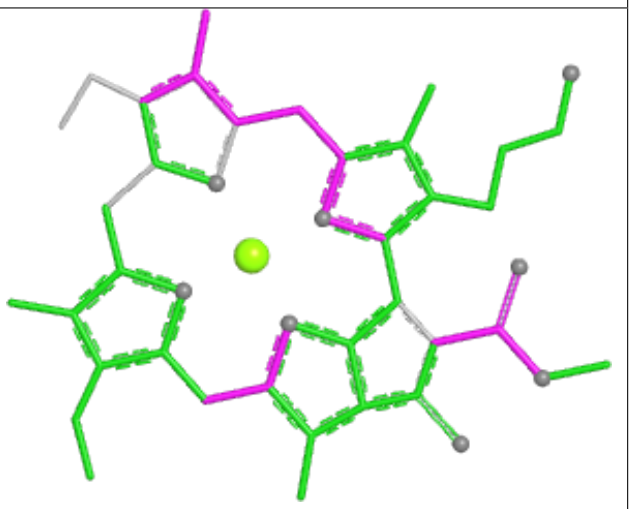
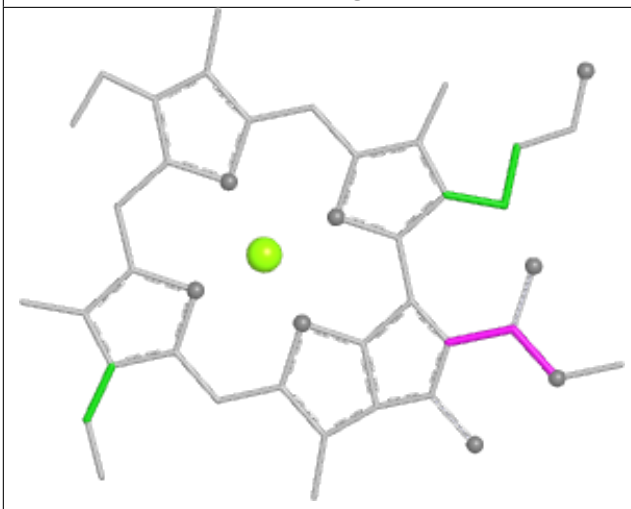
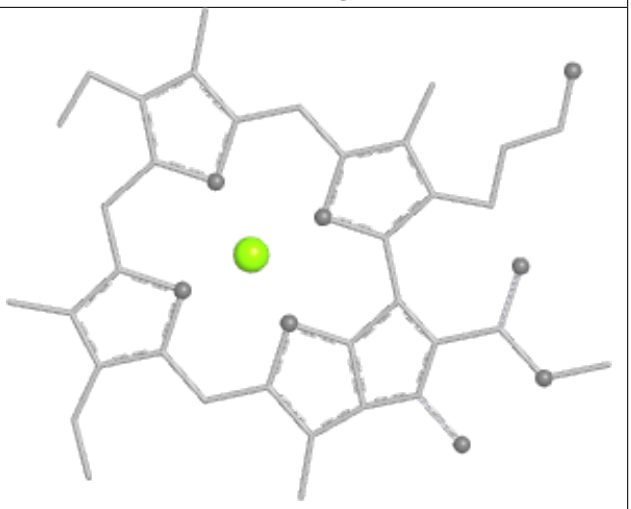
Bond angles

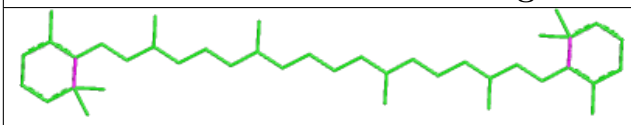
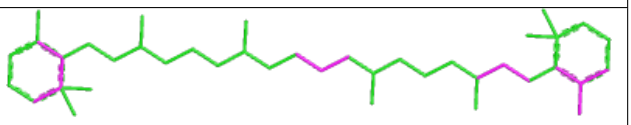
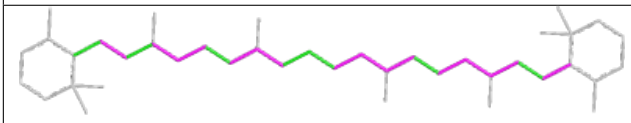
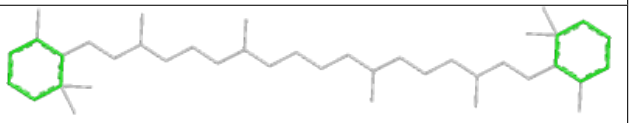


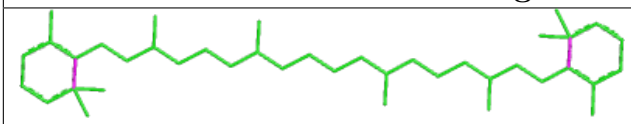
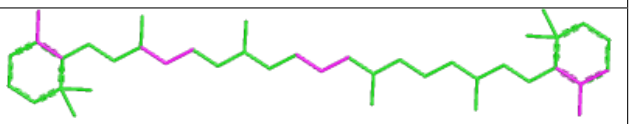
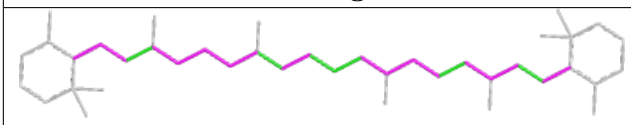
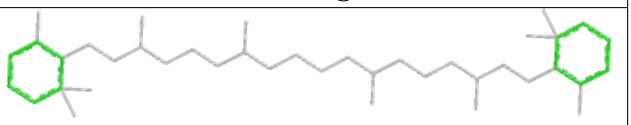
Torsions

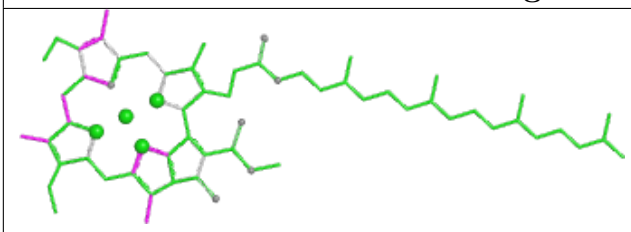
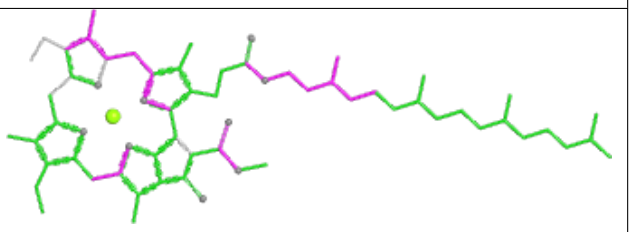
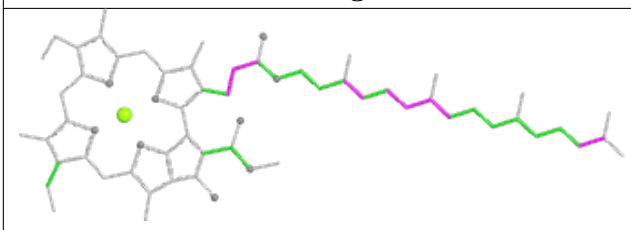
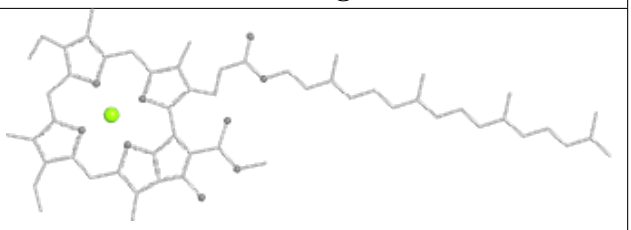


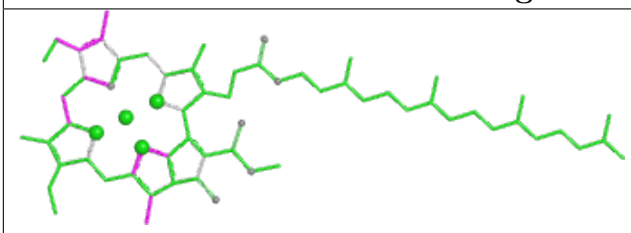
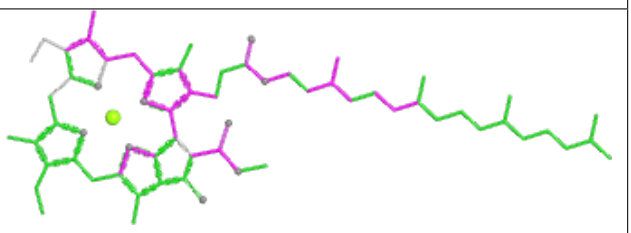
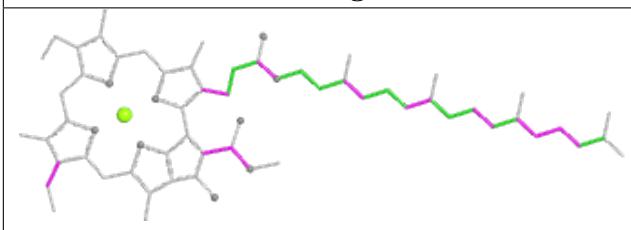
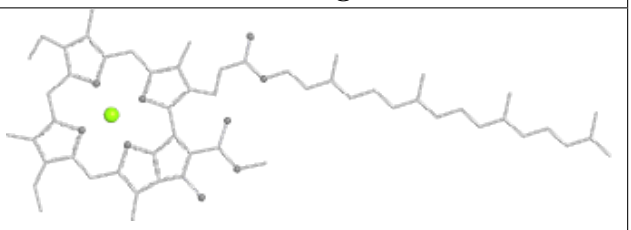
Rings

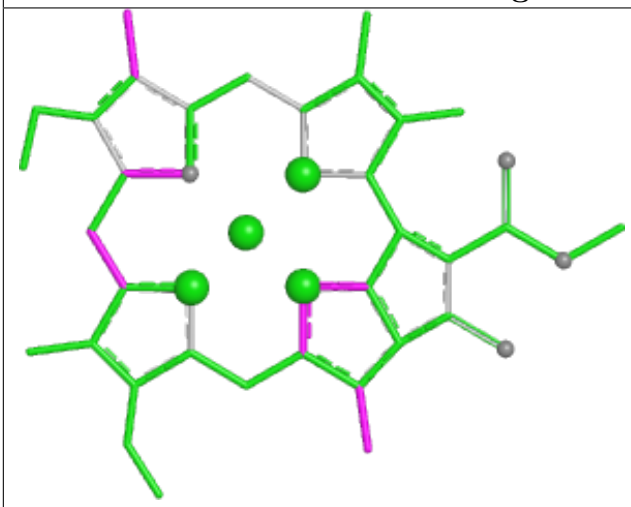
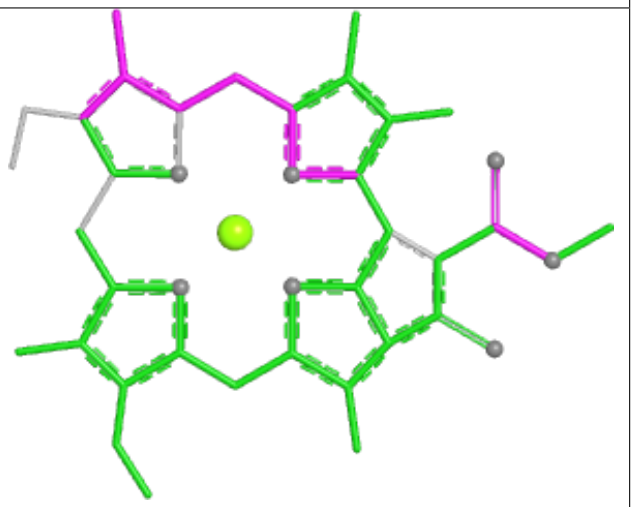
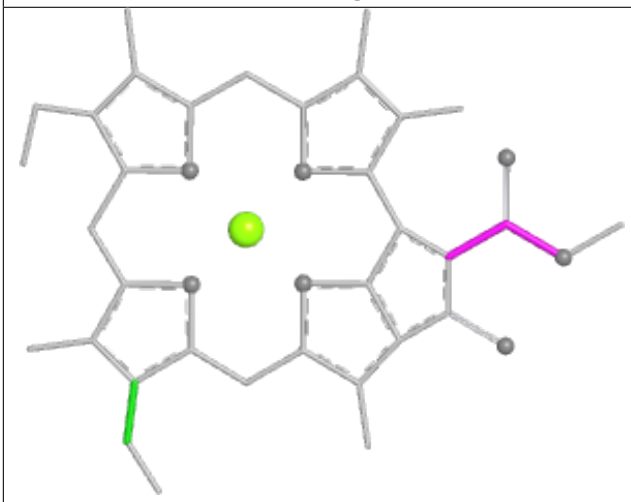
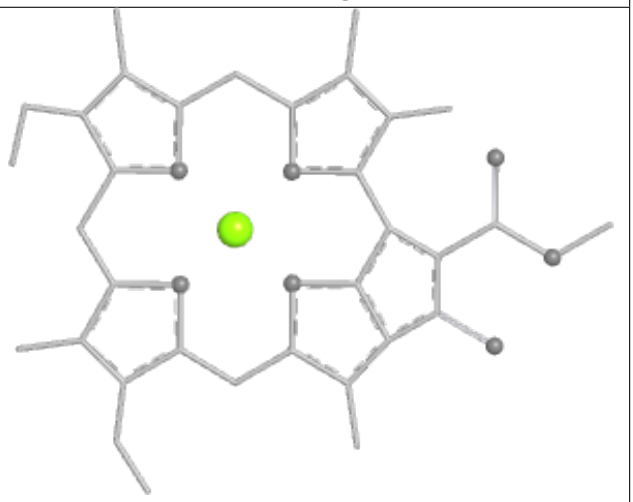
Ligand CLA AA 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

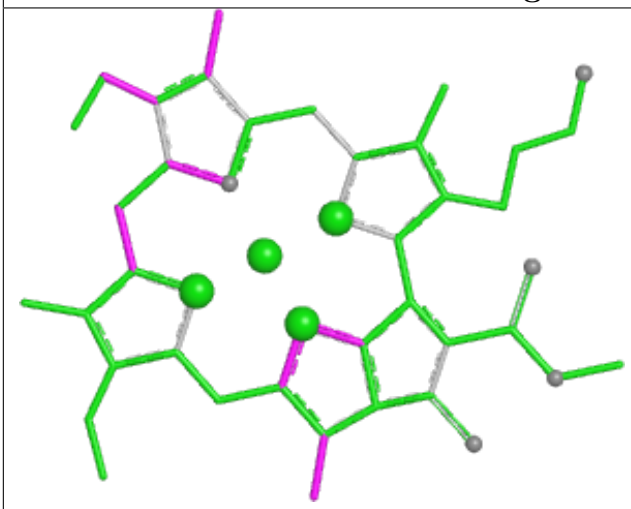
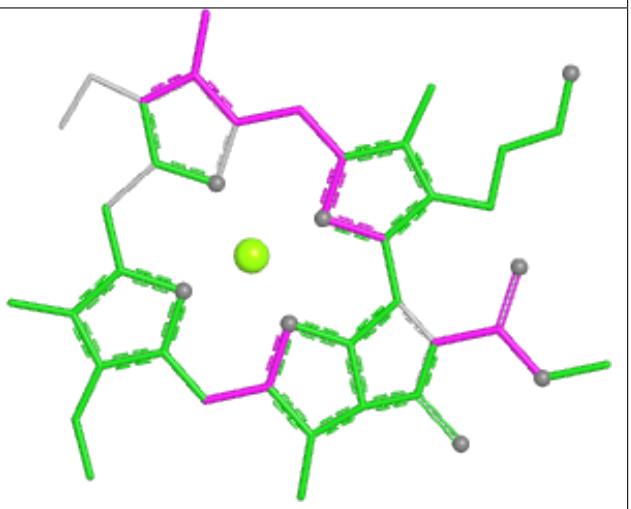
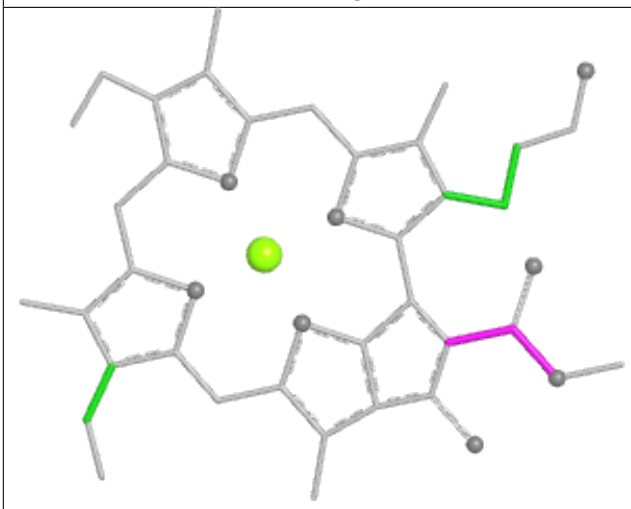
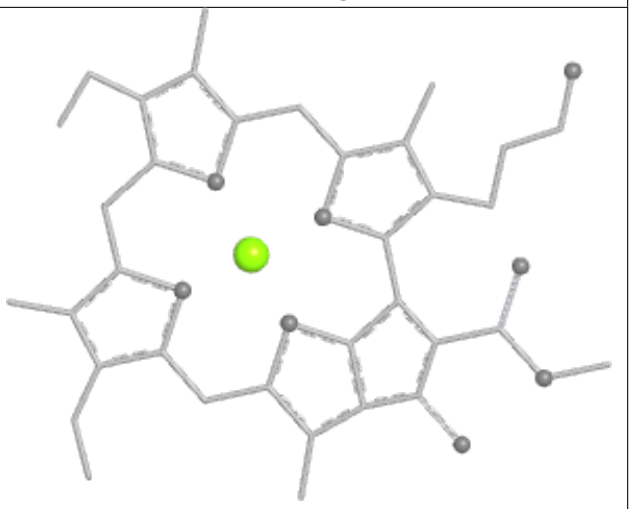
Ligand BCR J1 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

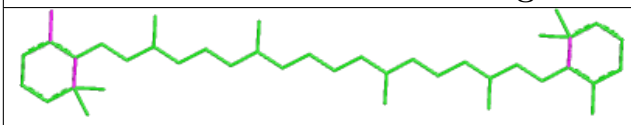
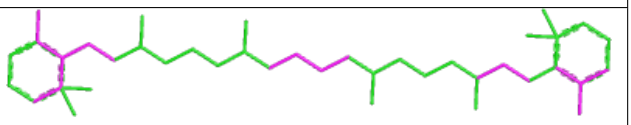
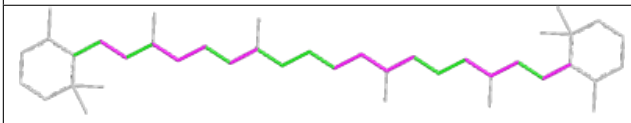
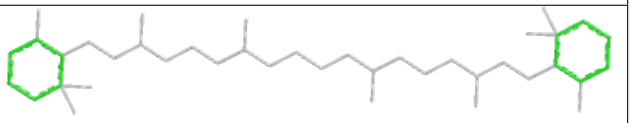
Ligand BCR LL 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

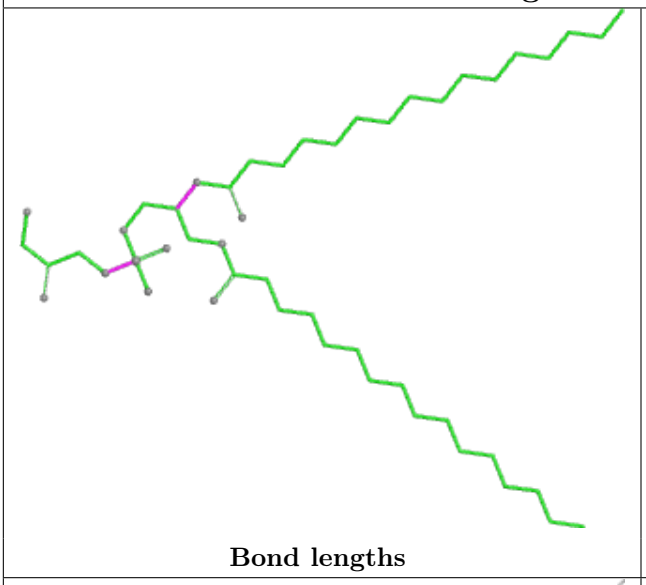
Ligand CLA B1 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 812	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

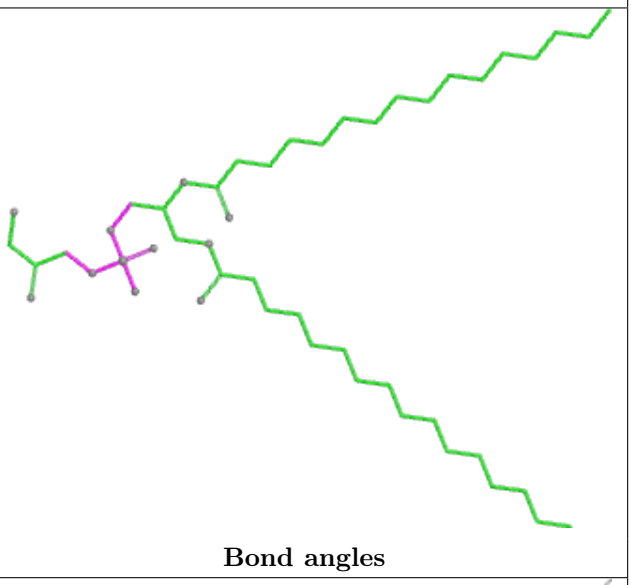
Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR JJ 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

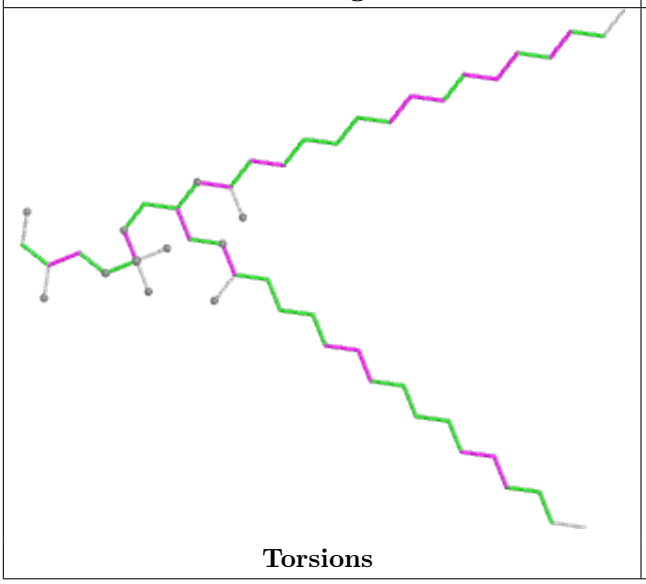
Ligand LHG A 845



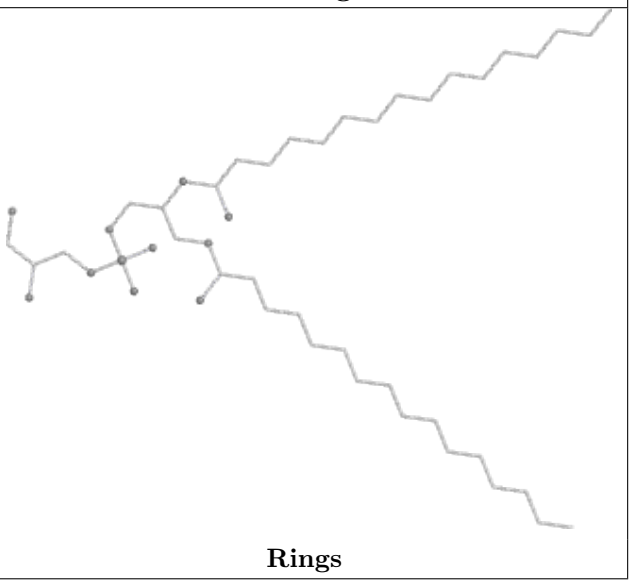
Bond lengths



Bond angles

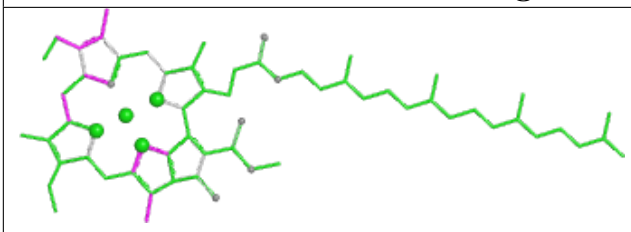


Torsions

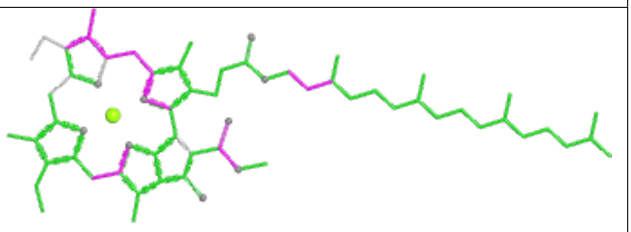


Rings

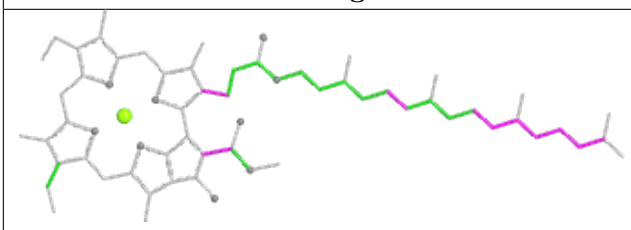
Ligand CLA A2 807



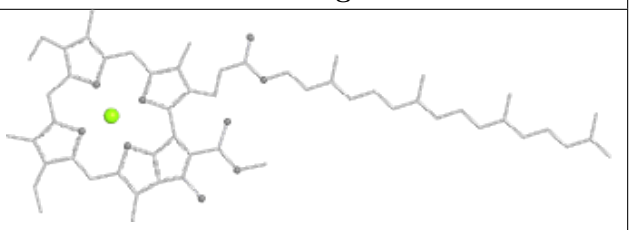
Bond lengths



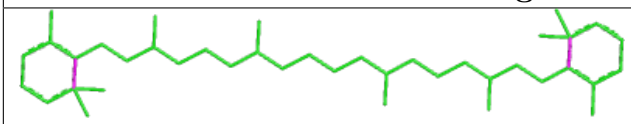
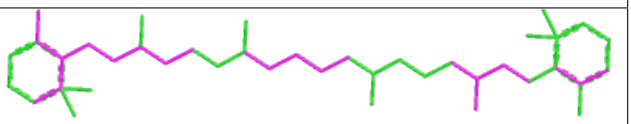
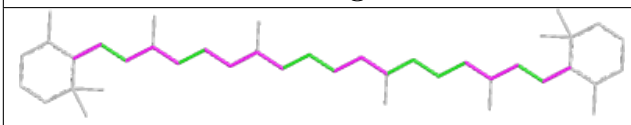
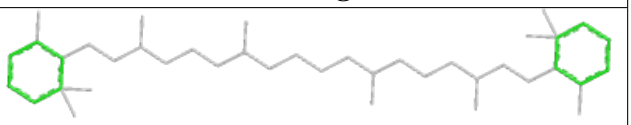
Bond angles

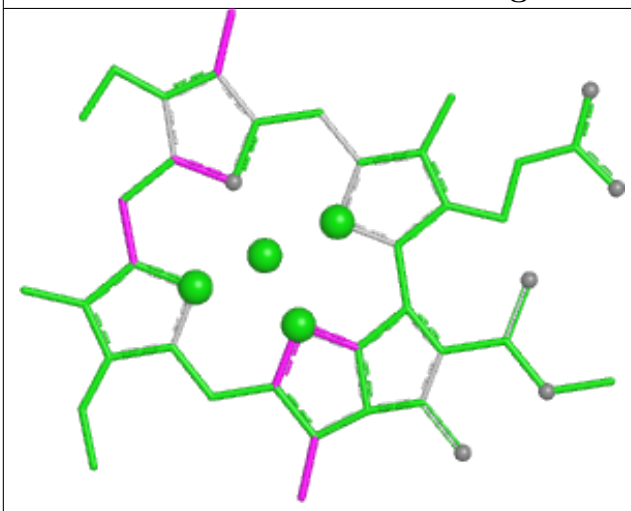
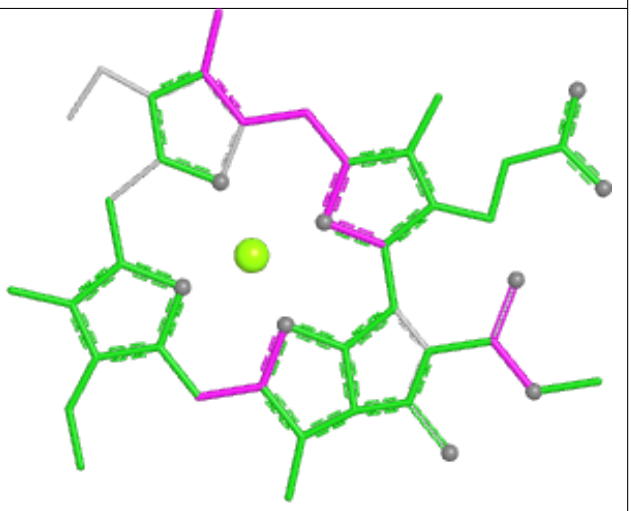
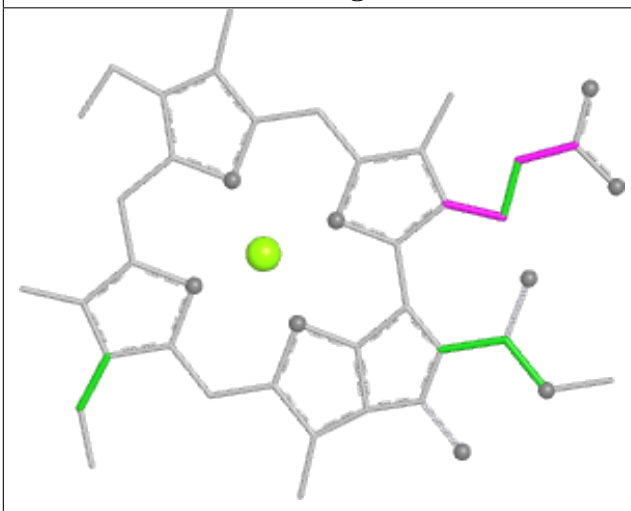
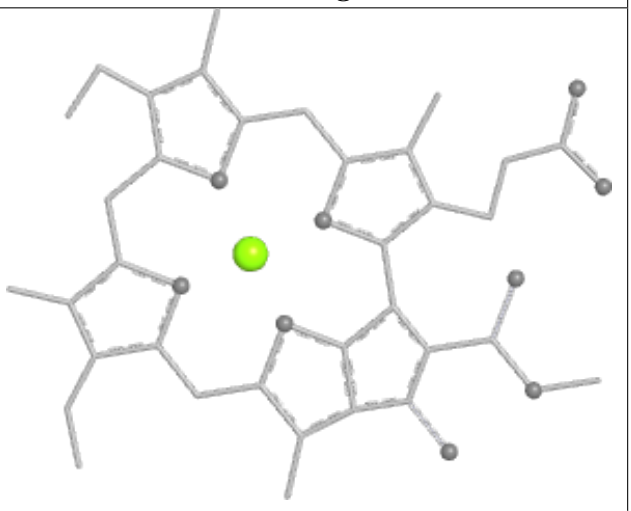


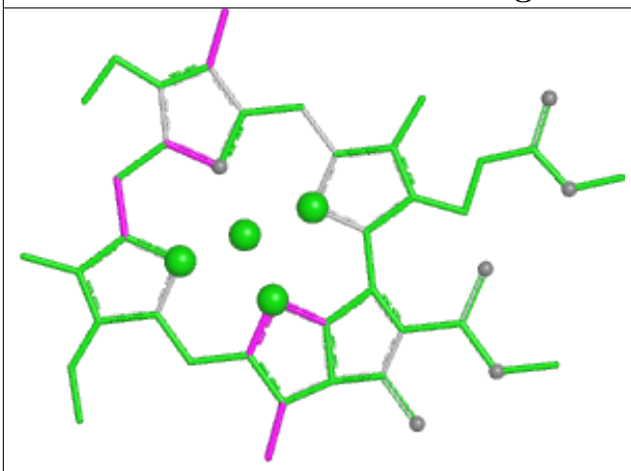
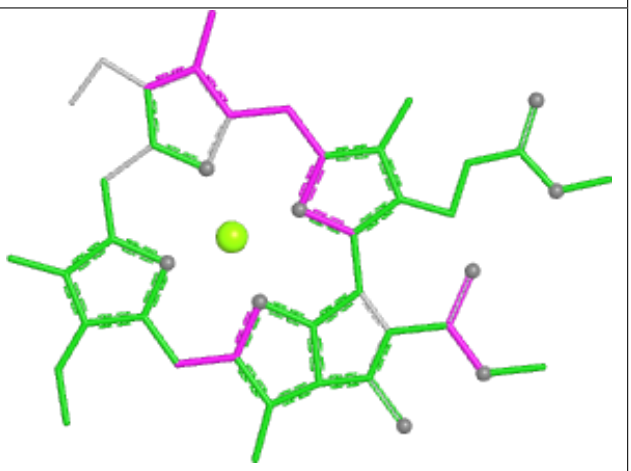
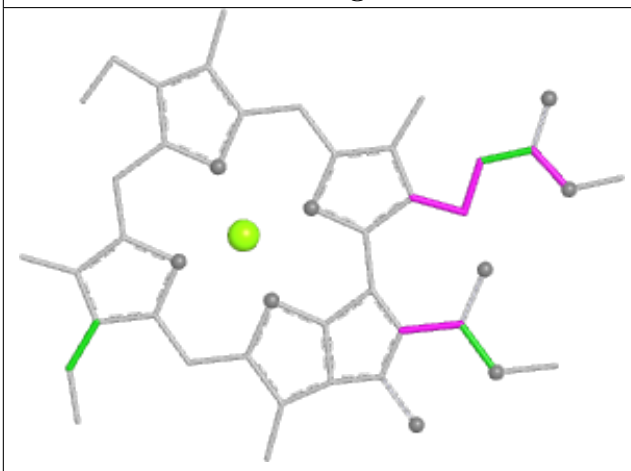
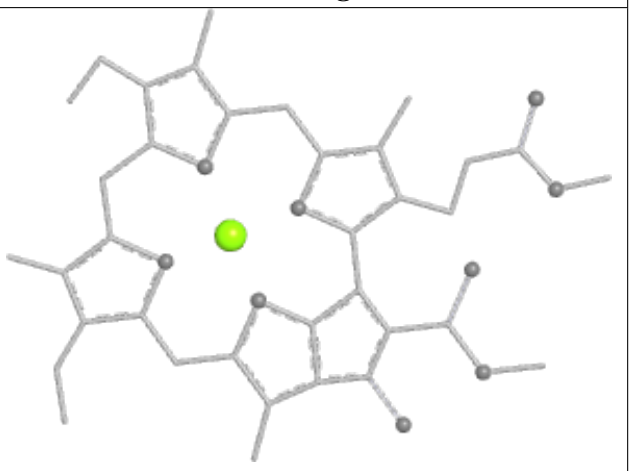
Torsions



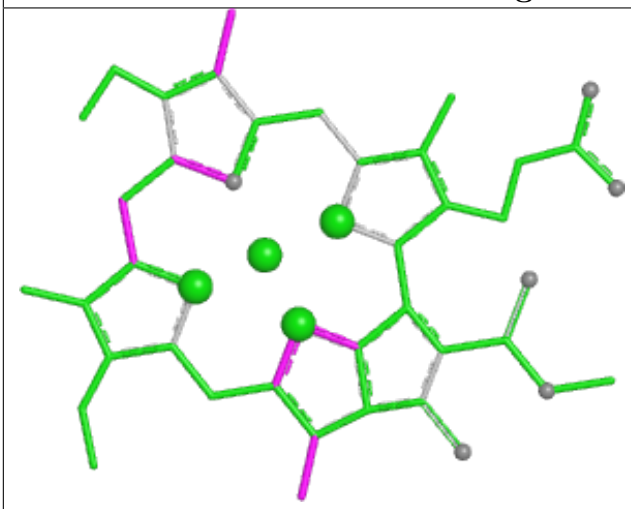
Rings

Ligand BCR L1 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

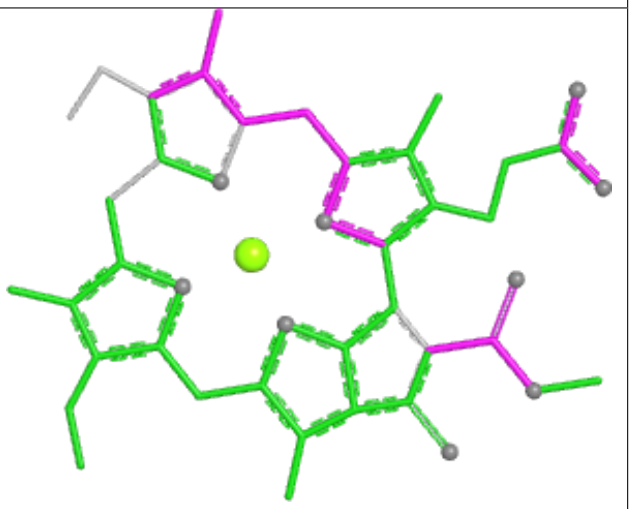
Ligand CLA AA 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

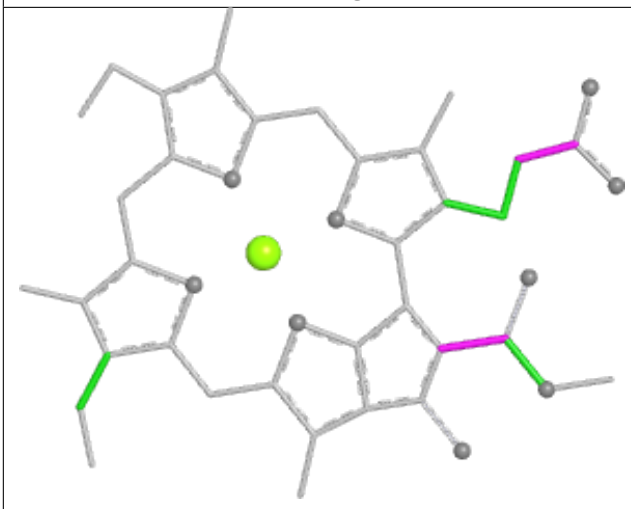
Ligand CLA B1 809



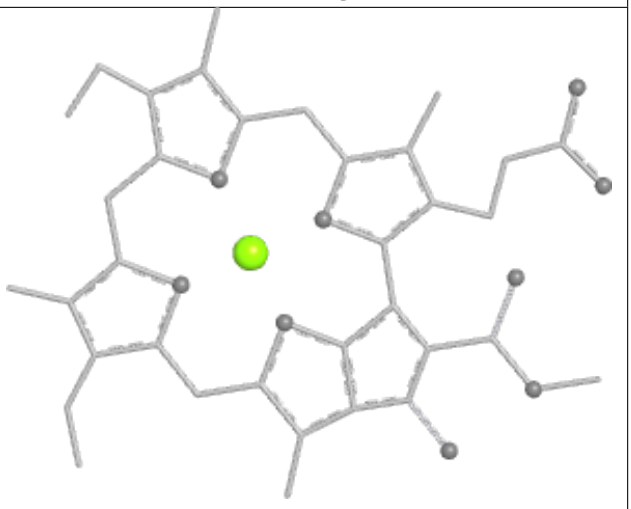
Bond lengths



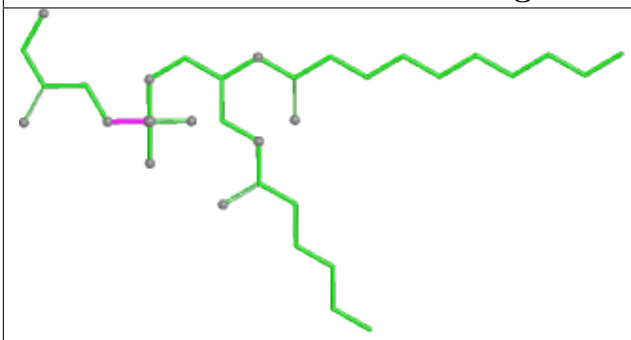
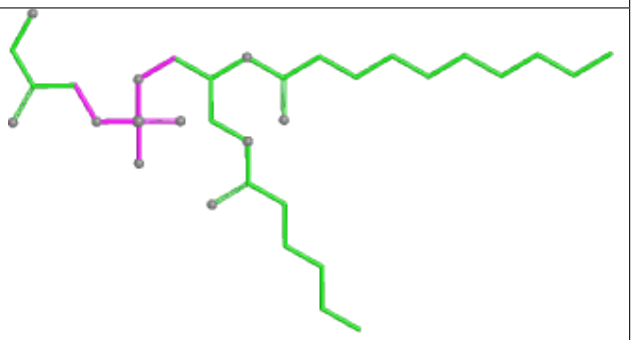
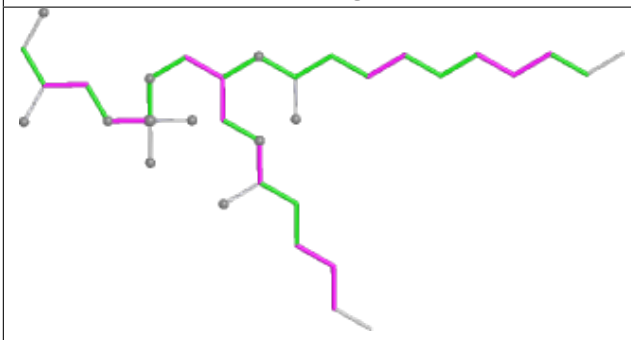
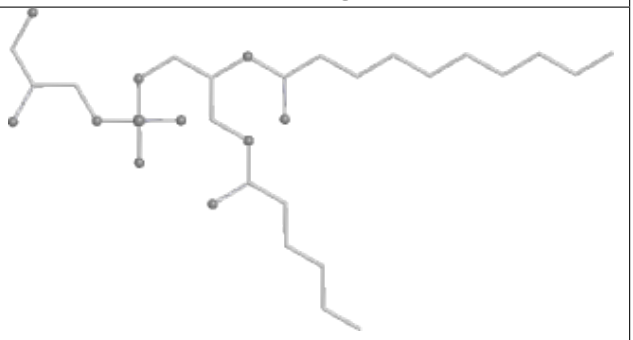
Bond angles

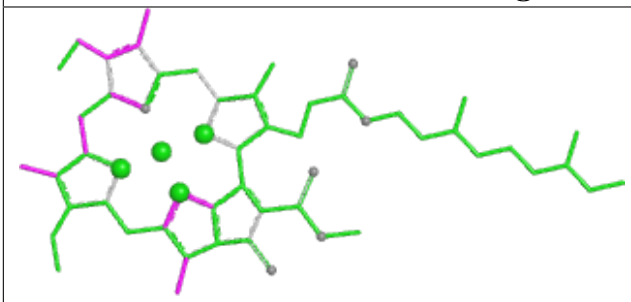
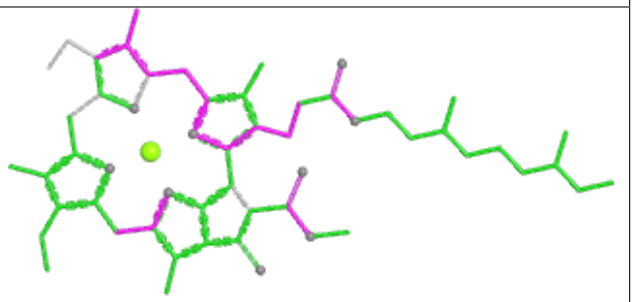
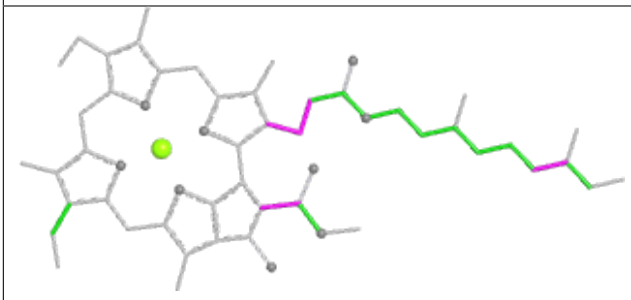
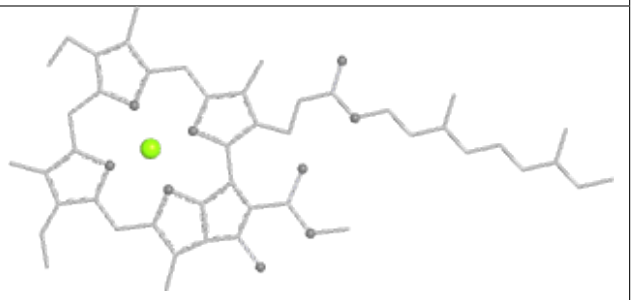


Torsions

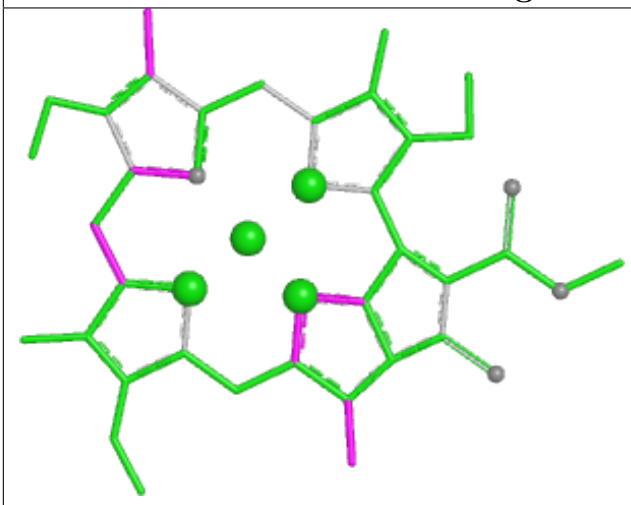


Rings

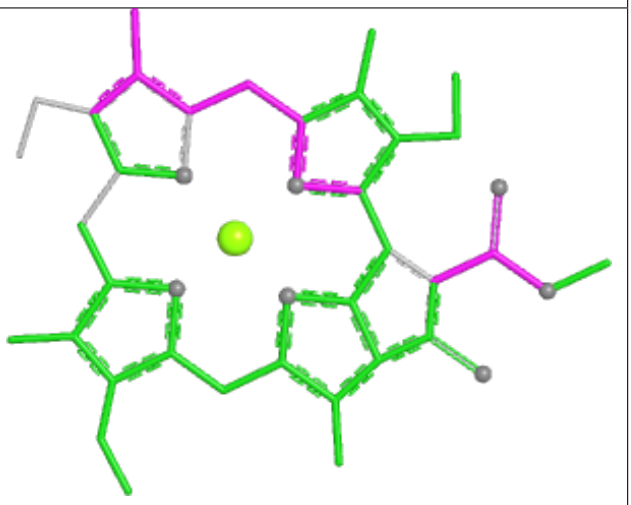
Ligand LHG B1 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

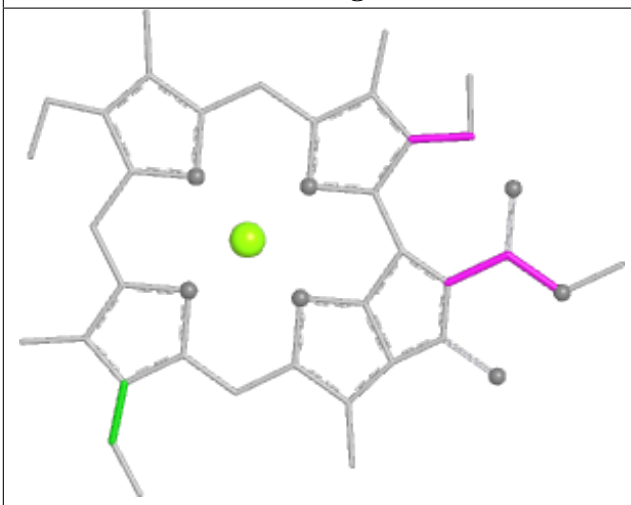
Ligand CLA B1 813



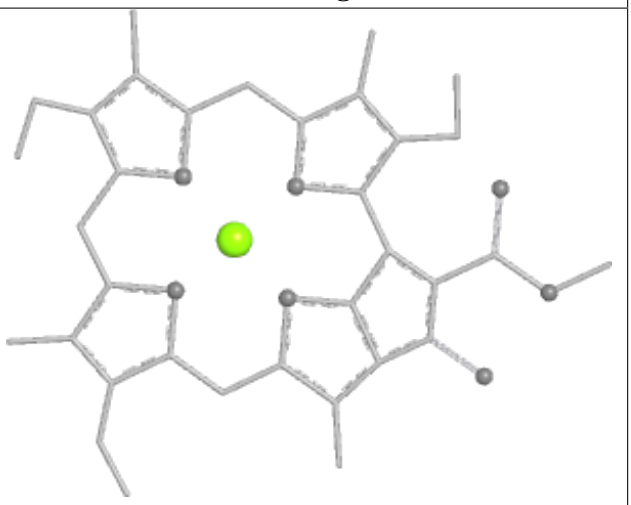
Bond lengths



Bond angles

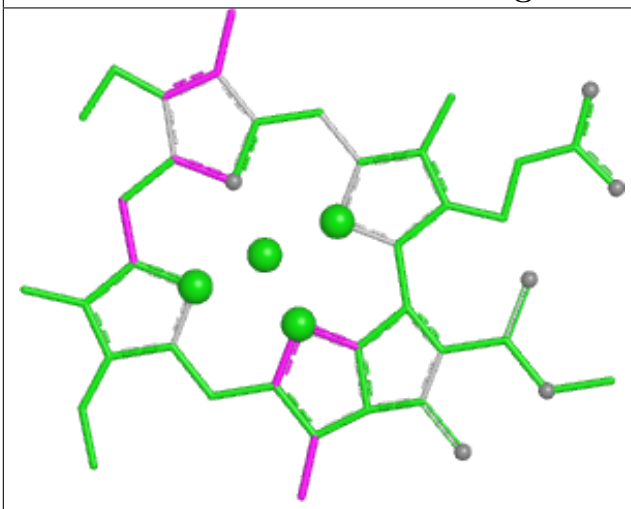


Torsions

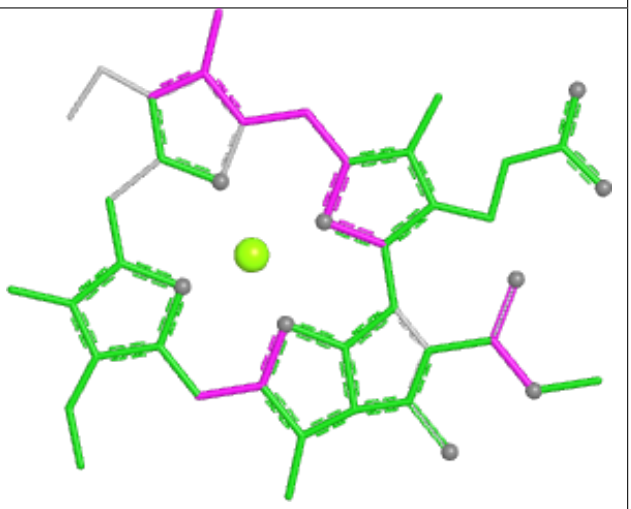


Rings

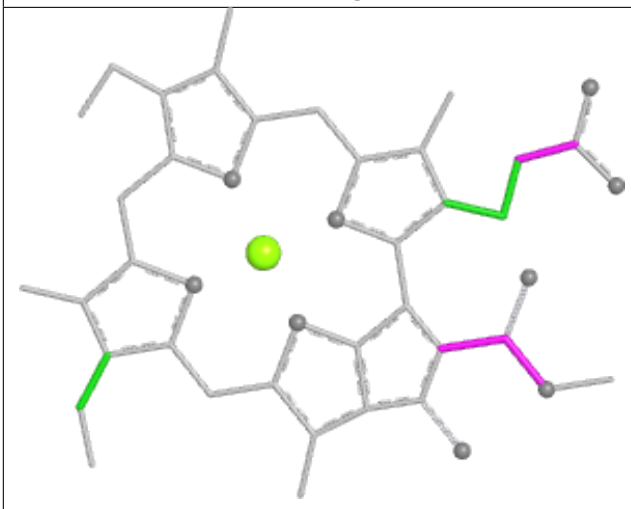
Ligand CLA A2 837



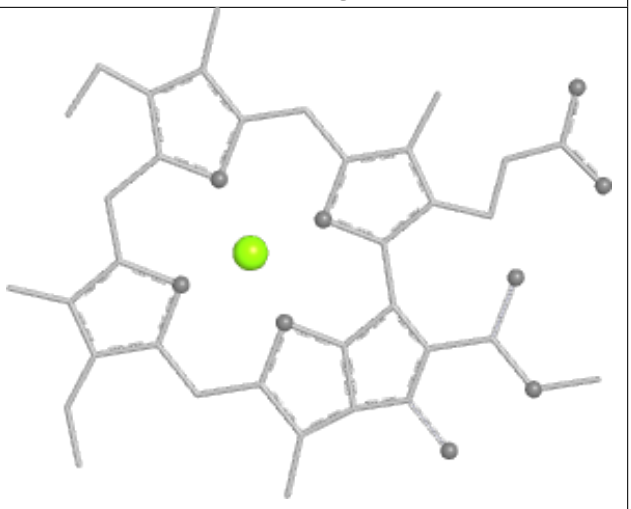
Bond lengths



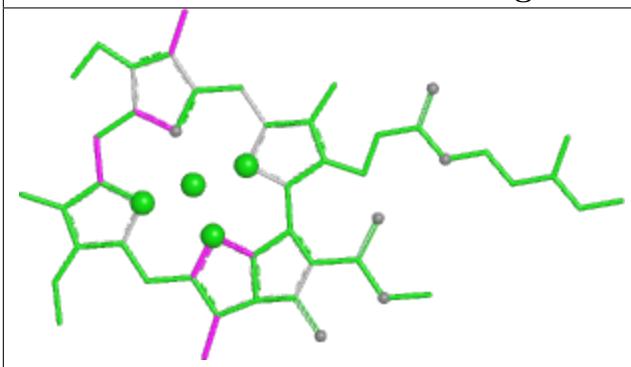
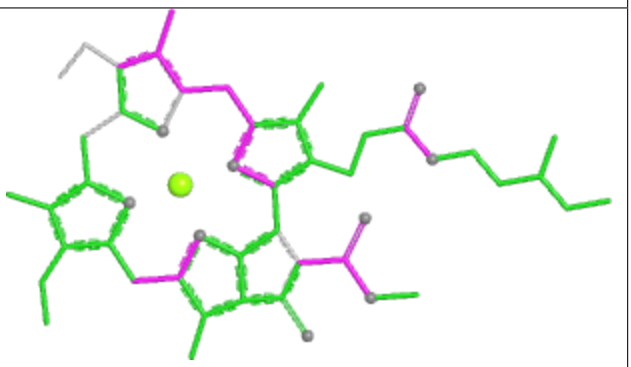
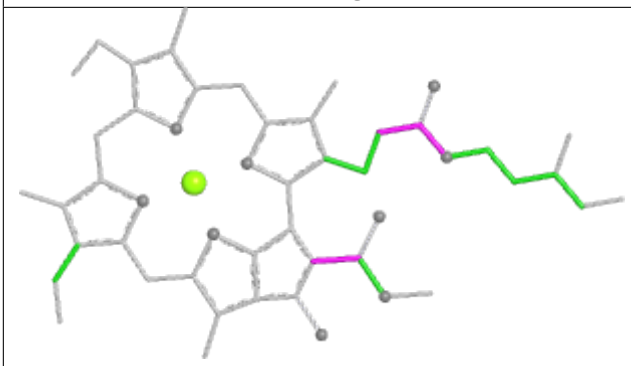
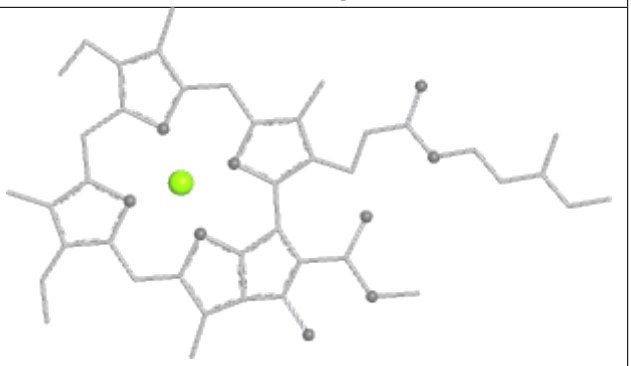
Bond angles

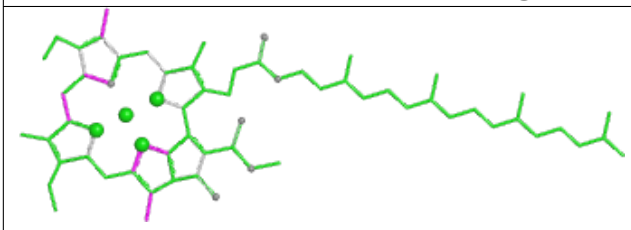
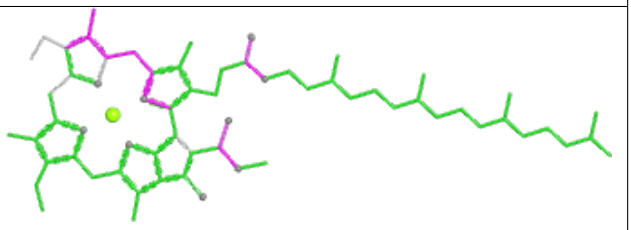
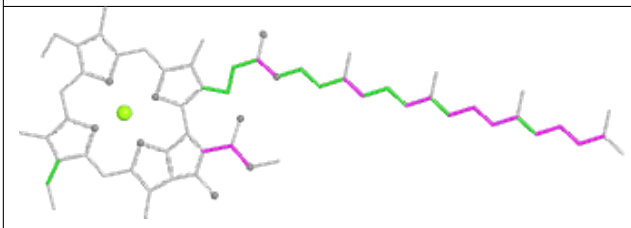
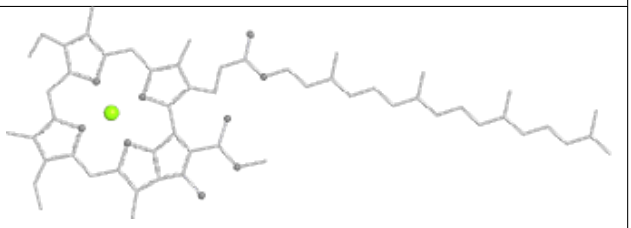


Torsions

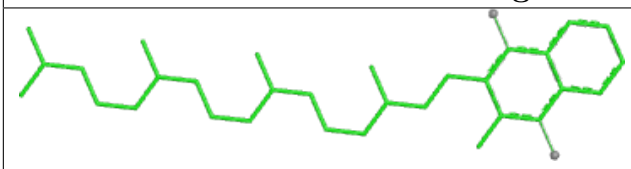


Rings

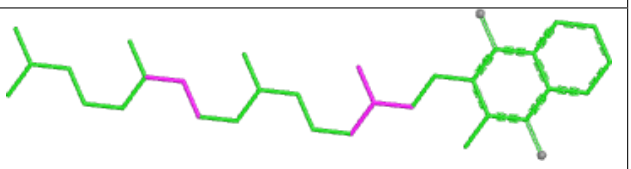
Ligand CLA A2 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

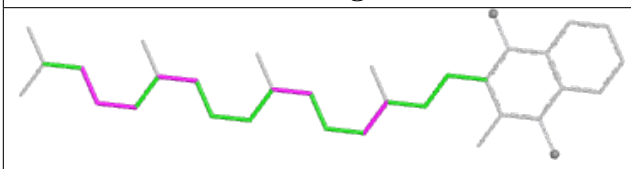
Ligand PQN A1 843



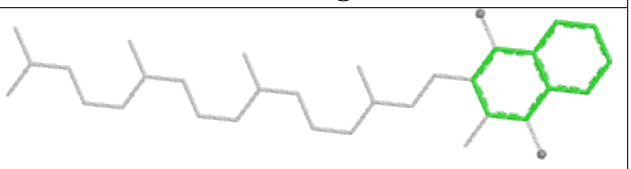
Bond lengths



Bond angles

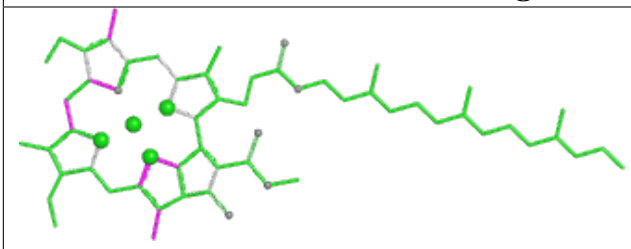


Torsions

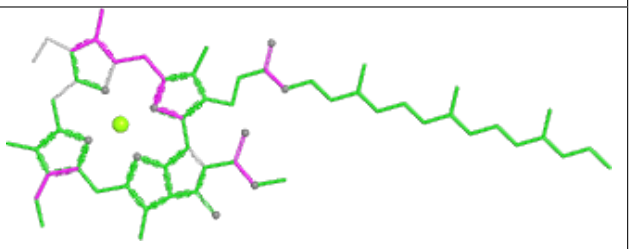


Rings

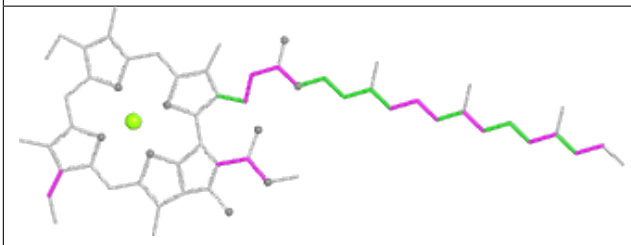
Ligand CLA A1 829



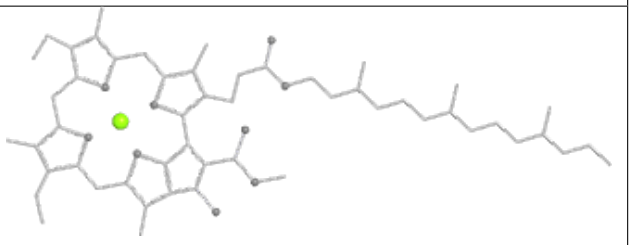
Bond lengths



Bond angles

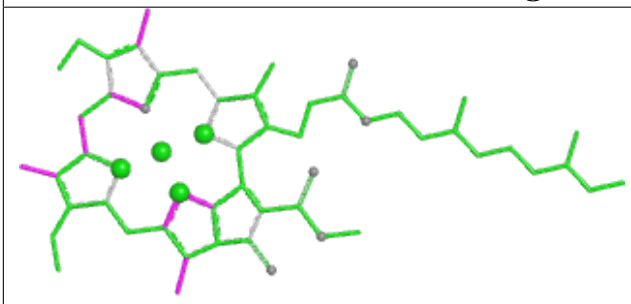


Torsions

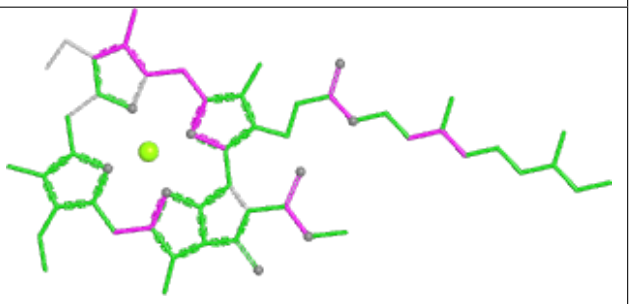


Rings

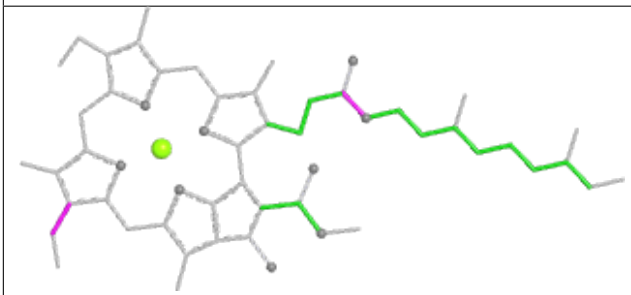
Ligand CLA B 830



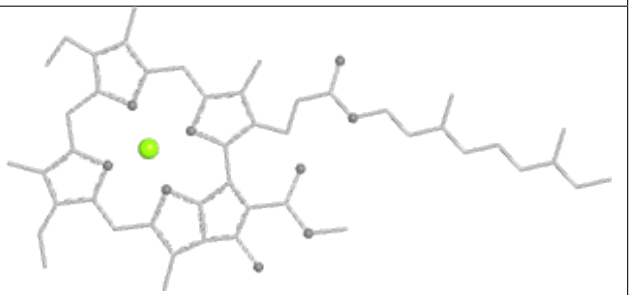
Bond lengths



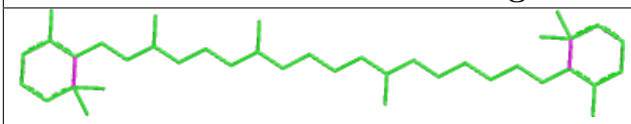
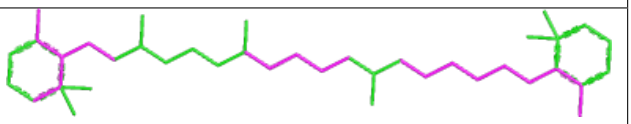
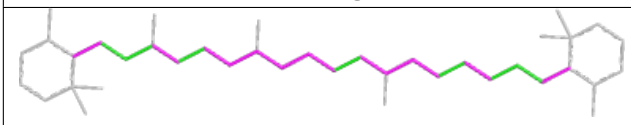
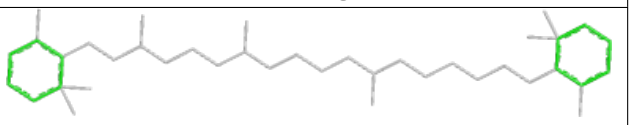
Bond angles

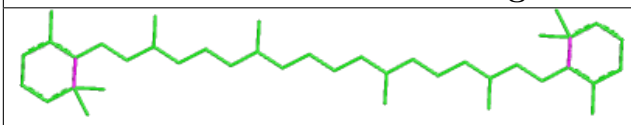
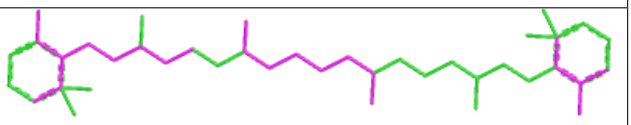
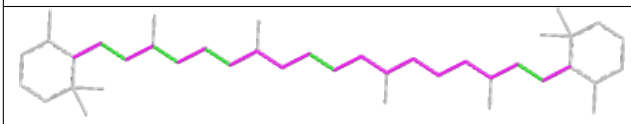
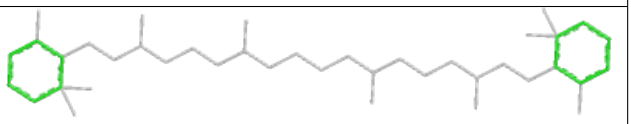


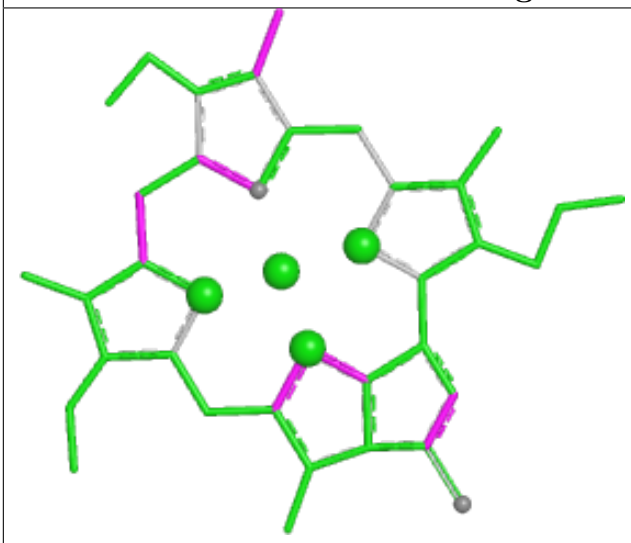
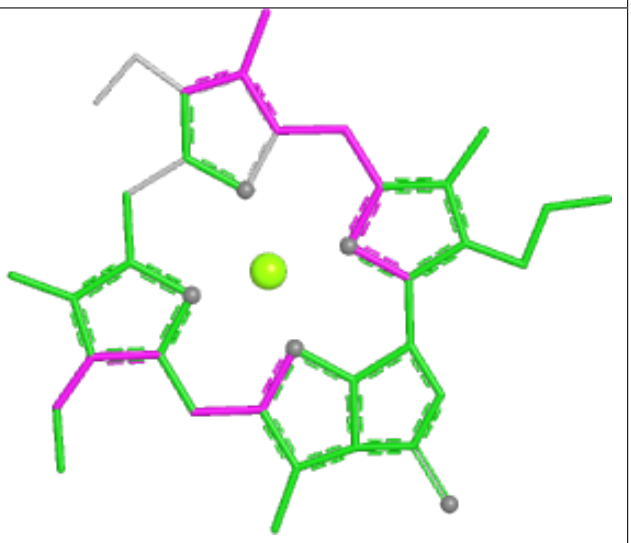
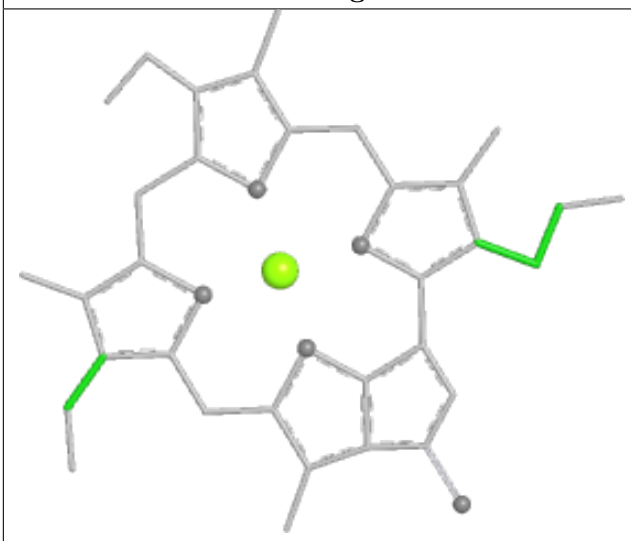
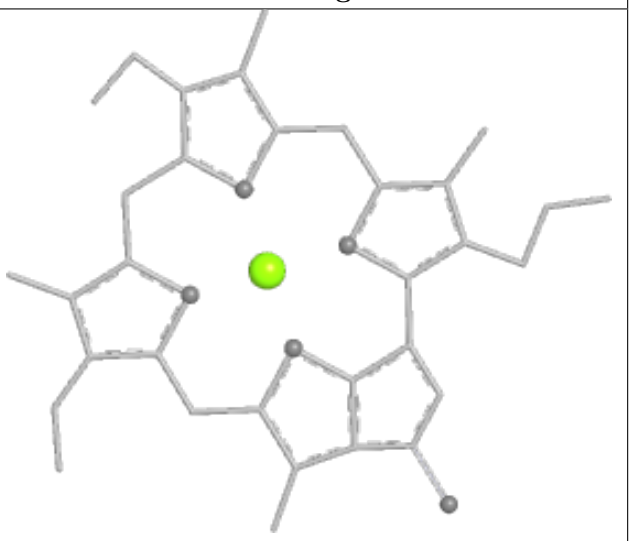
Torsions

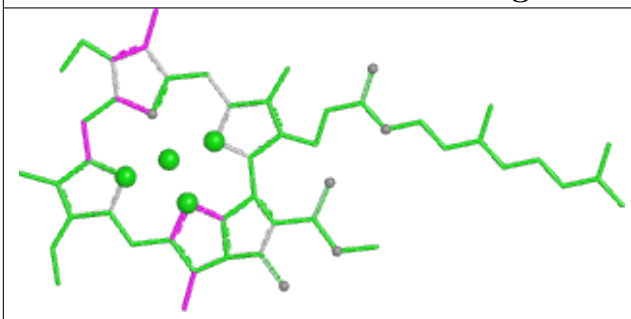
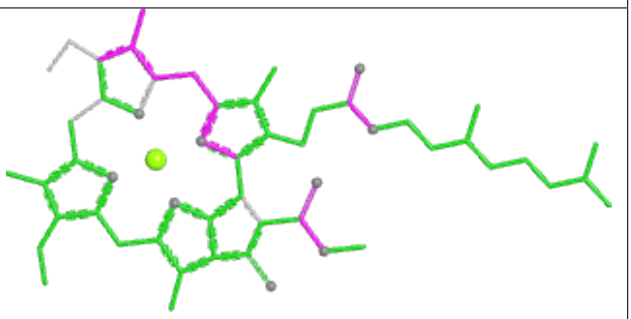
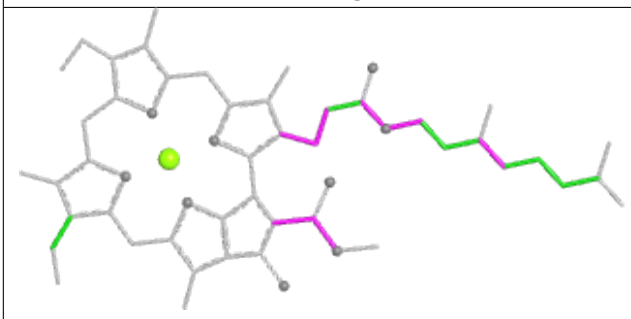
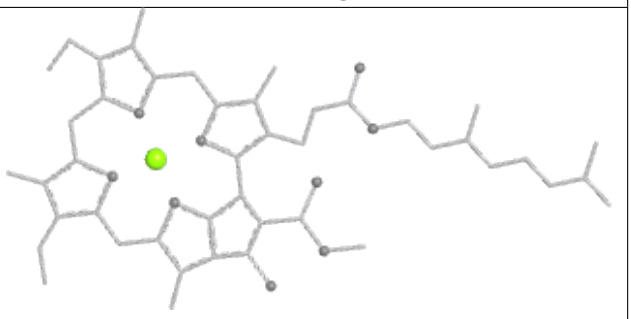


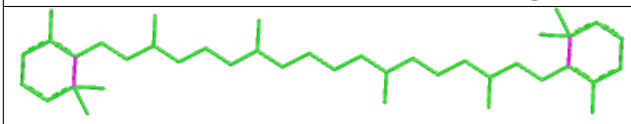
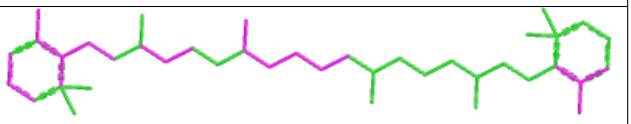
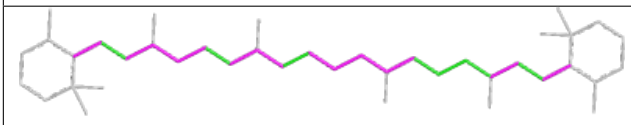
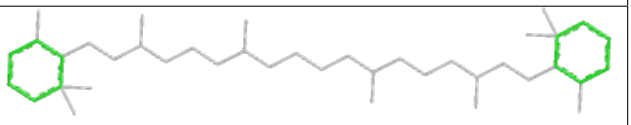
Rings

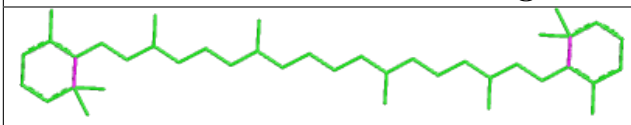
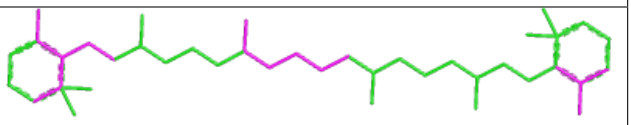
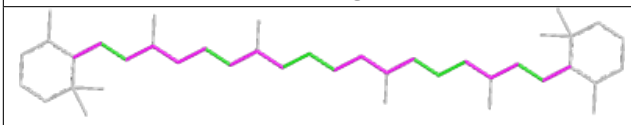
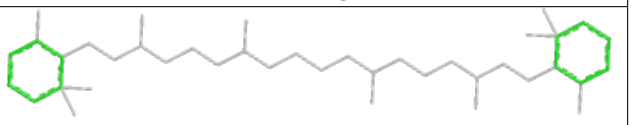
Ligand BCR AA 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

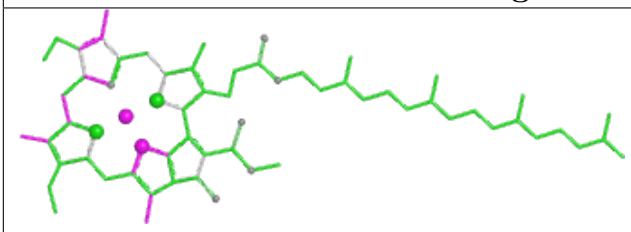
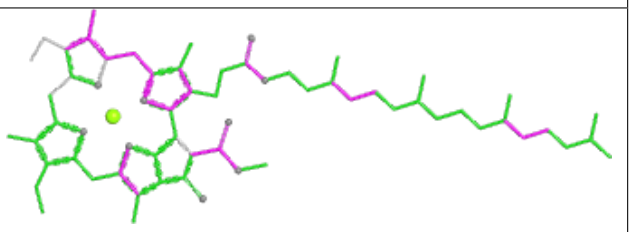
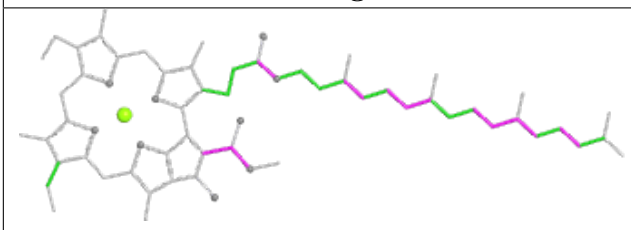
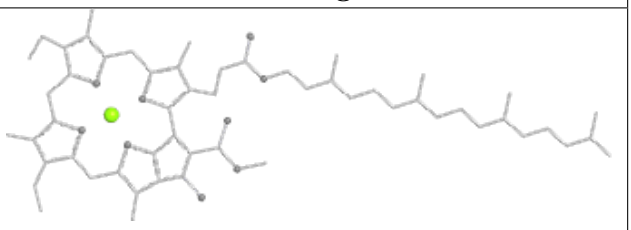
Ligand BCR AA 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

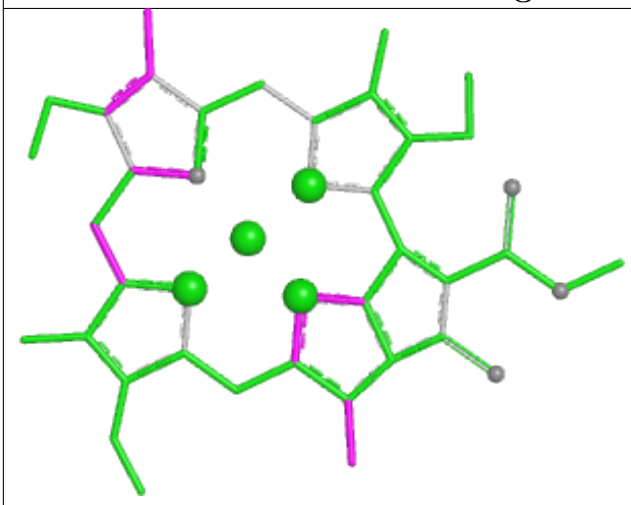
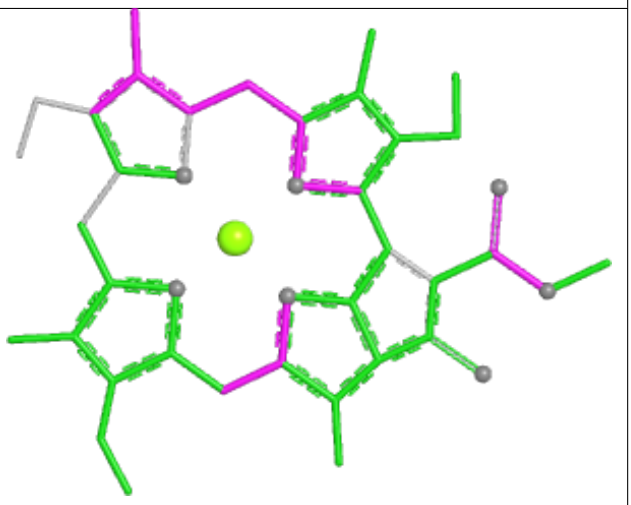
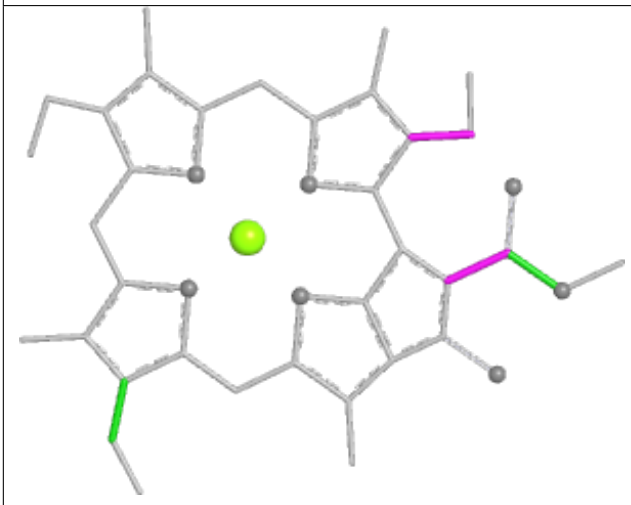
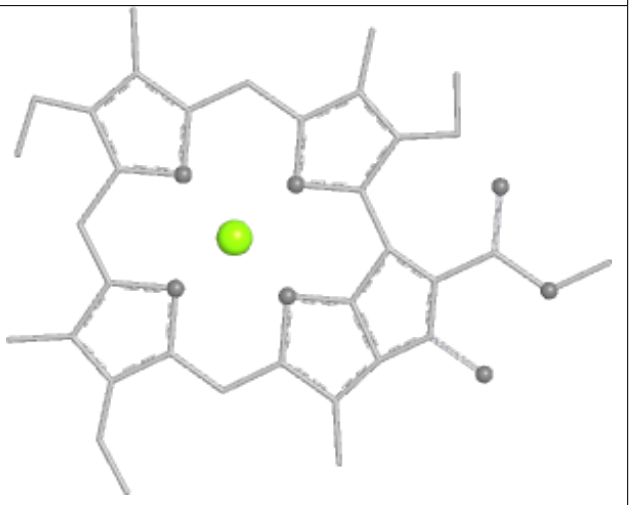
Ligand CLA B1 845	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

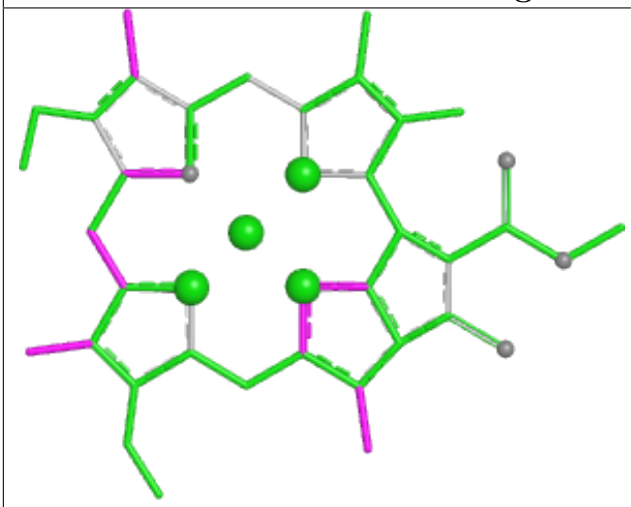
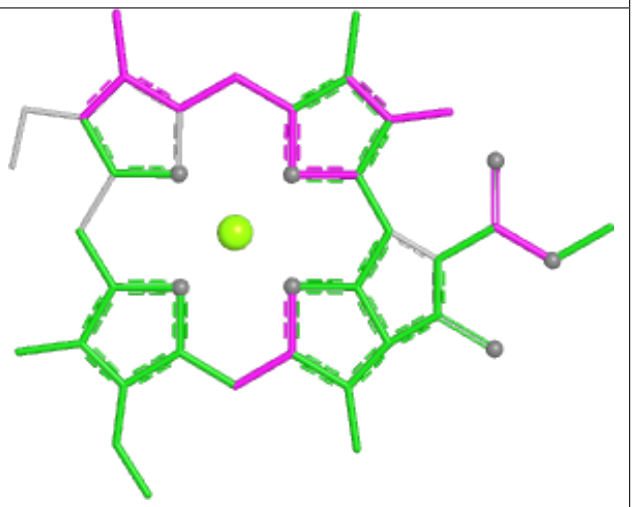
Ligand CLA BB 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 833	
	
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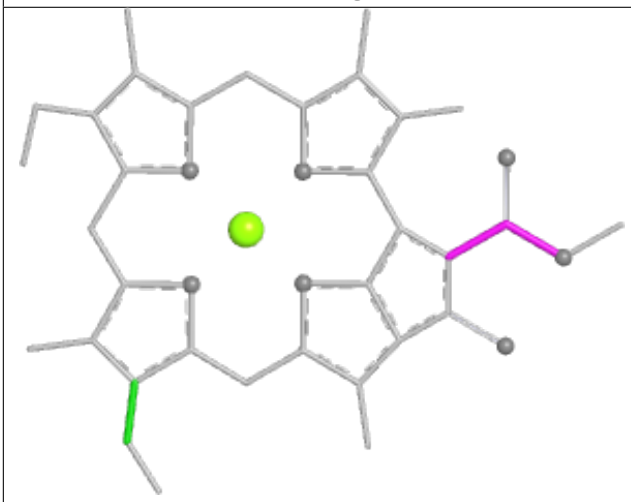
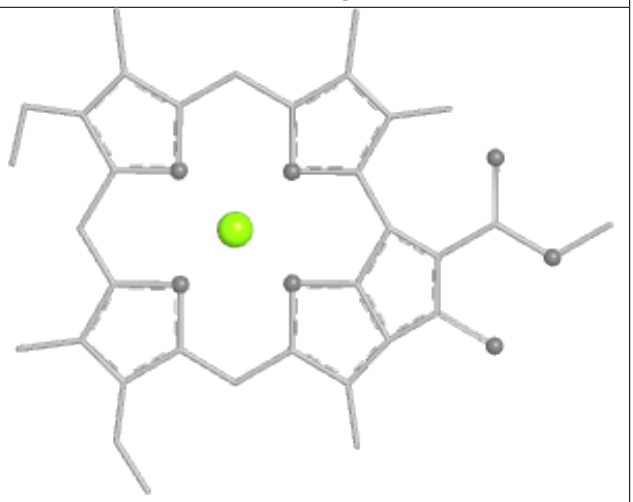
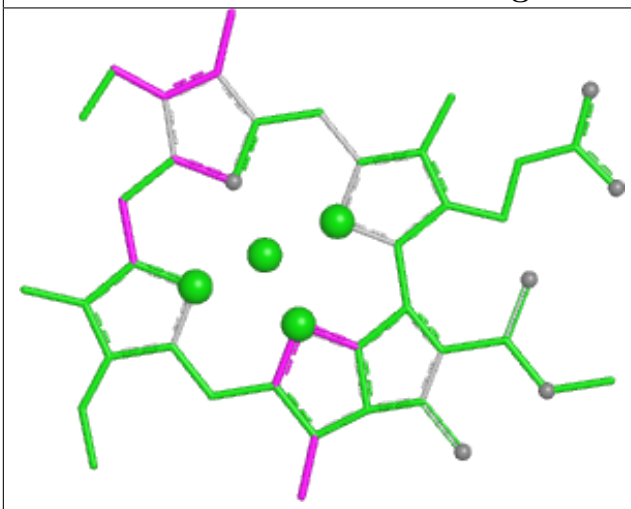
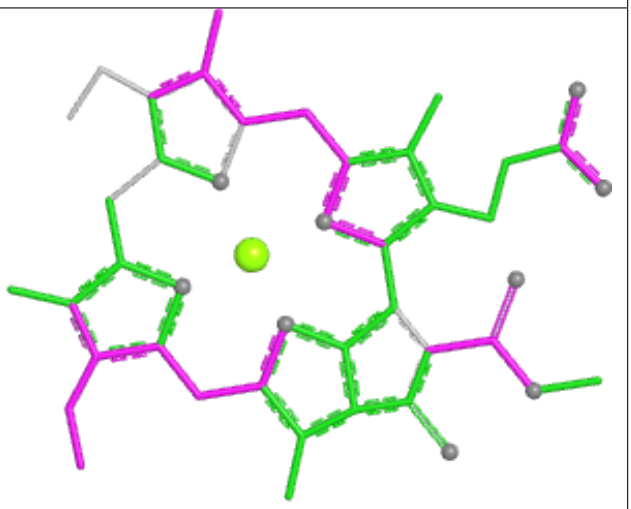
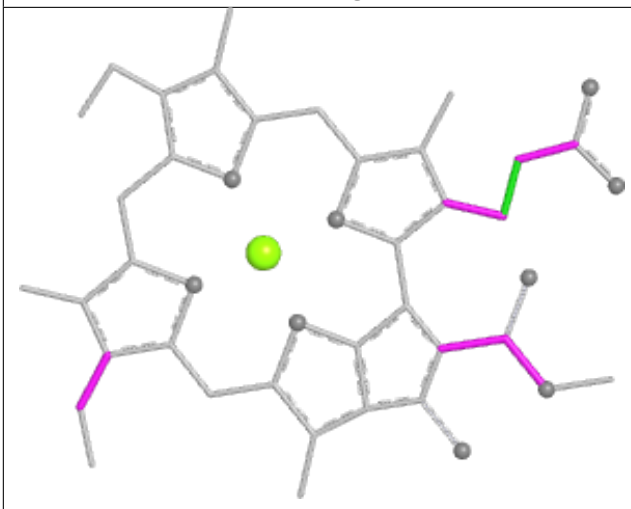
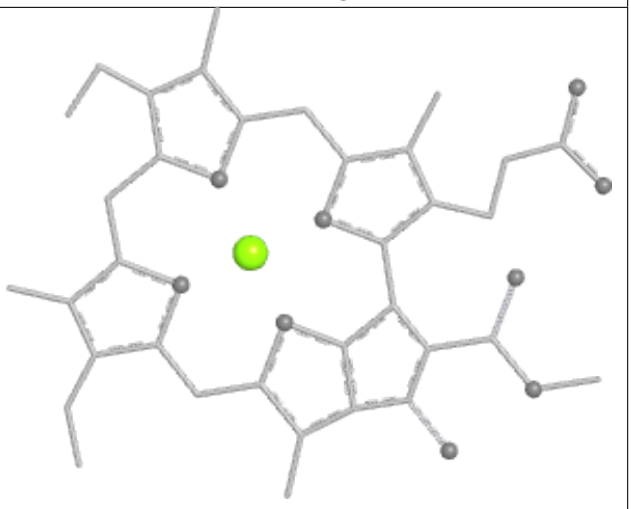
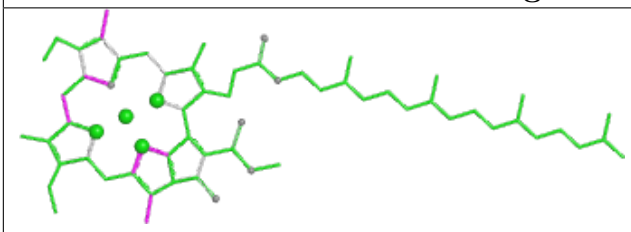
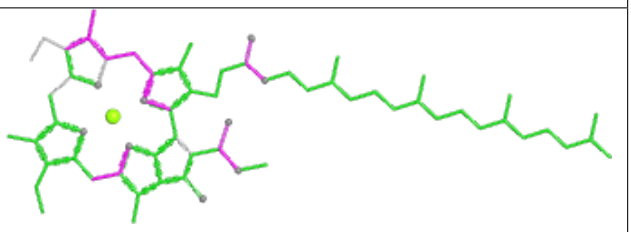
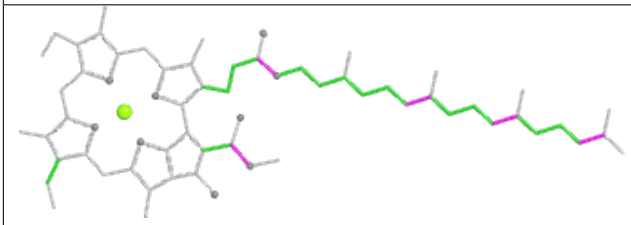
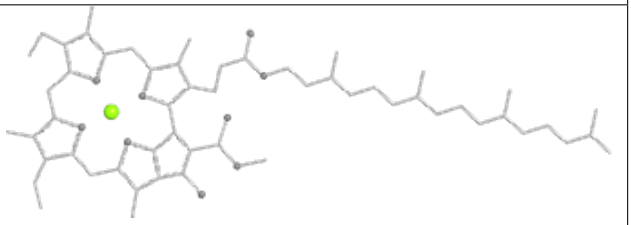
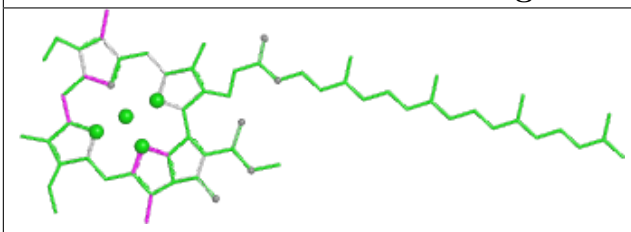
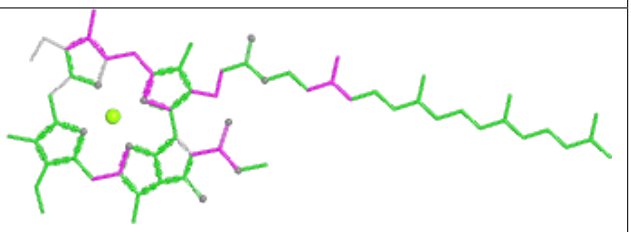
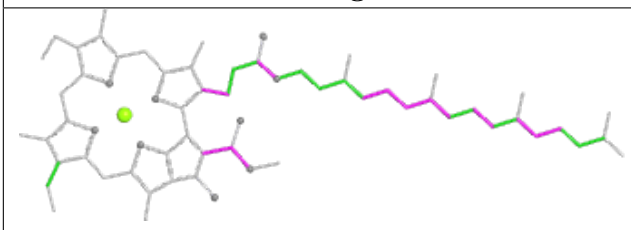
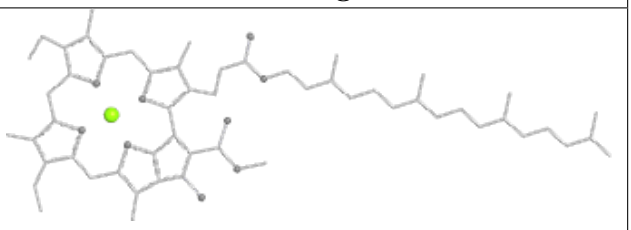
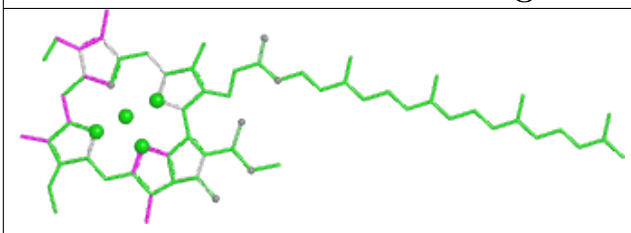
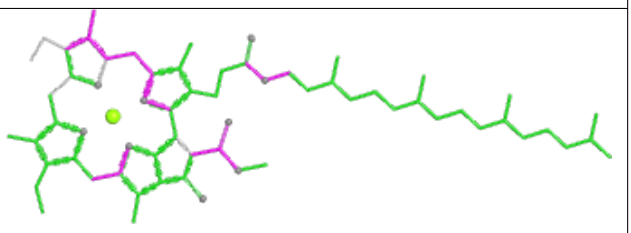
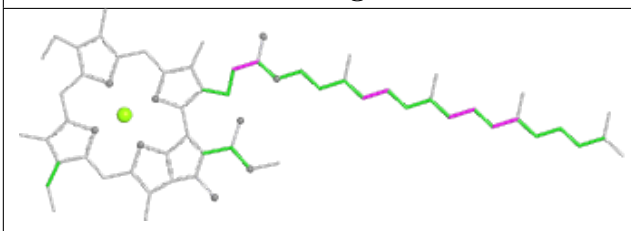
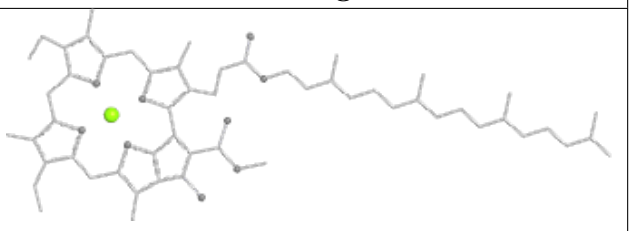
	
Torsions	**Rings**

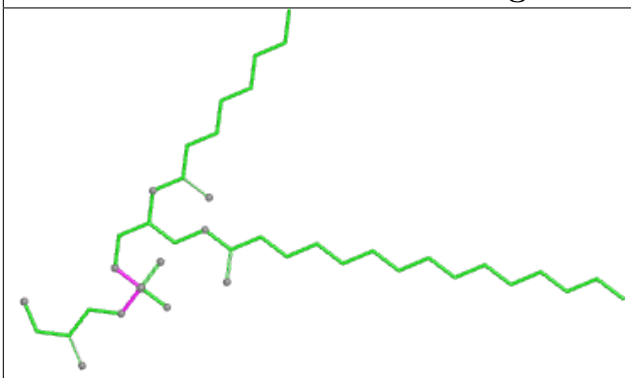
Ligand CLA BB 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

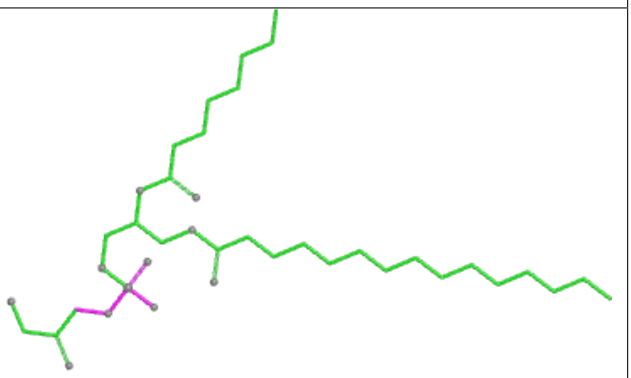
Ligand CLA B1 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA LL 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

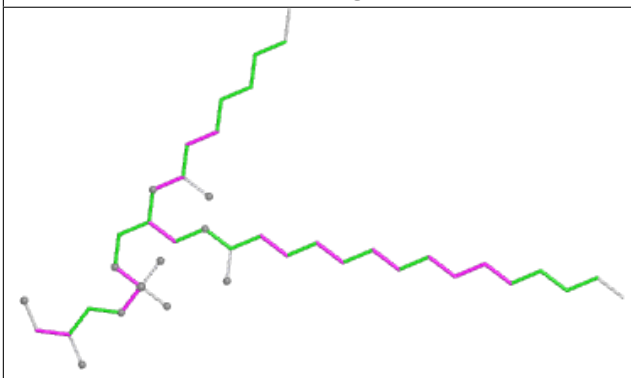
Ligand LHG XX 102



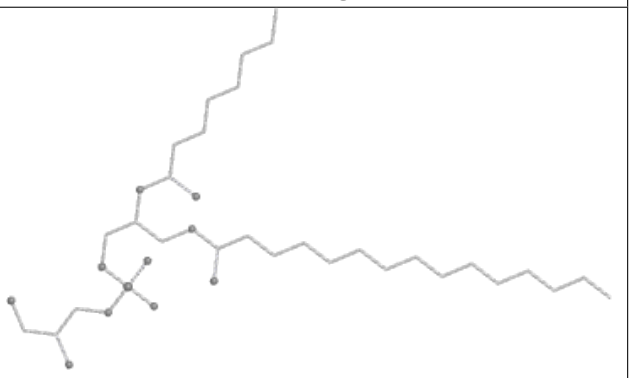
Bond lengths



Bond angles

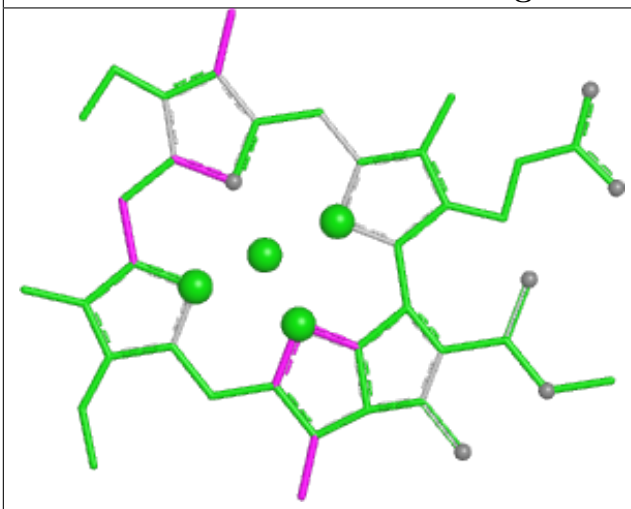


Torsions

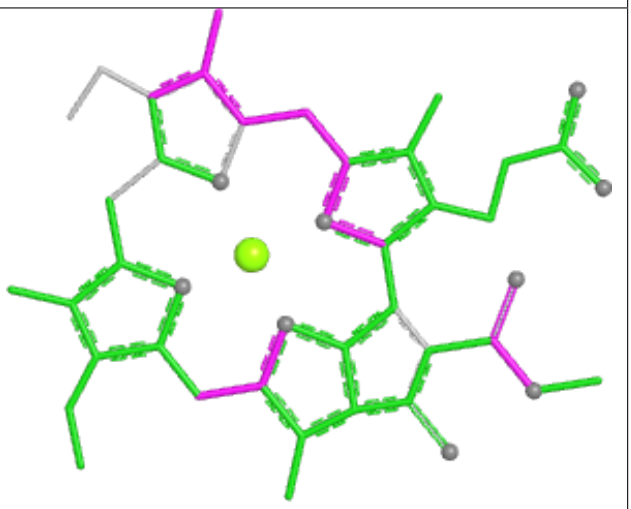


Rings

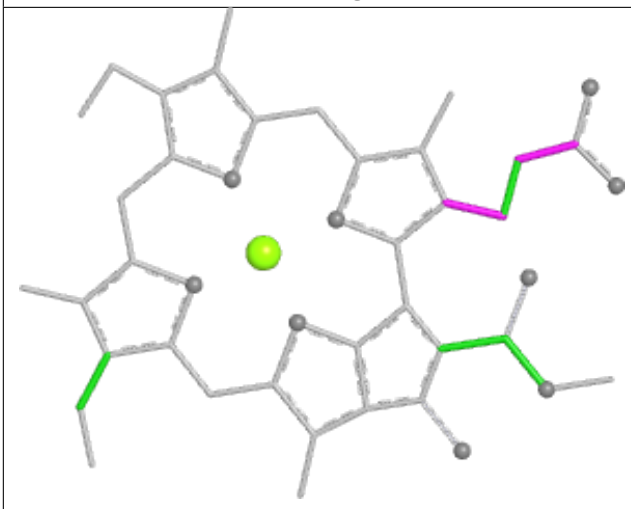
Ligand CLA A2 818



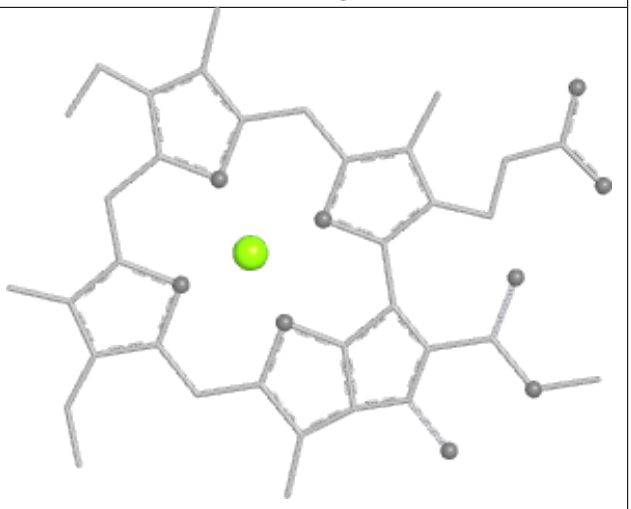
Bond lengths



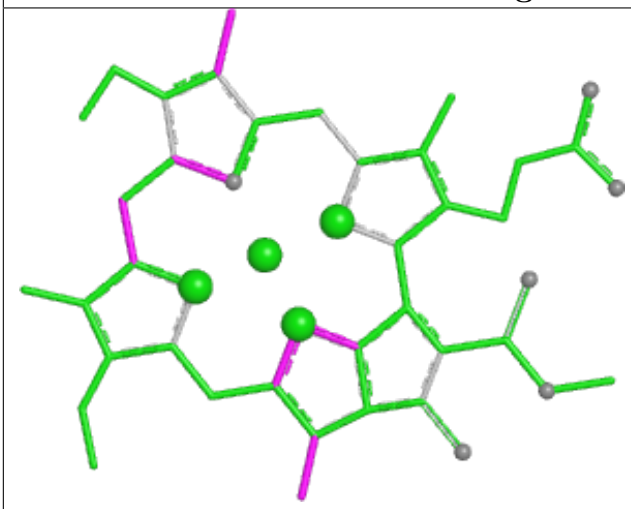
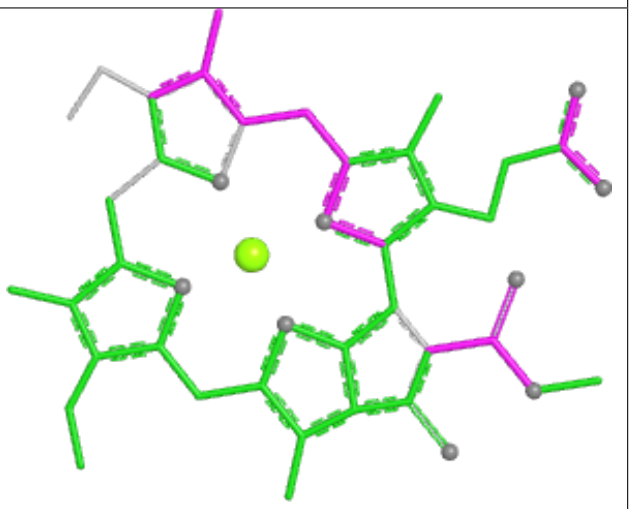
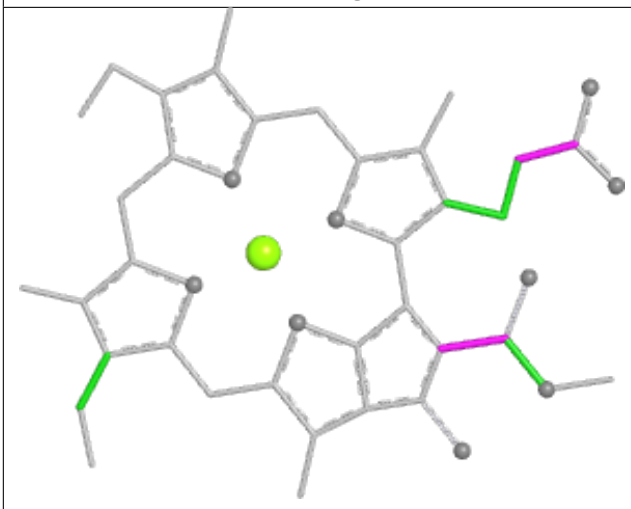
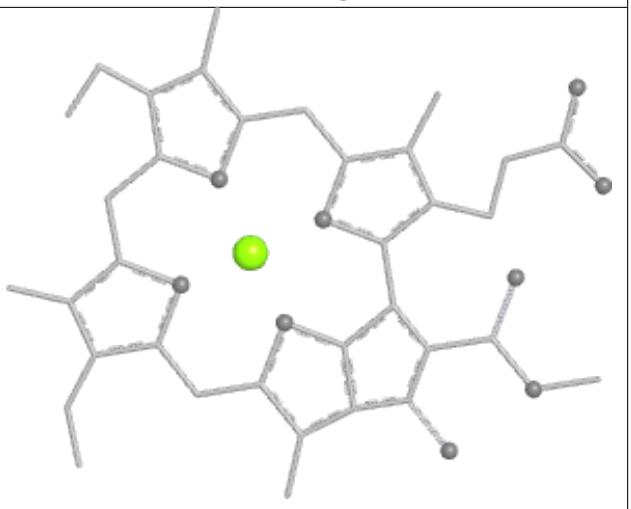
Bond angles

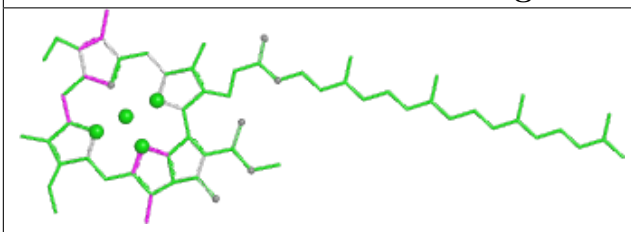
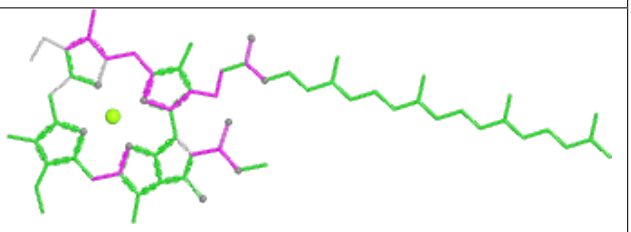
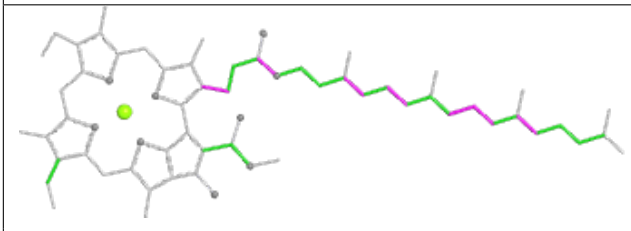
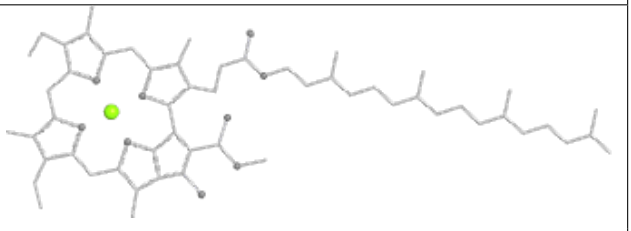


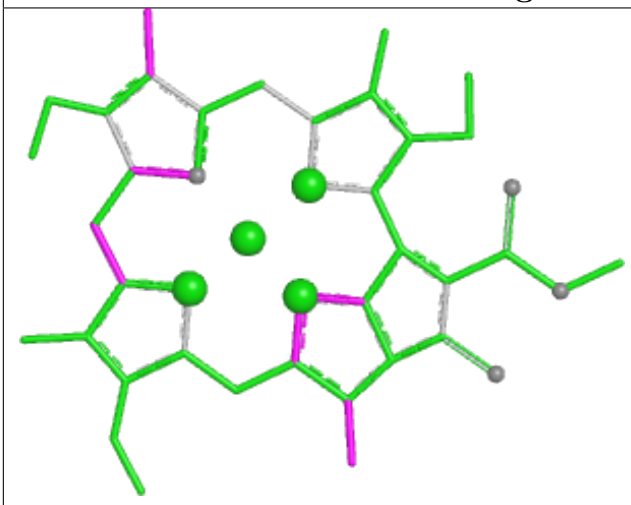
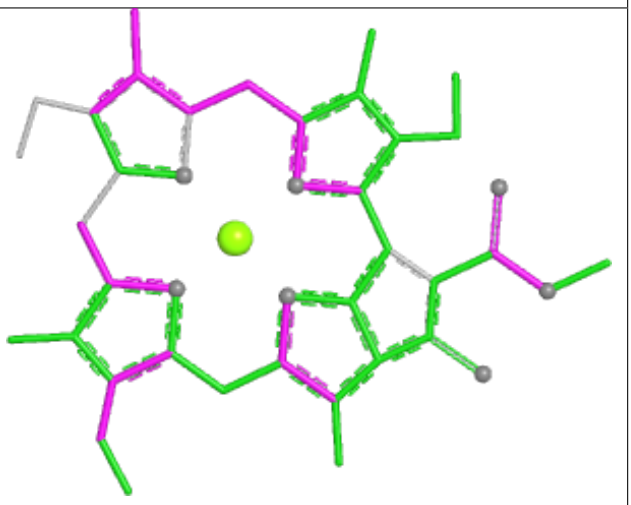
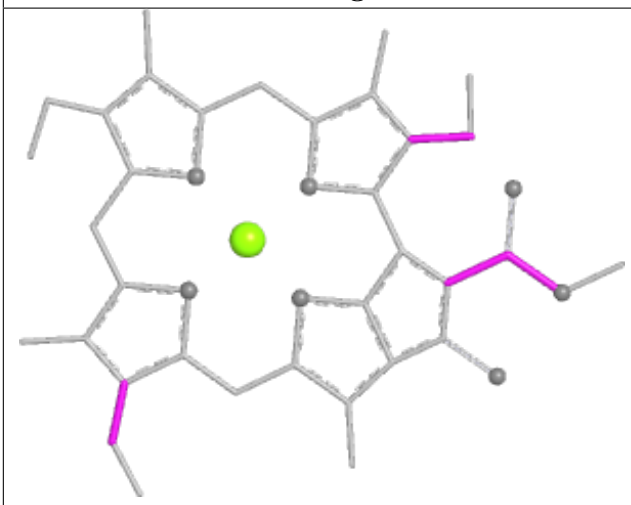
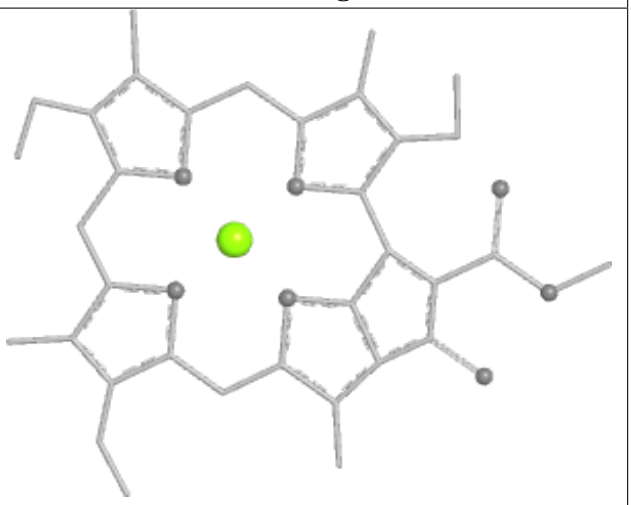
Torsions

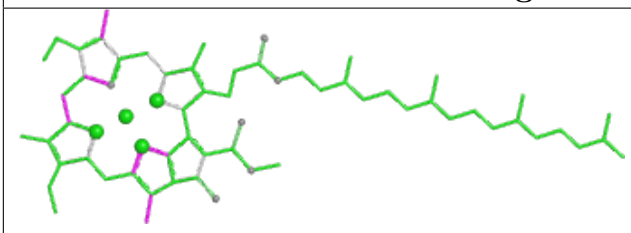
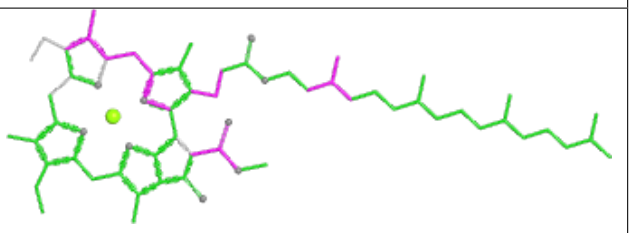
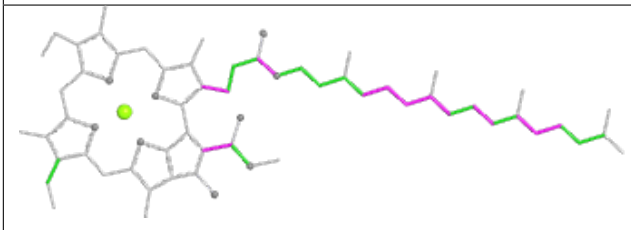
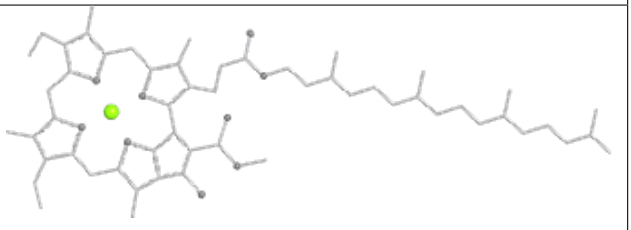


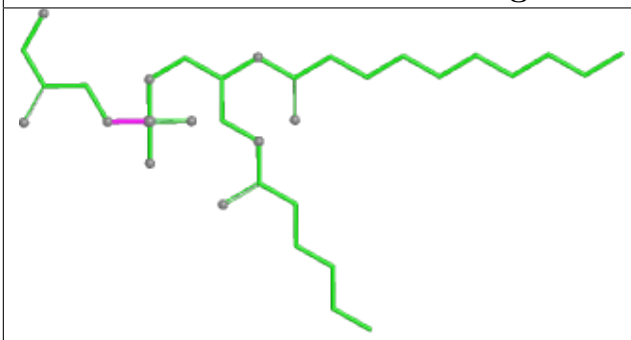
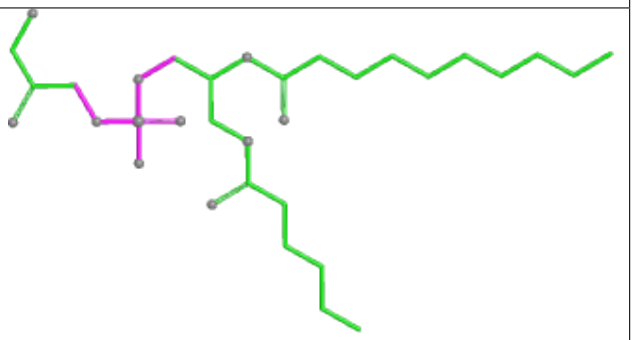
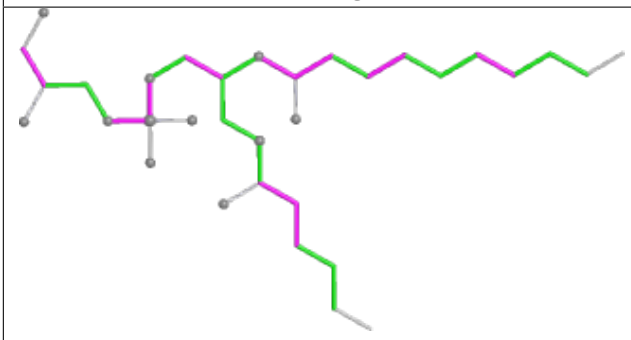
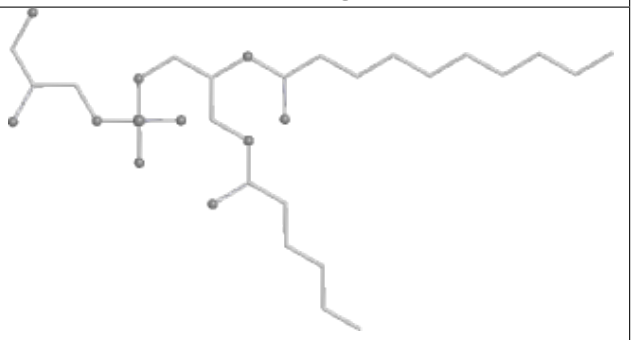
Rings

Ligand CLA B2 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA LL 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG BB 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

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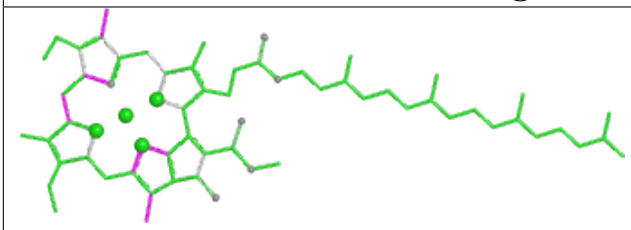
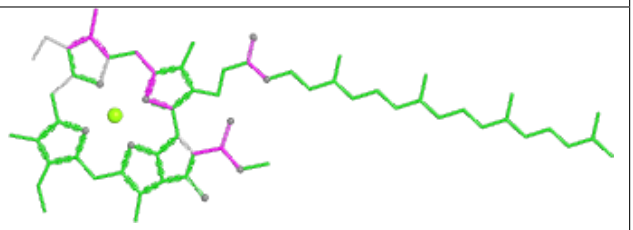
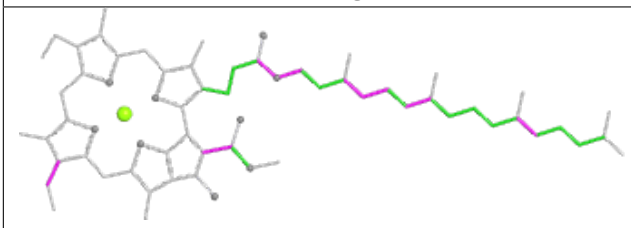
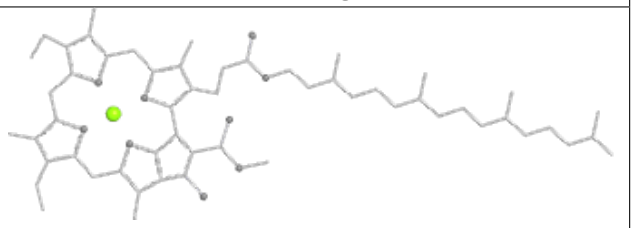
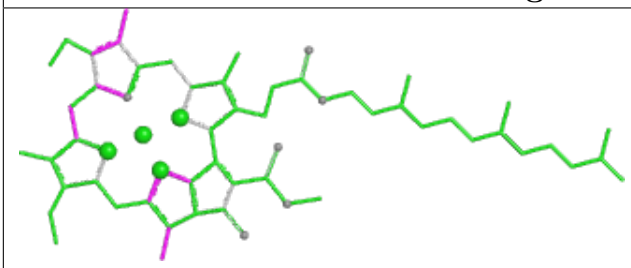
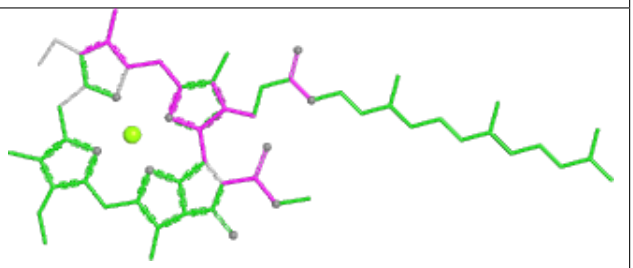
 Bond lengths	 Bond angles
 Torsions	 Rings

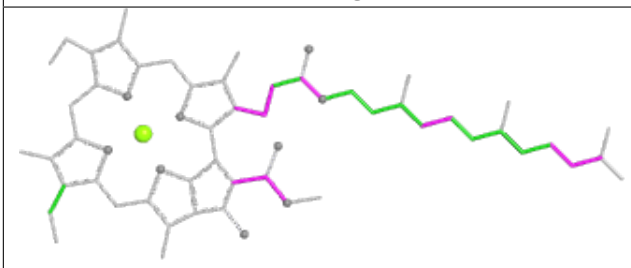
Ligand CLA F 301



Bond lengths



Bond angles



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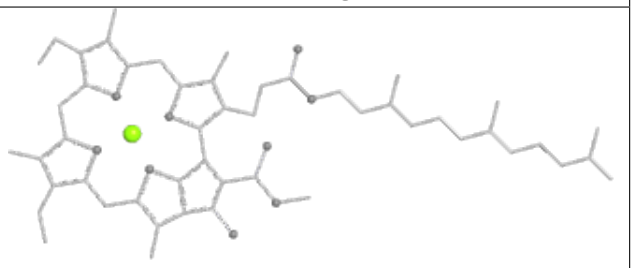
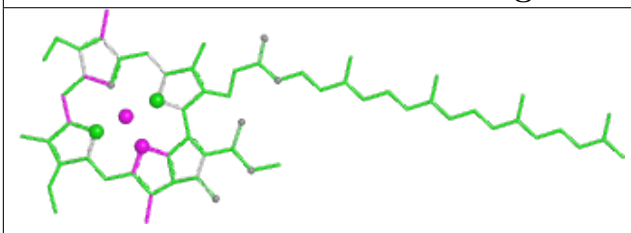
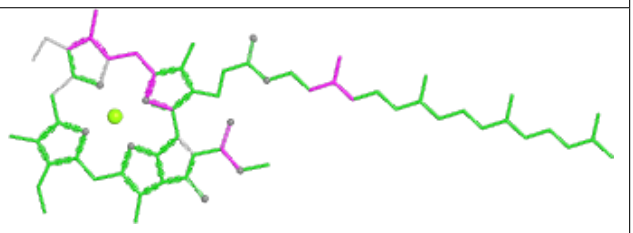


Rings

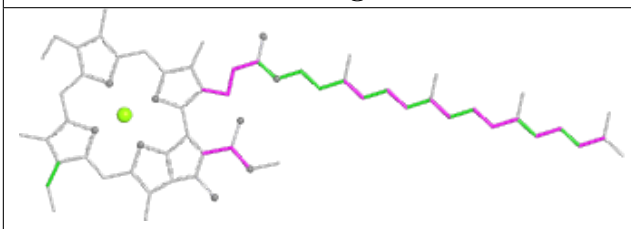
Ligand CLA A1 828



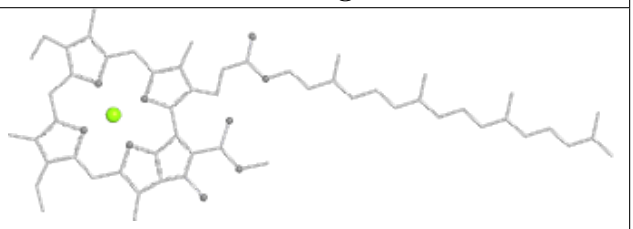
Bond lengths



Bond angles

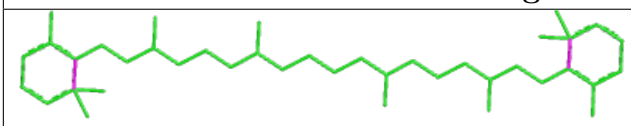


Torsions

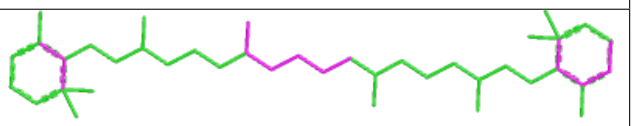


Rings

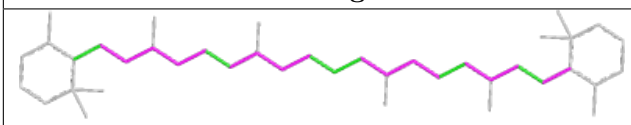
Ligand BCR B 842



Bond lengths



Bond angles



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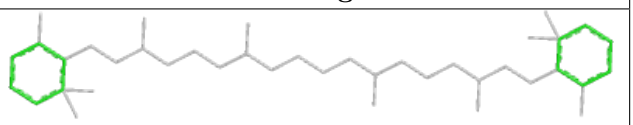
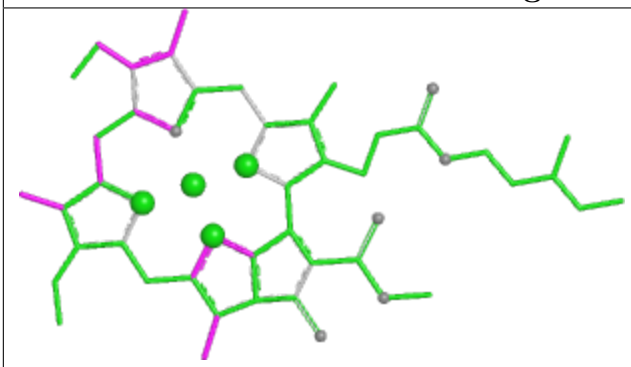
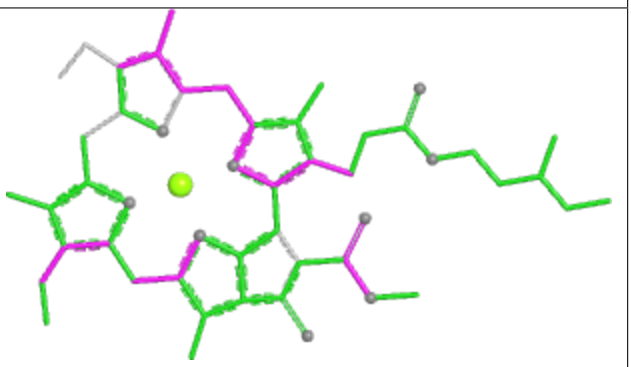
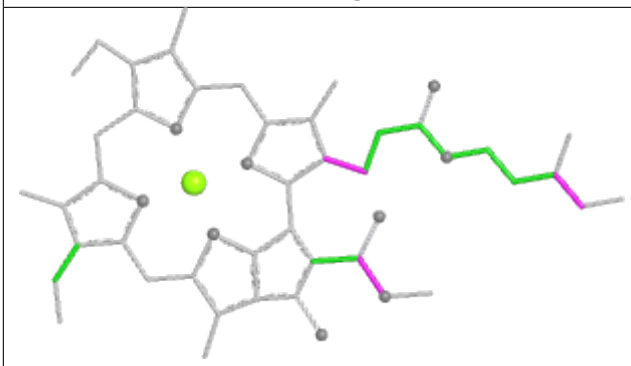
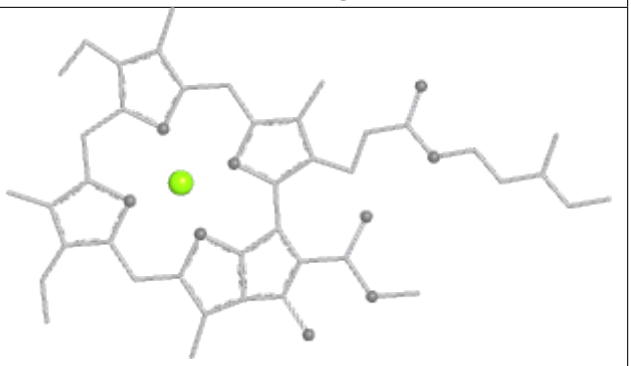
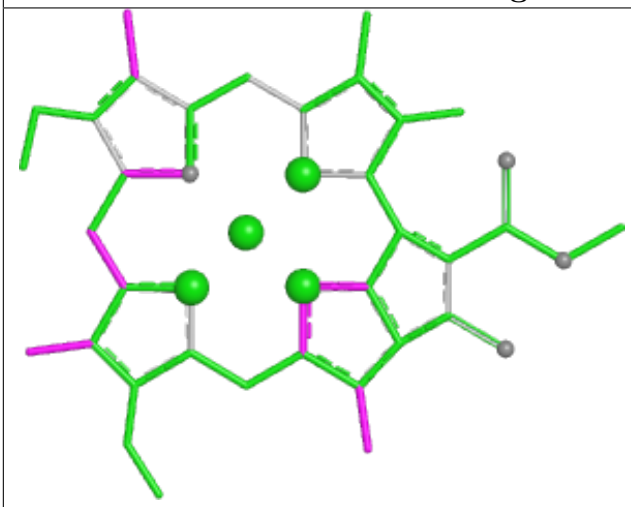


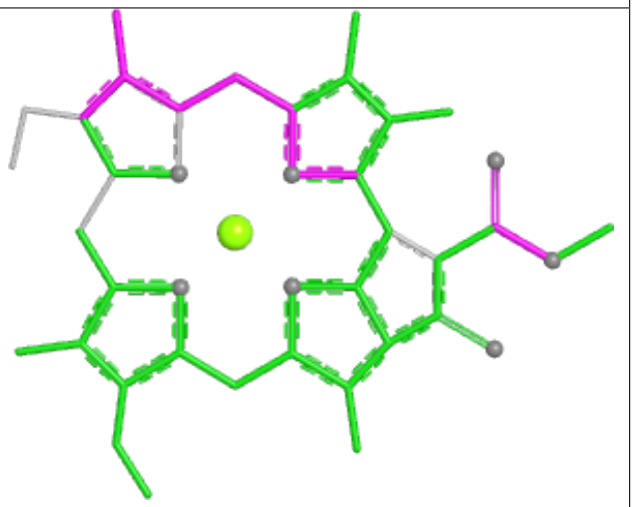
Rings

Ligand CLA A 811	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

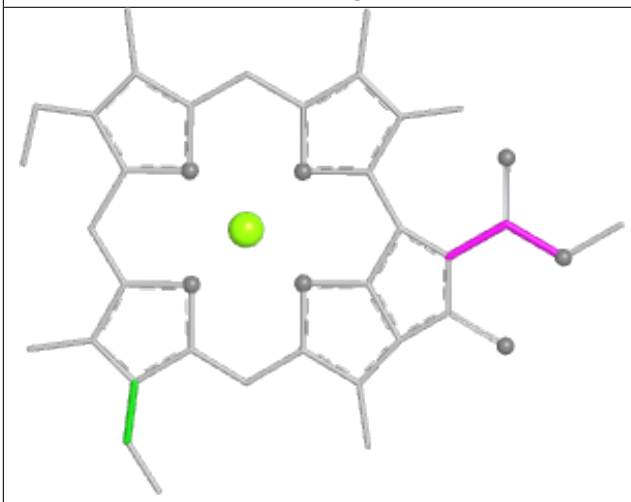
Ligand CLA AA 834



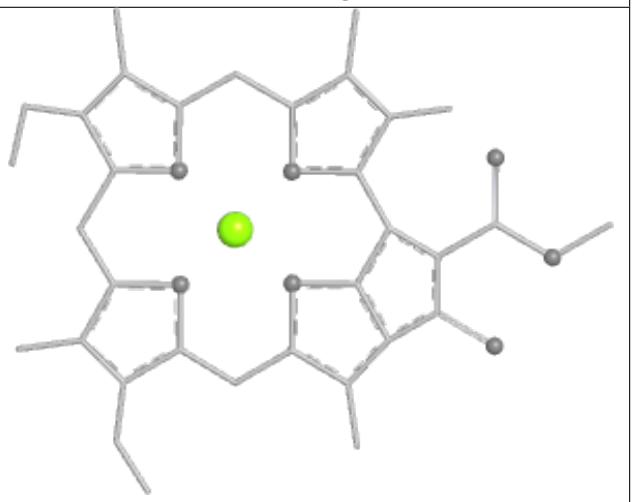
Bond lengths



Bond angles

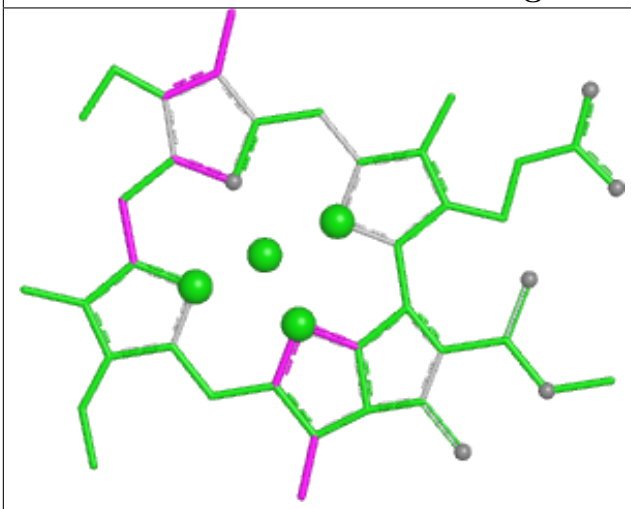


Torsions

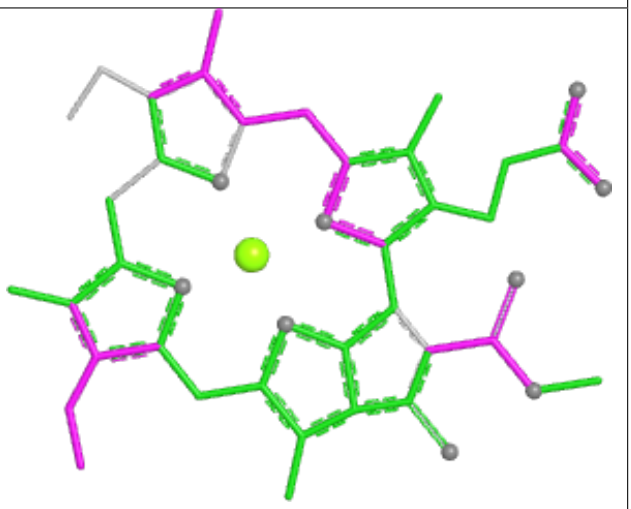


Rings

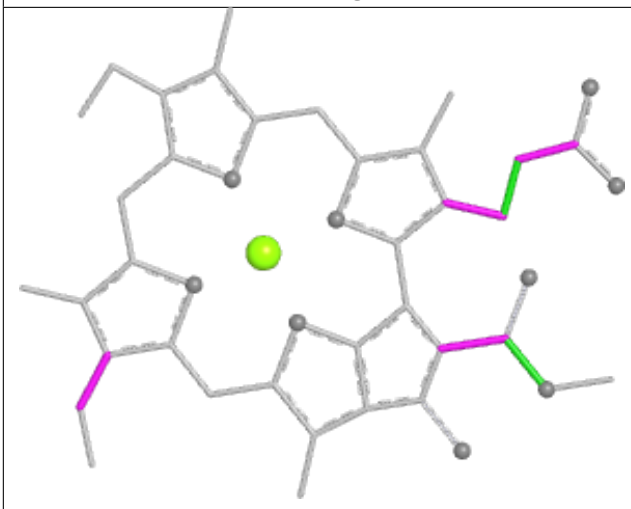
Ligand CLA B 820



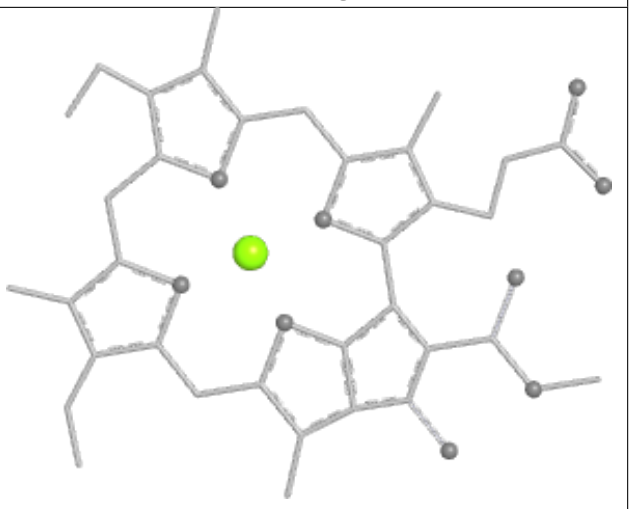
Bond lengths



Bond angles

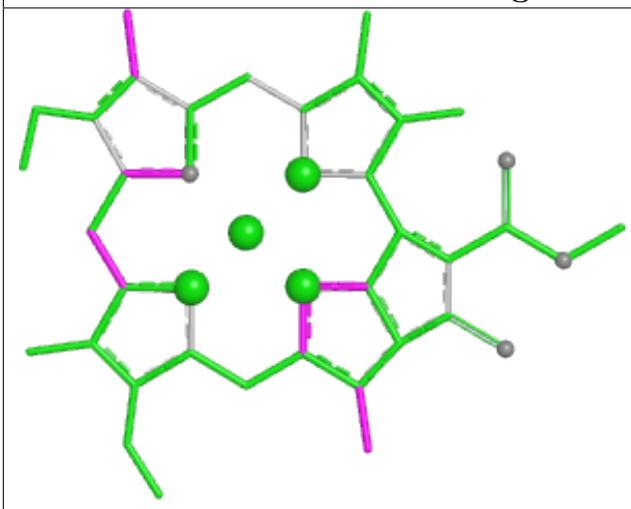


Torsions

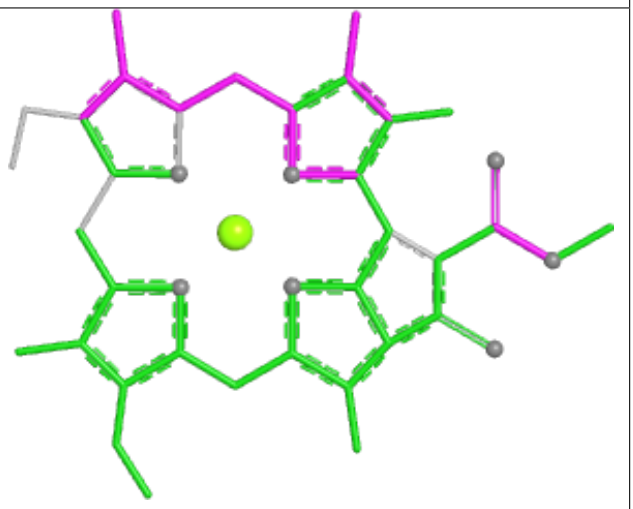


Rings

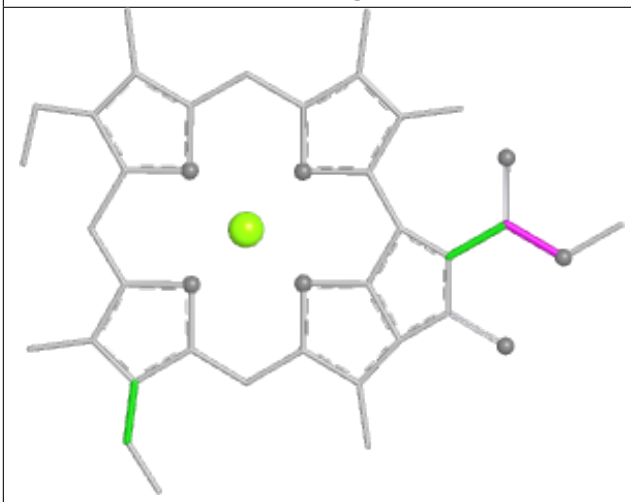
Ligand CLA BB 819



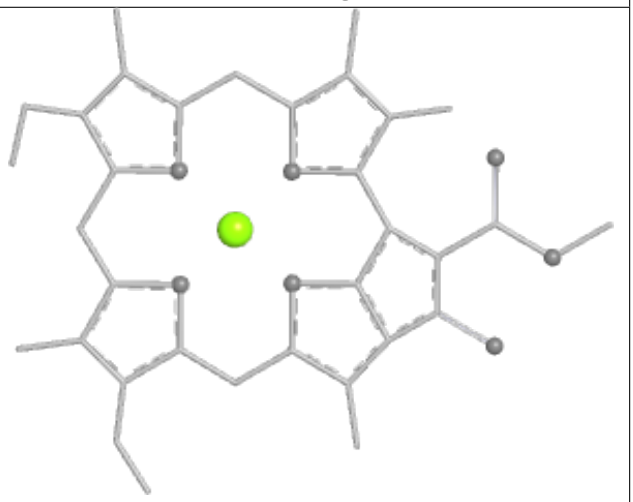
Bond lengths



Bond angles

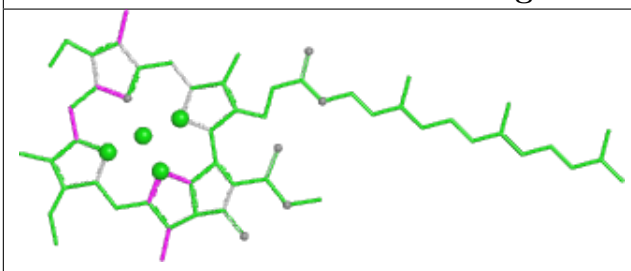


Torsions

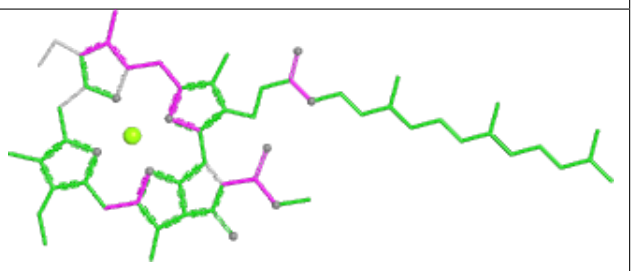


Rings

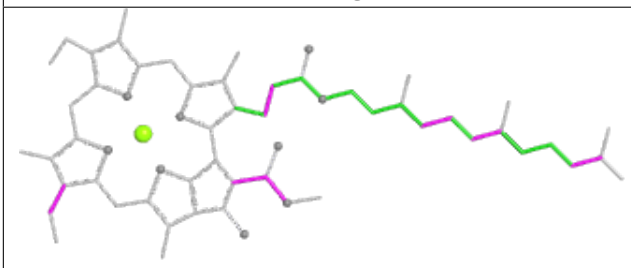
Ligand CLA B1 836



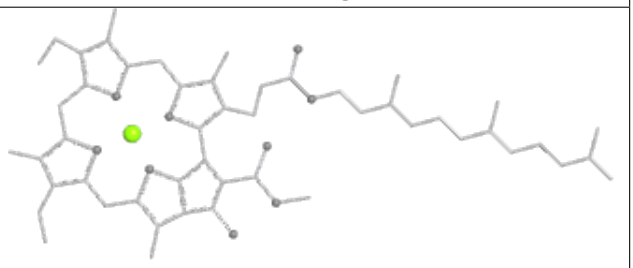
Bond lengths



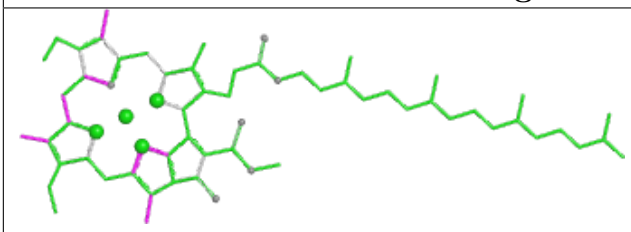
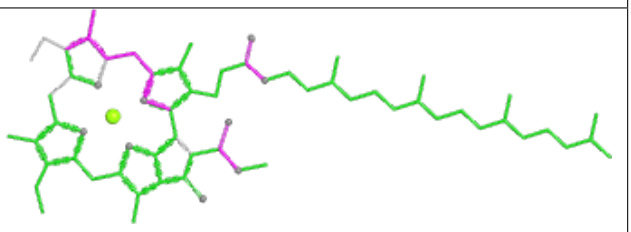
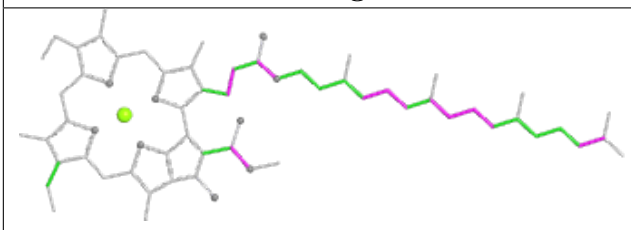
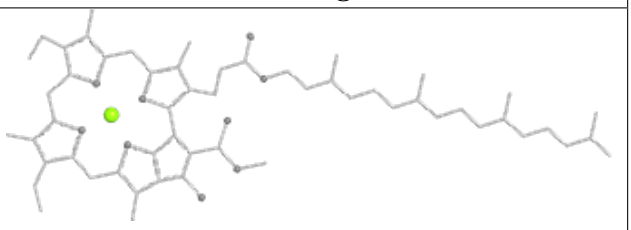
Bond angles

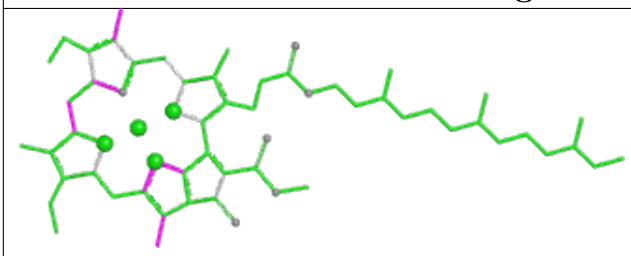
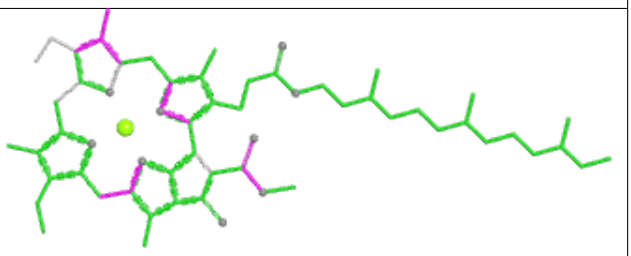
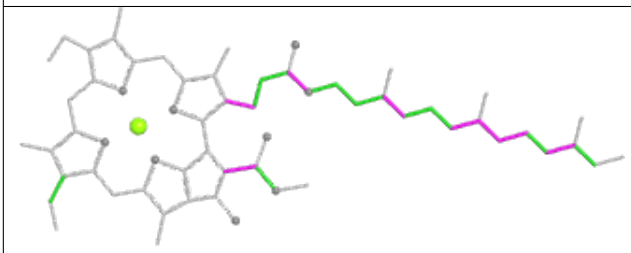
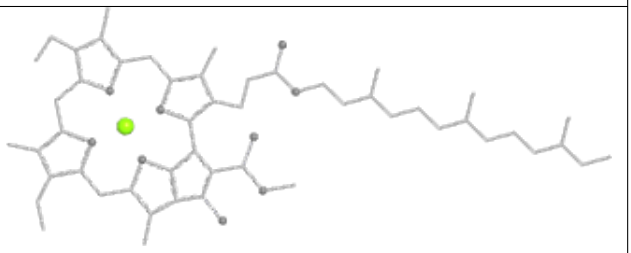


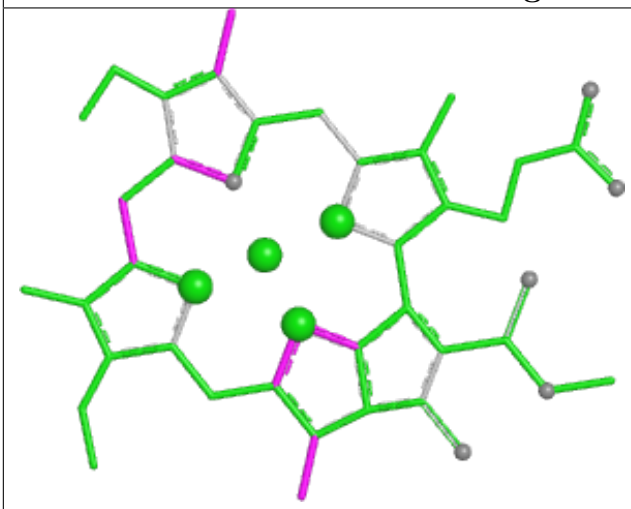
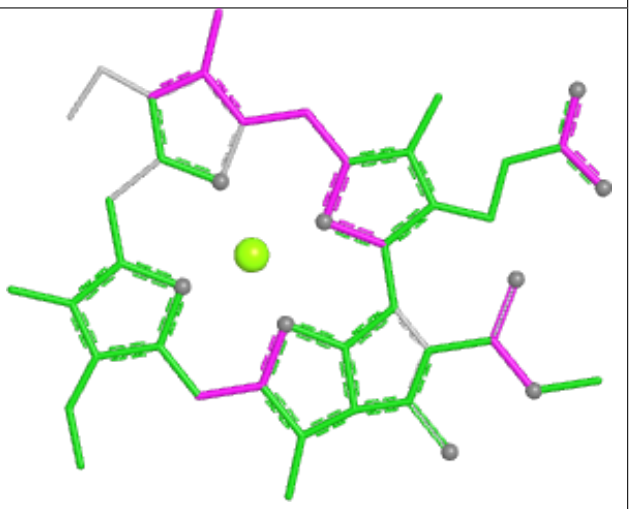
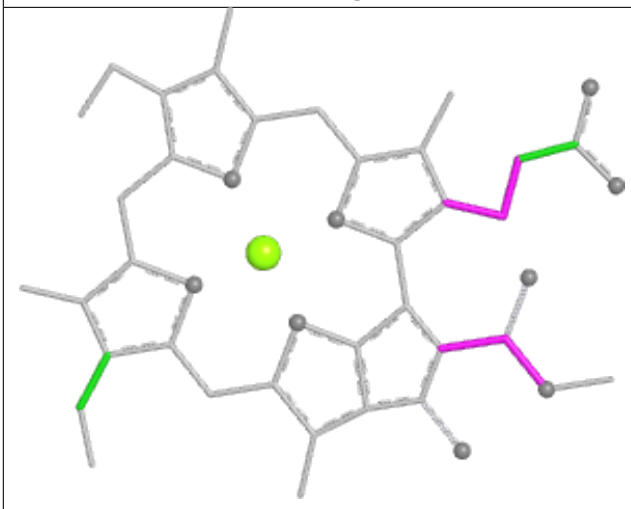
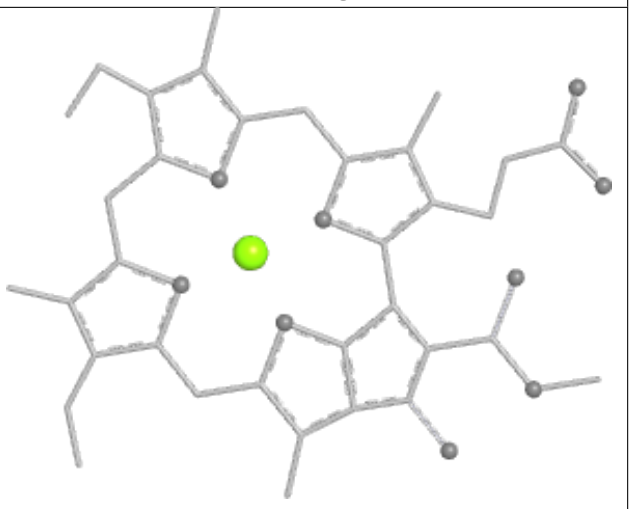
Torsions

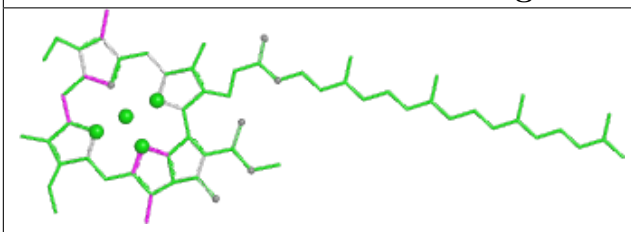
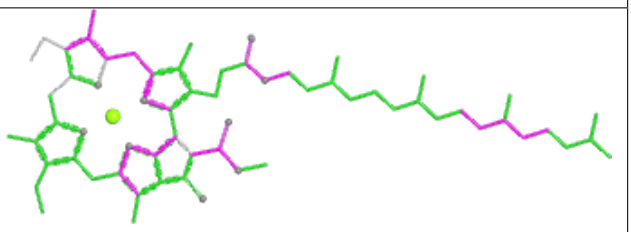
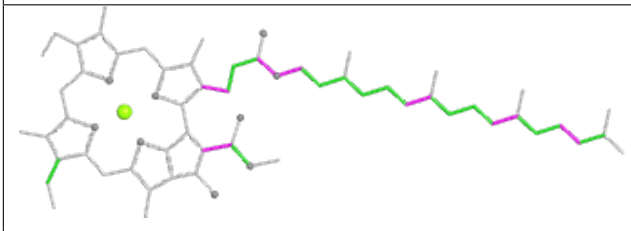
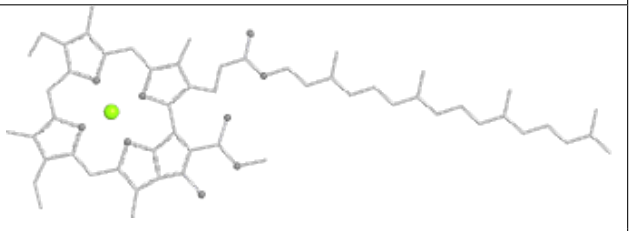


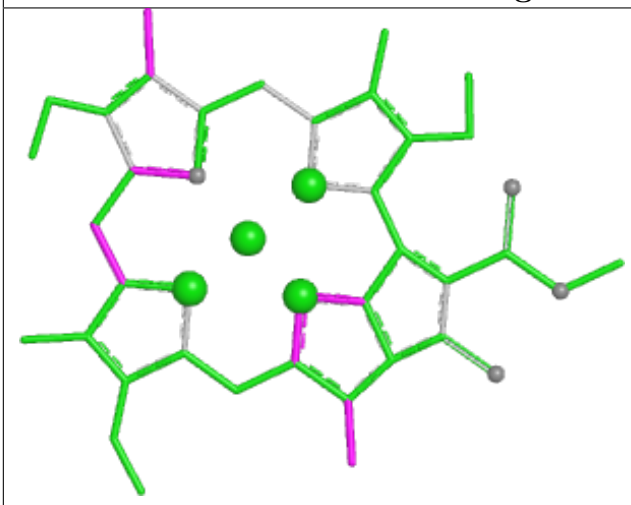
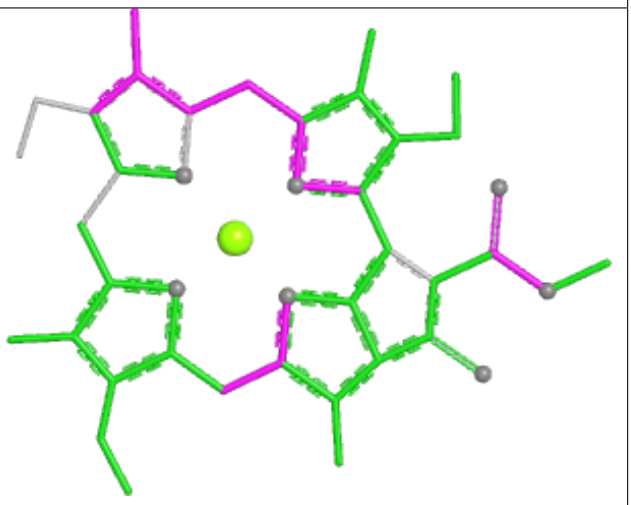
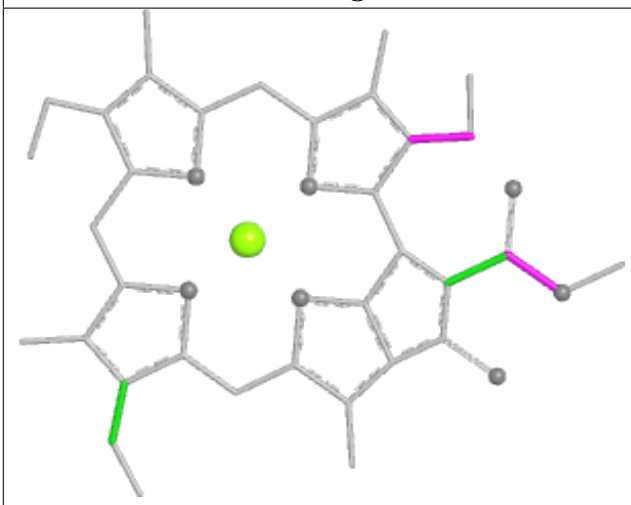
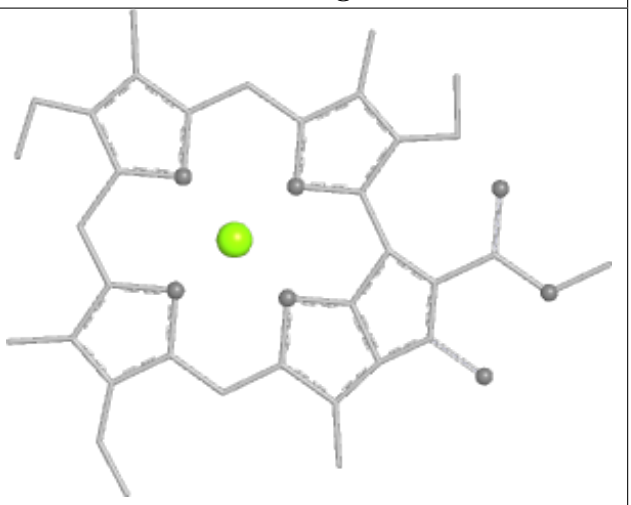
Rings

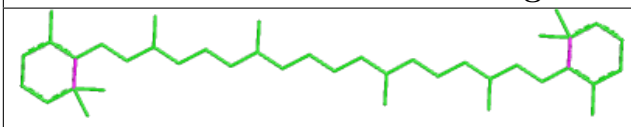
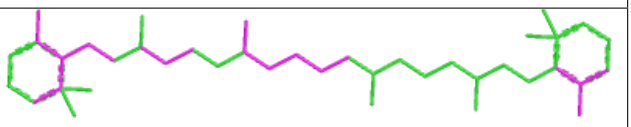
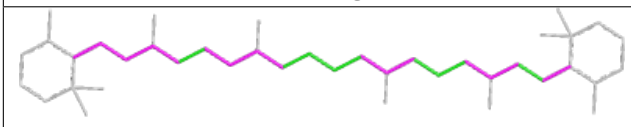
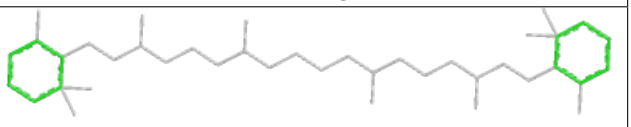
Ligand CLA A2 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

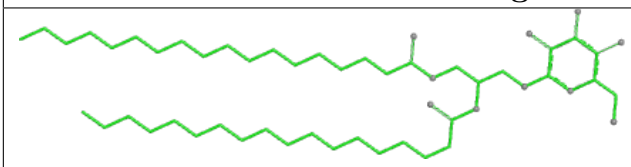
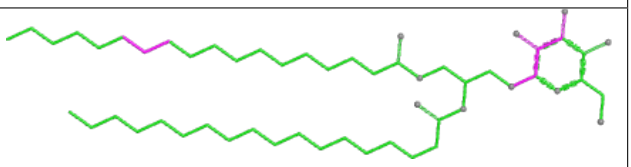
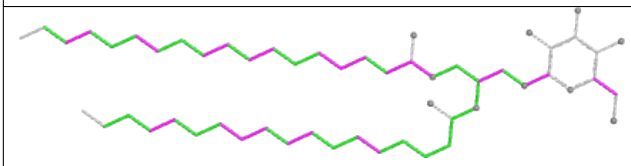
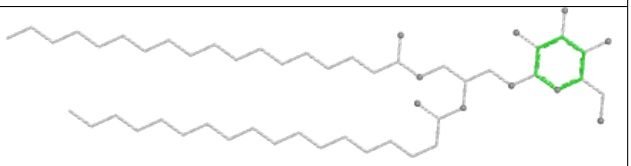
Ligand CLA B2 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

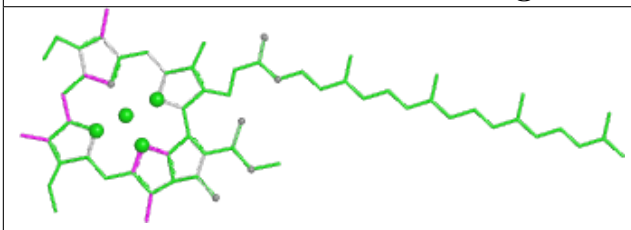
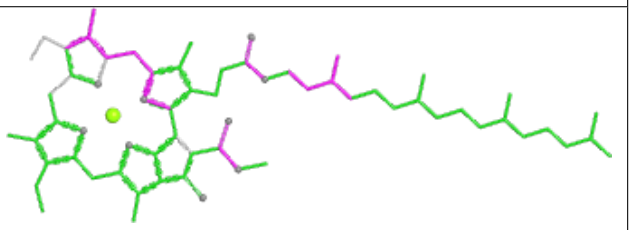
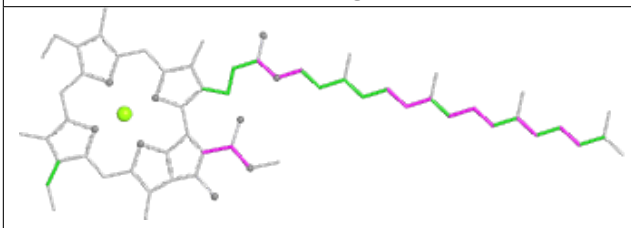
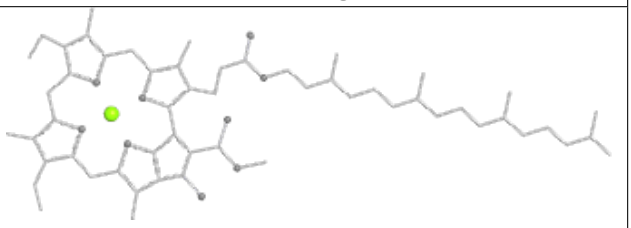
Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

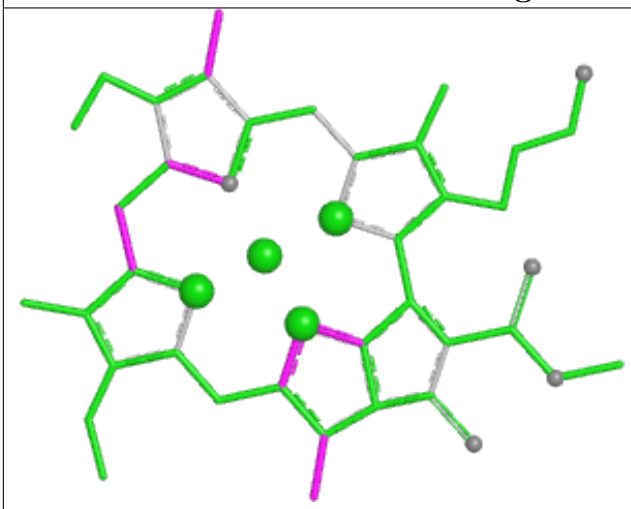
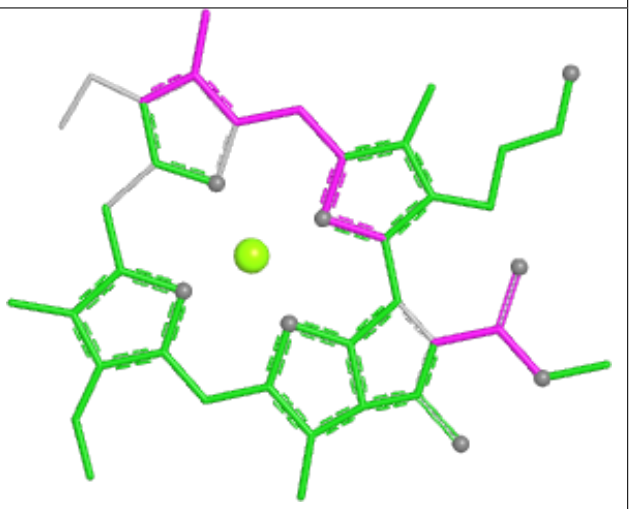
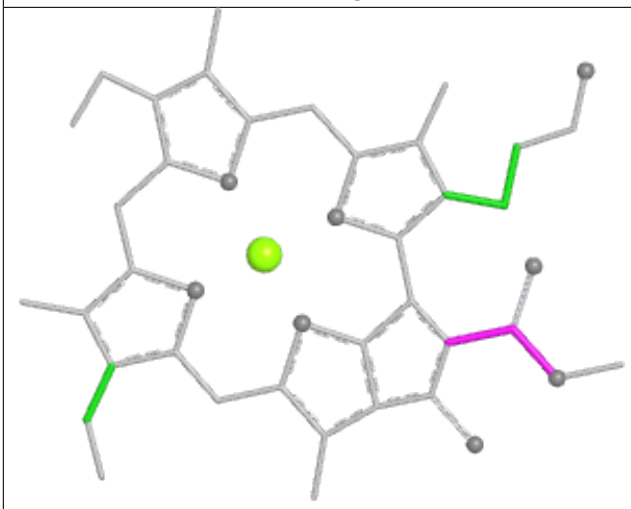
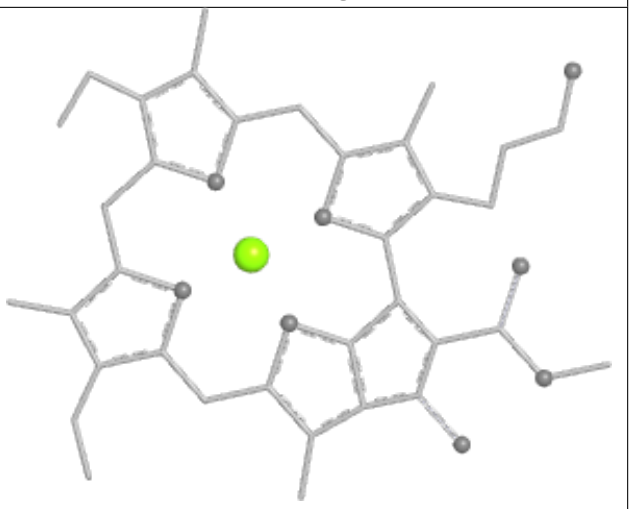
Ligand CLA B1 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

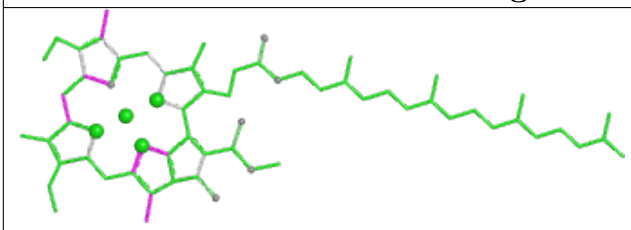
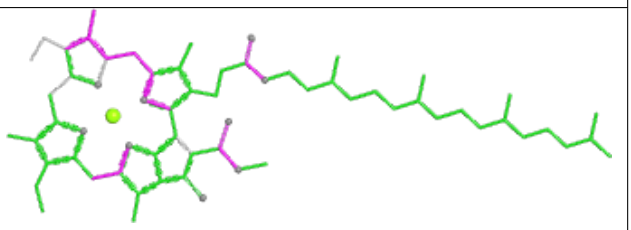
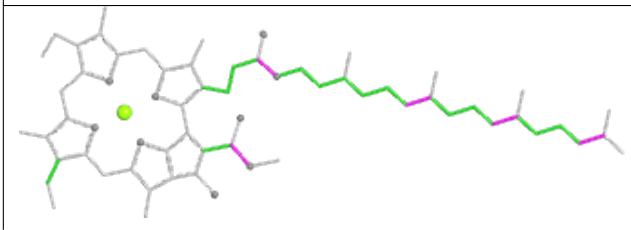
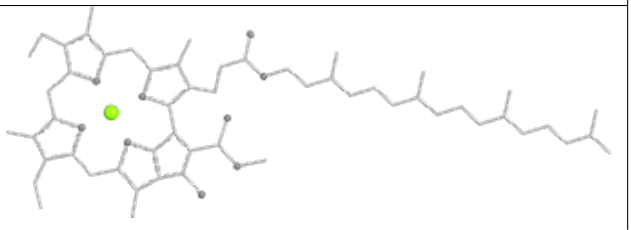
Ligand CLA A1 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

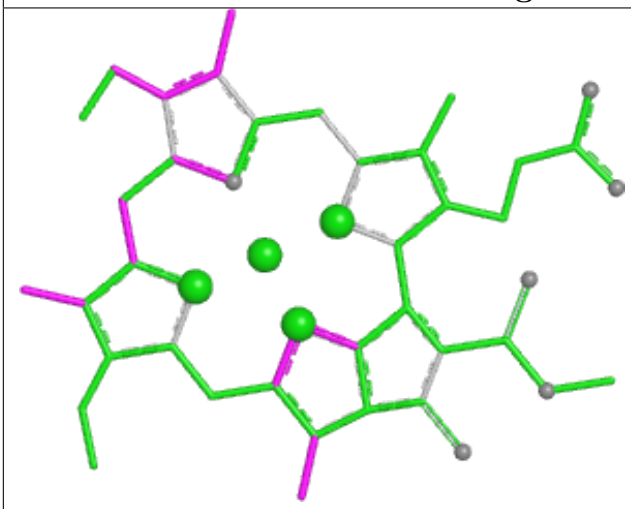
Ligand LMG B1 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

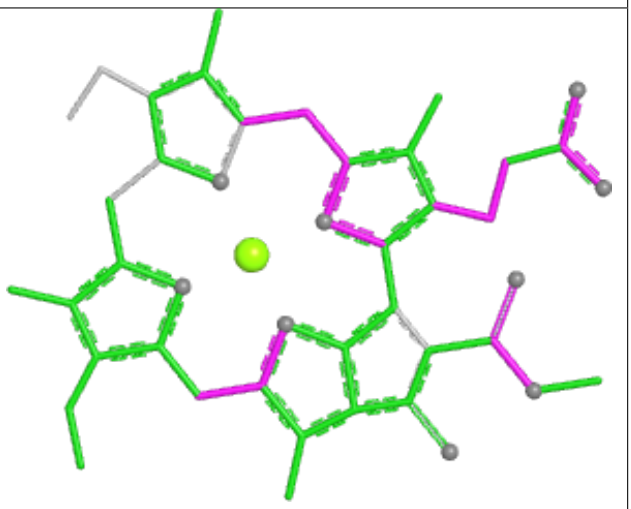
Ligand CLA A2 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

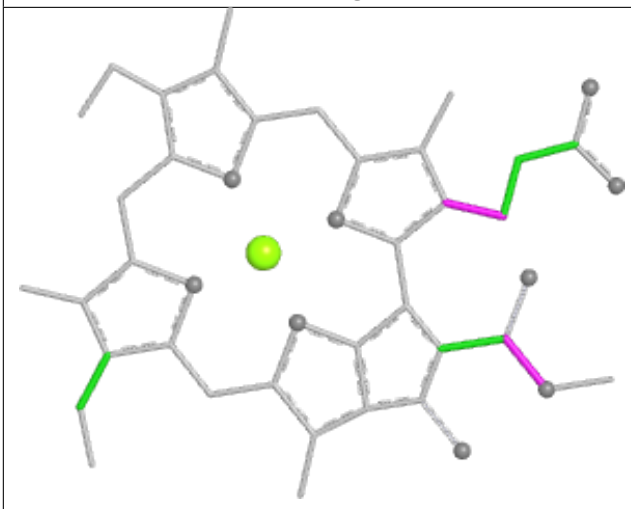
Ligand CLA B2 827



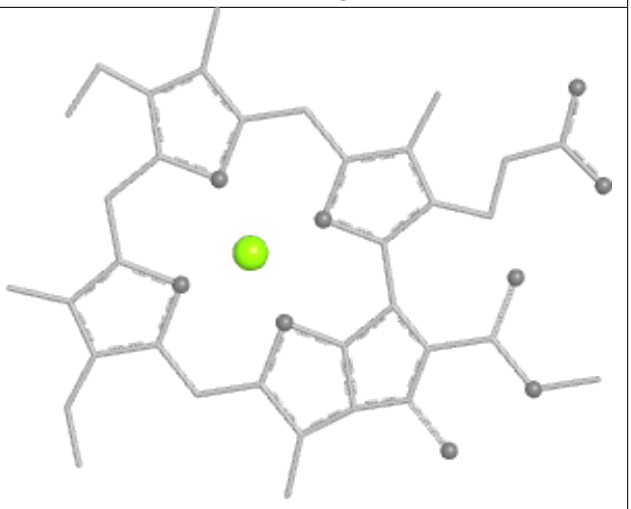
Bond lengths



Bond angles

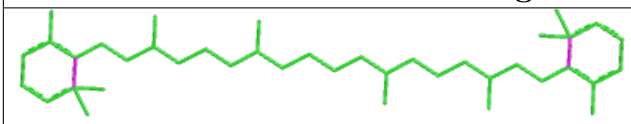


Torsions

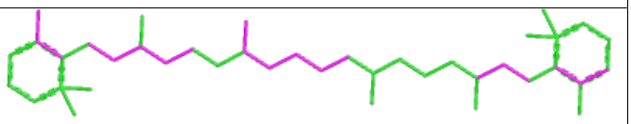


Rings

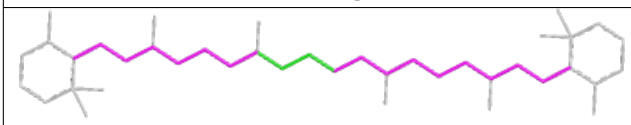
Ligand BCR F1 306



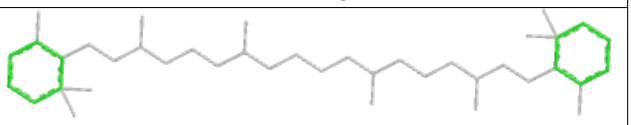
Bond lengths



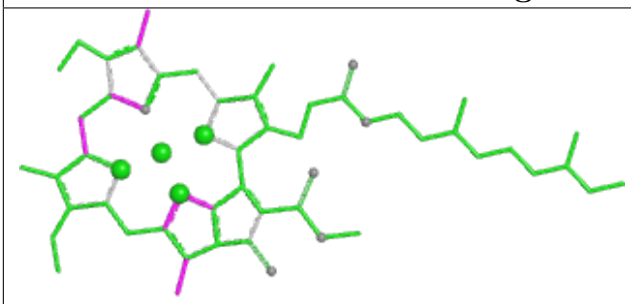
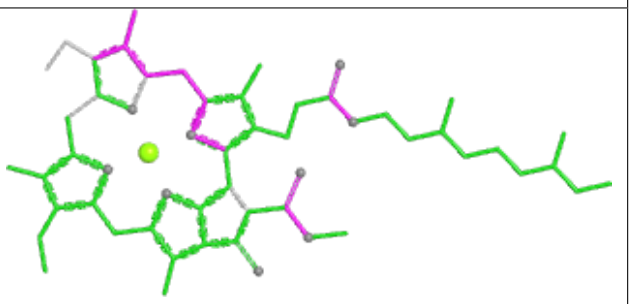
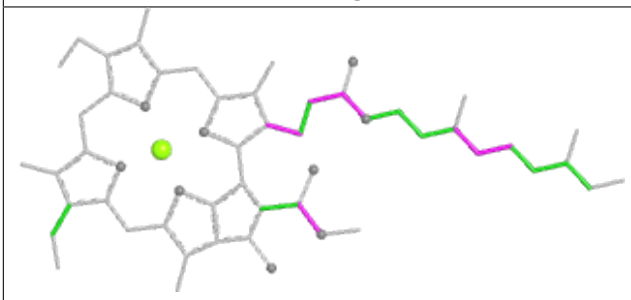
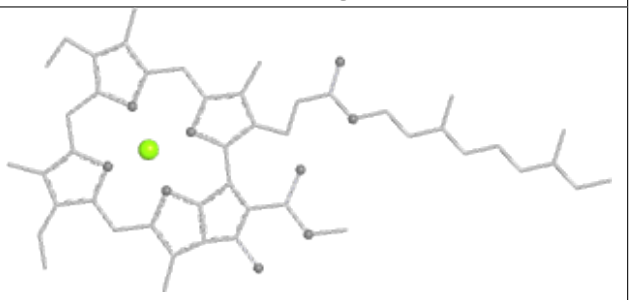
Bond angles

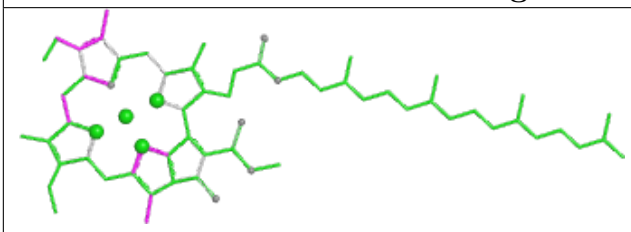
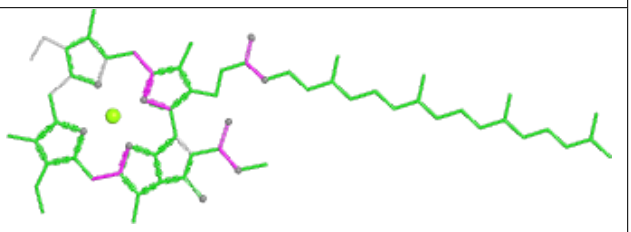
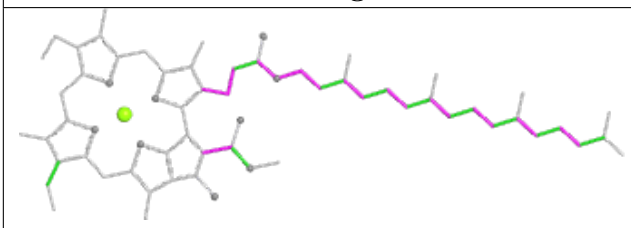
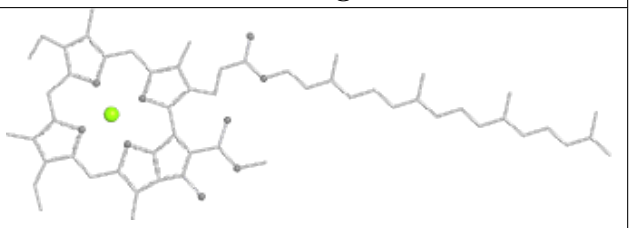


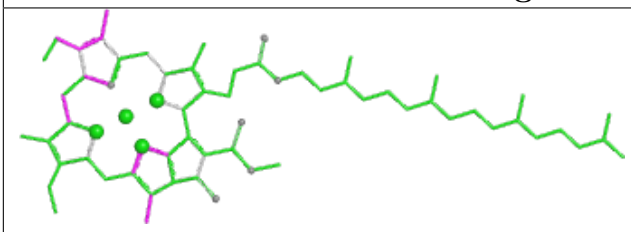
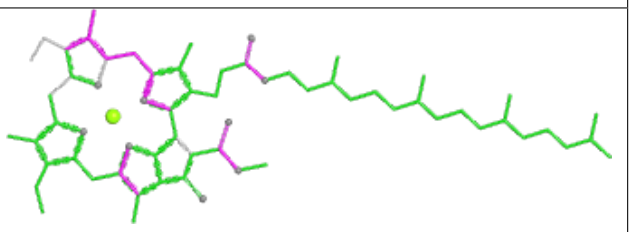
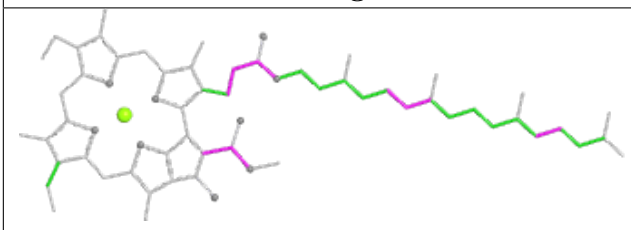
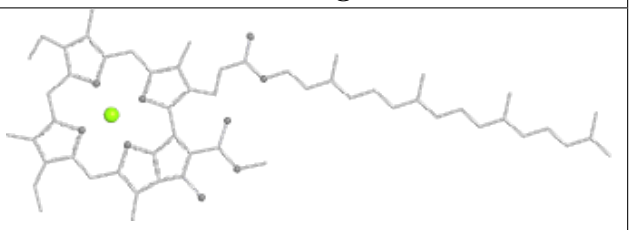
Torsions

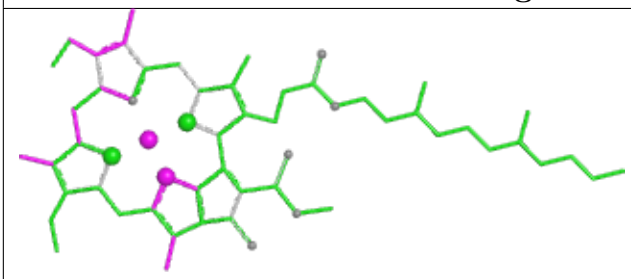
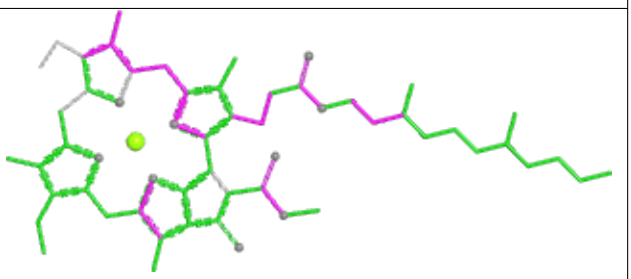
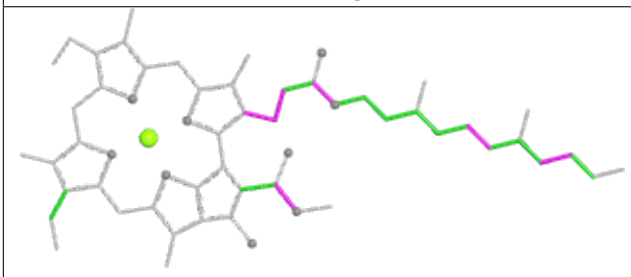
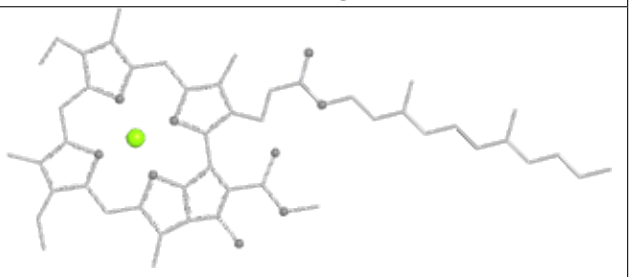


Rings

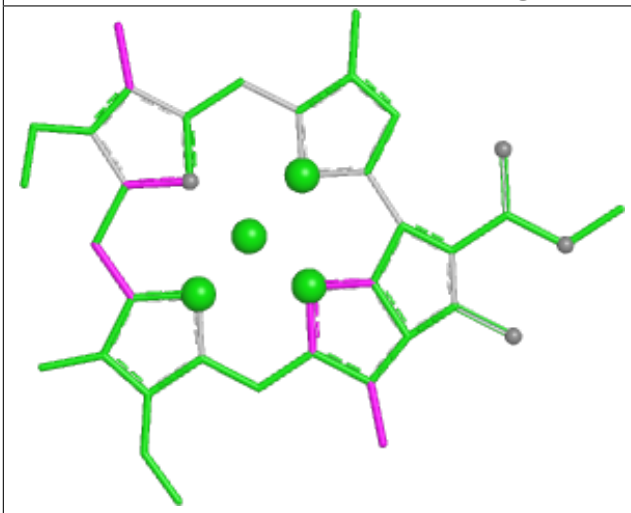
Ligand CLA A1 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

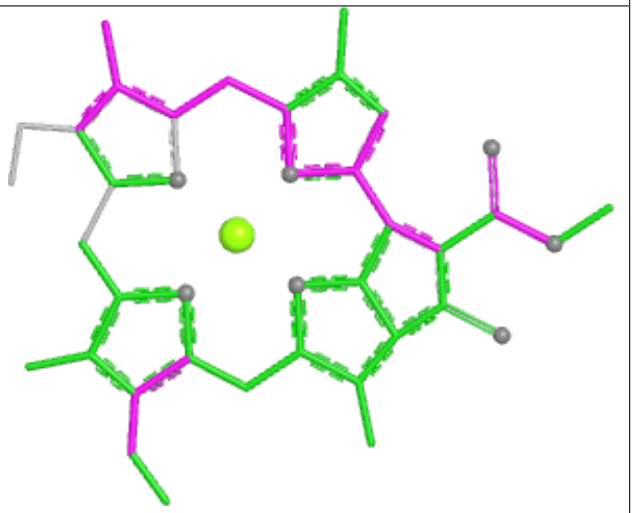
Ligand CLA A2 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

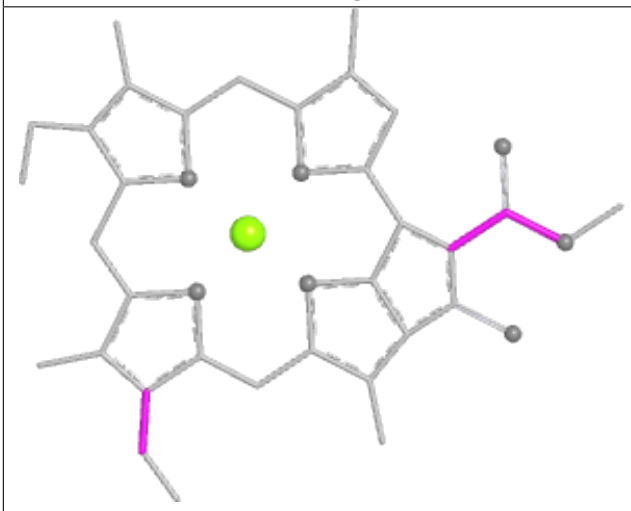
Ligand CLA K1 105



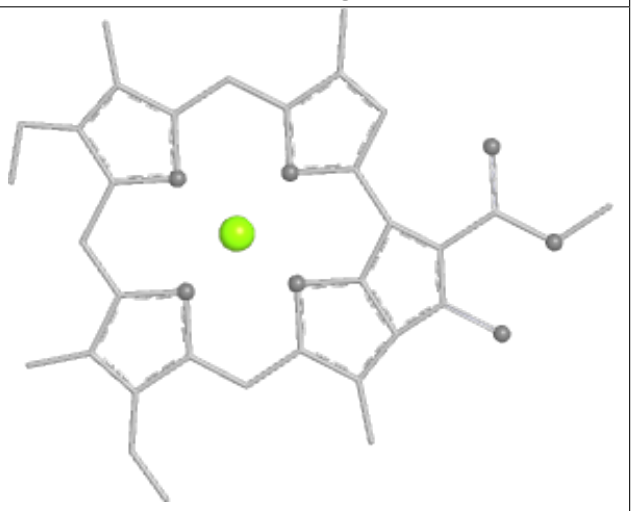
Bond lengths



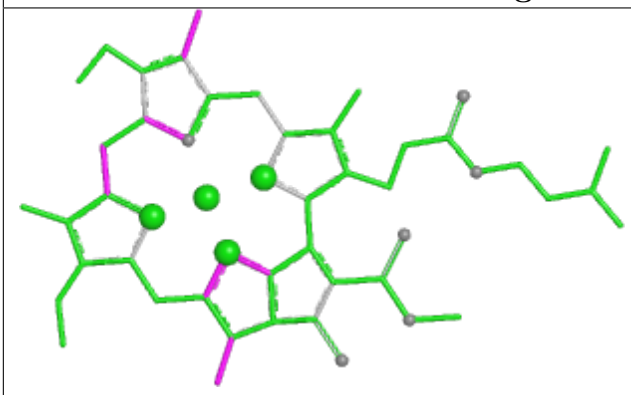
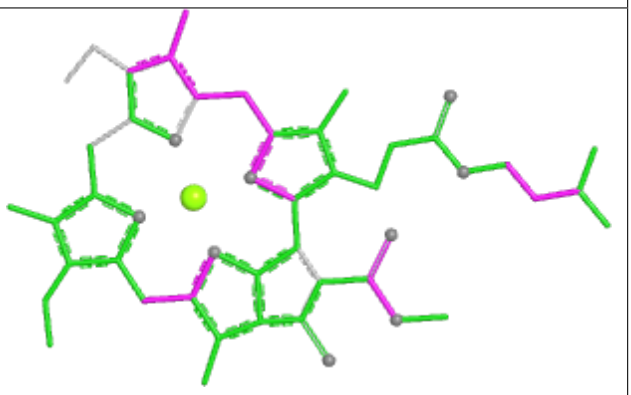
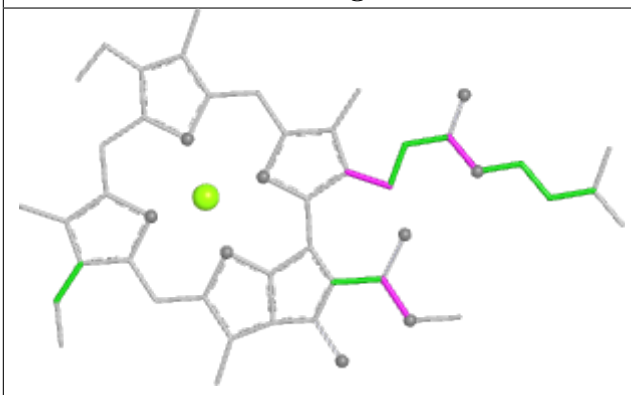
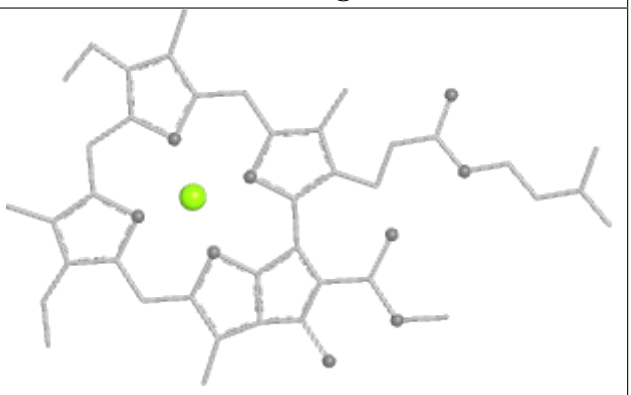
Bond angles



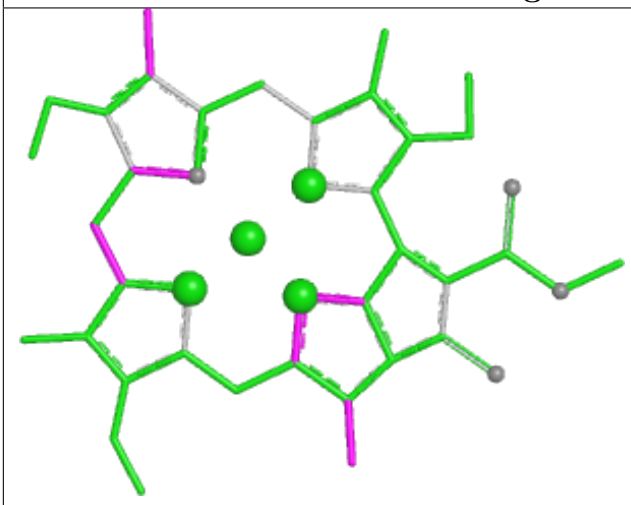
Torsions



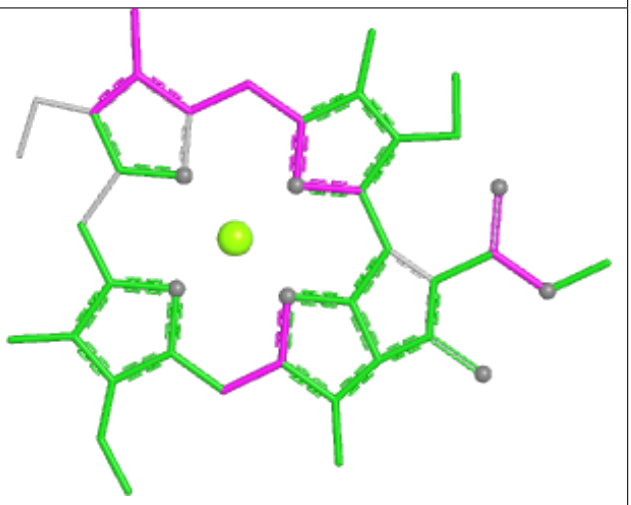
Rings

Ligand CLA A2 816	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

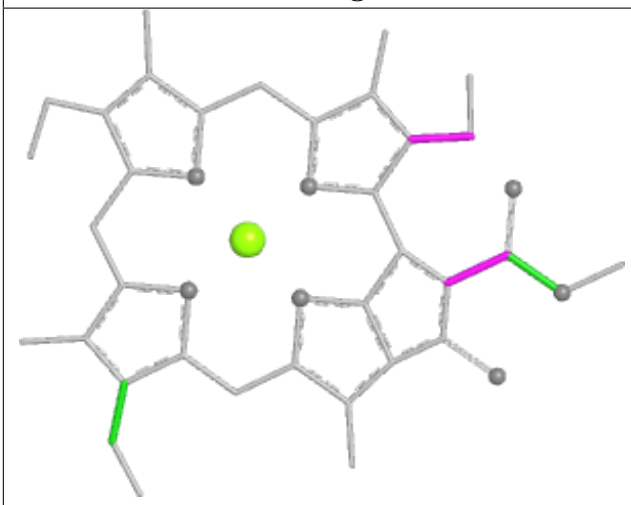
Ligand CLA A 814



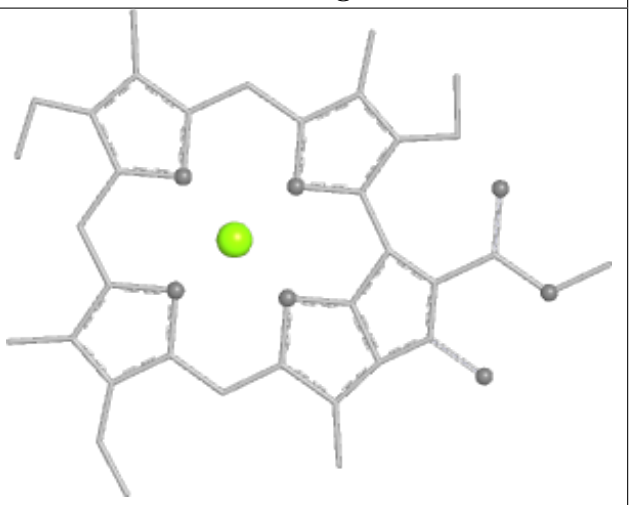
Bond lengths



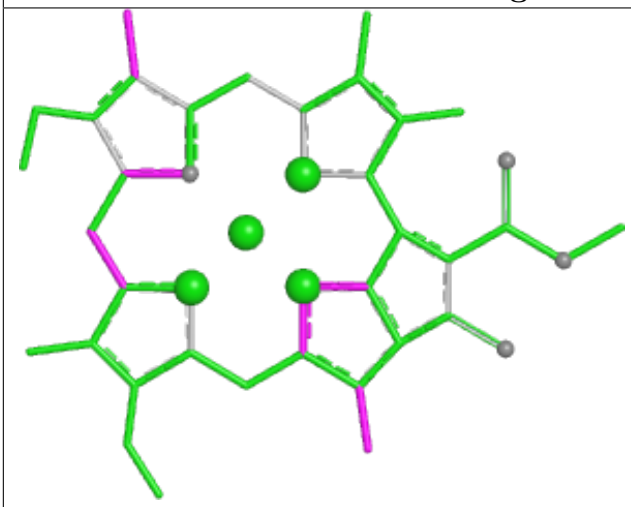
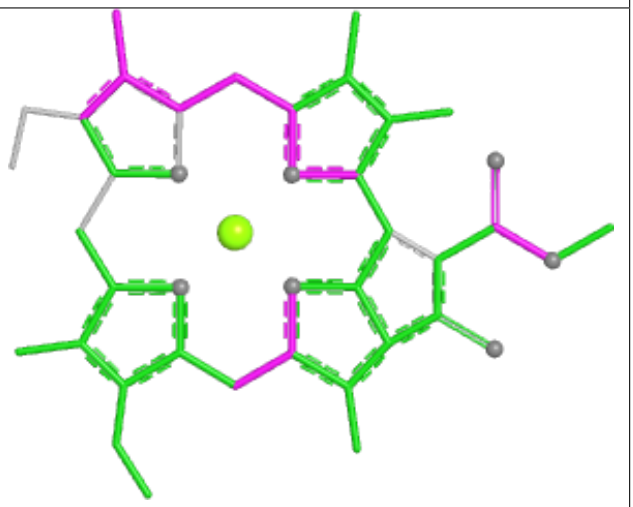
Bond angles



Torsions



Rings

Ligand CLA AA 845	
	
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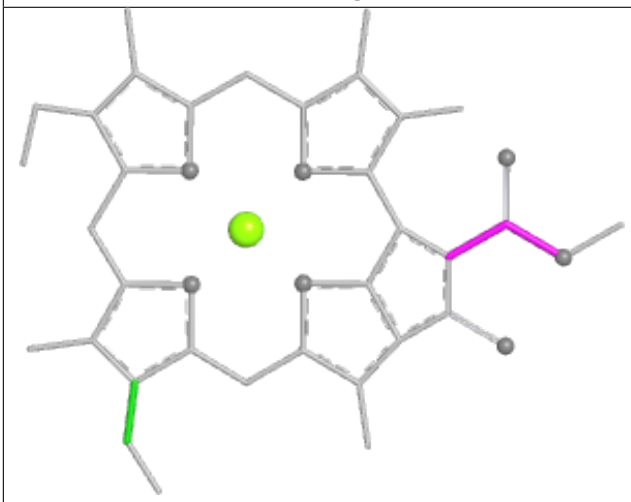
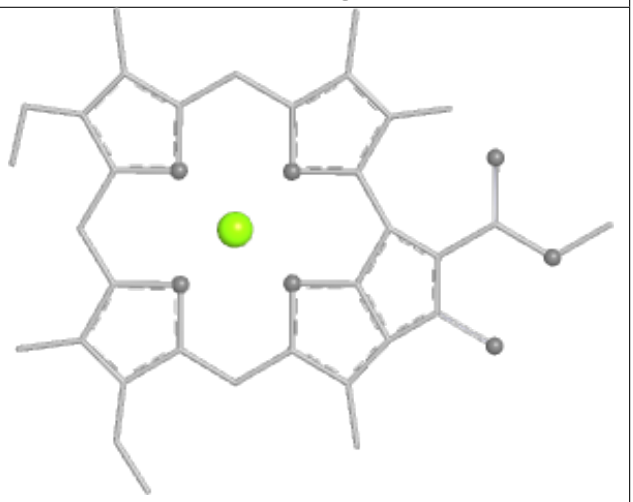
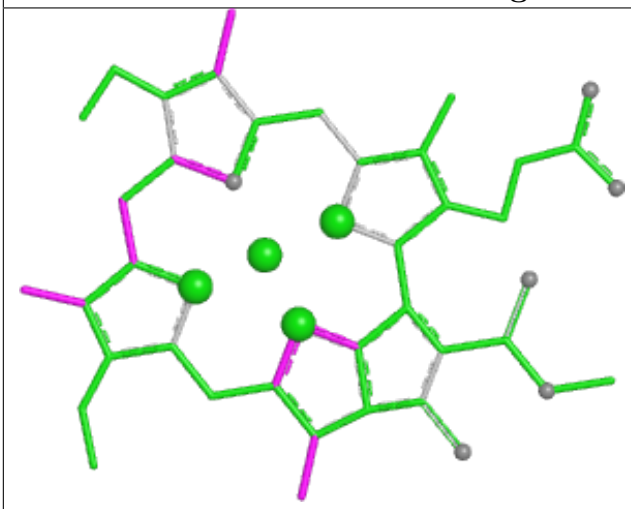
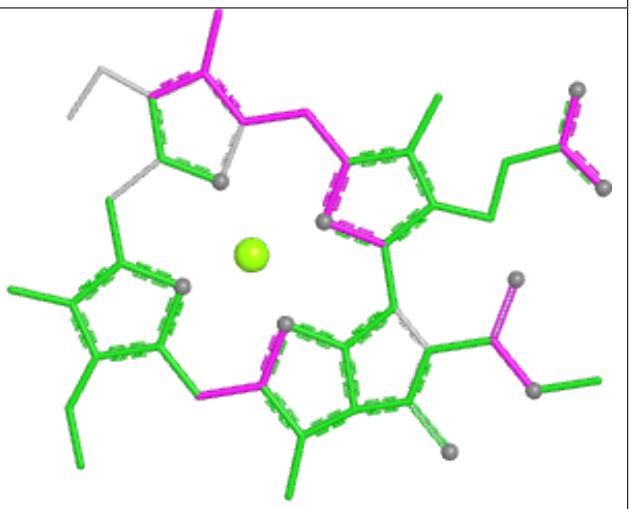
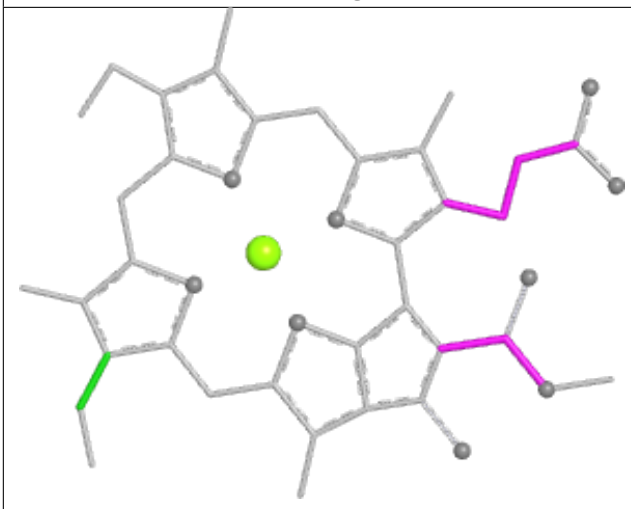
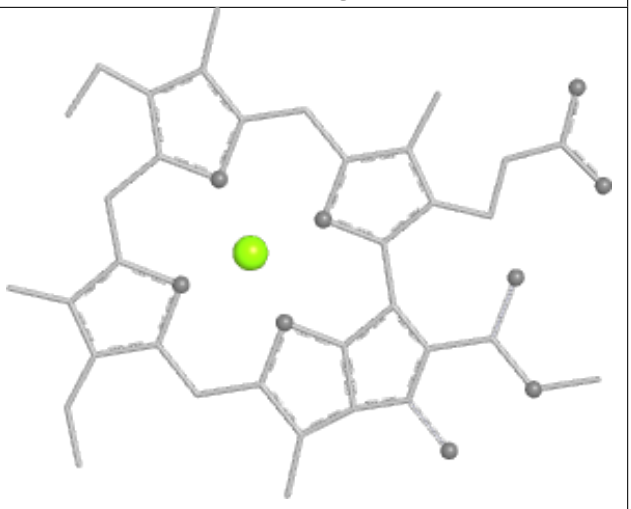
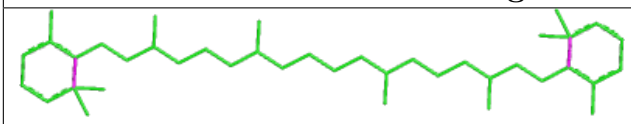
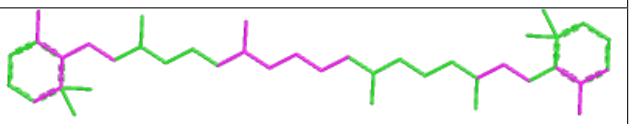
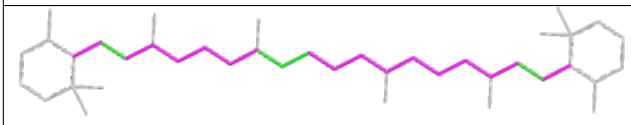
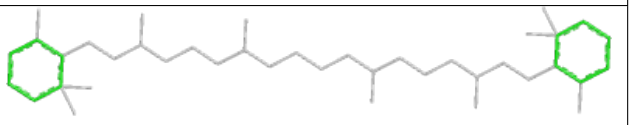
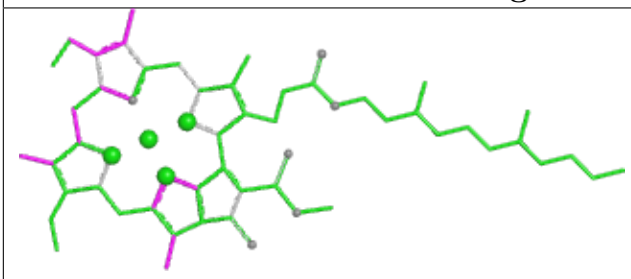
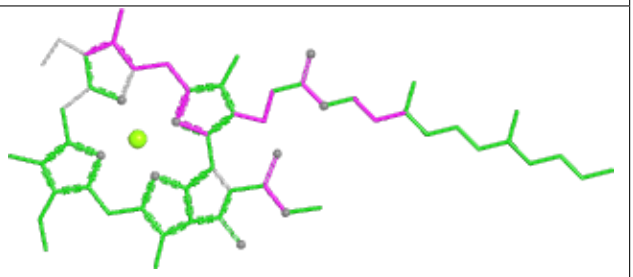
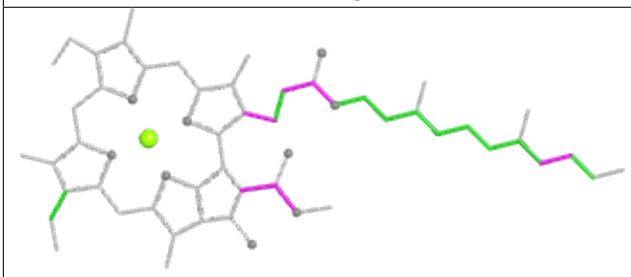
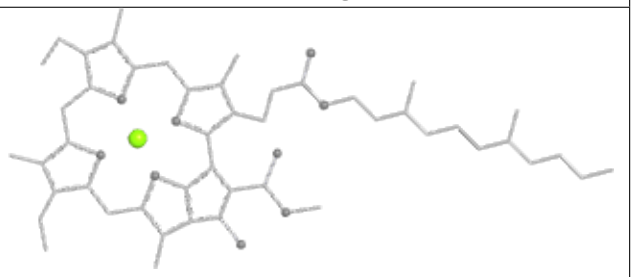
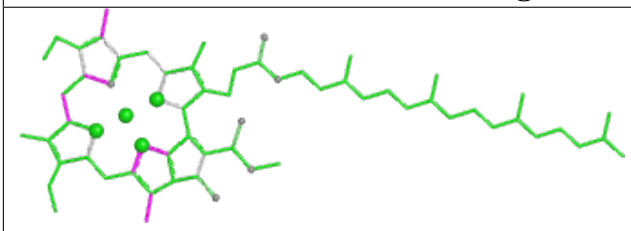
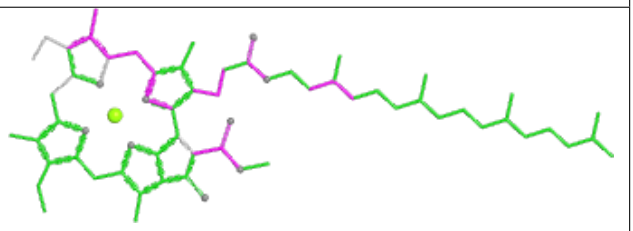
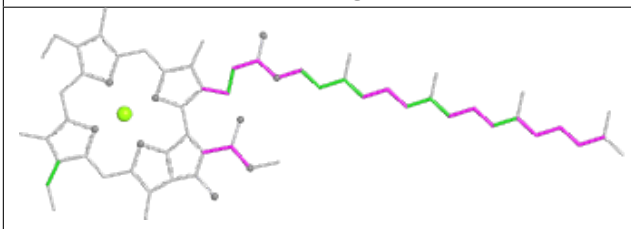
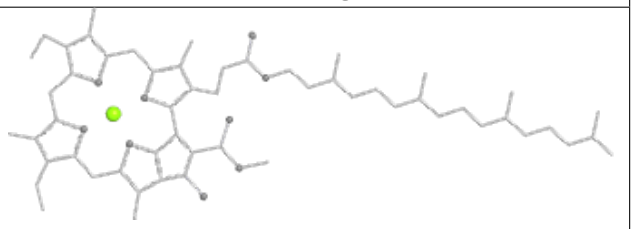
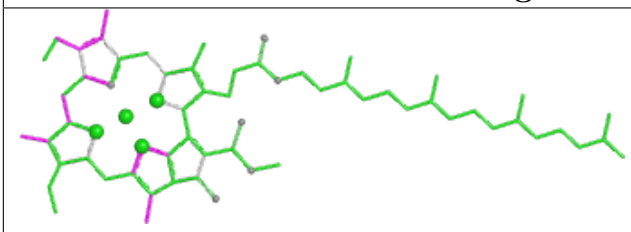
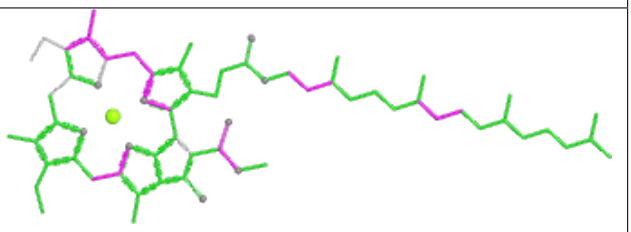
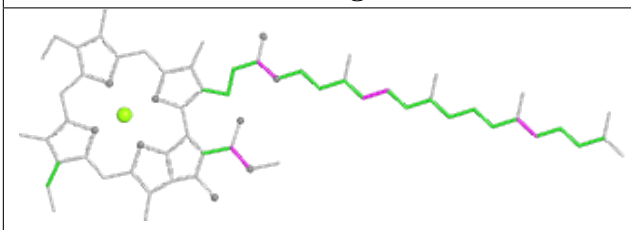
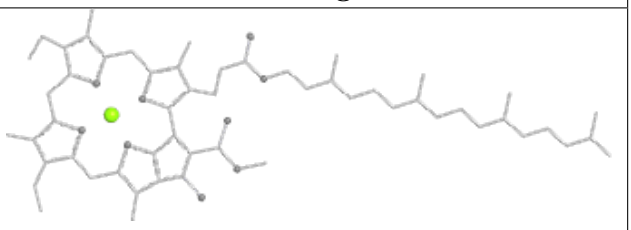
	
Torsions	**Rings**

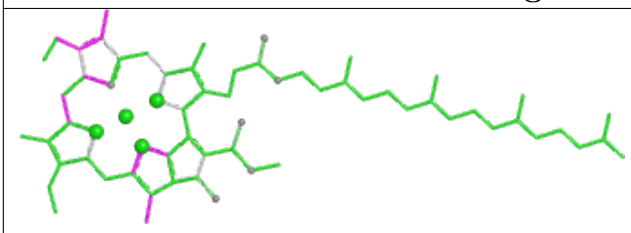
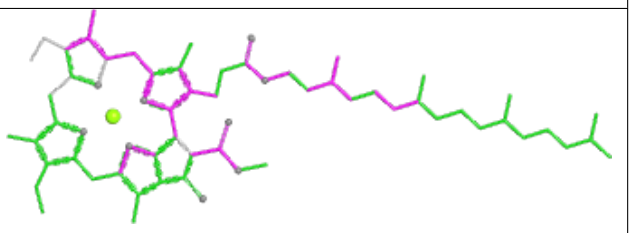
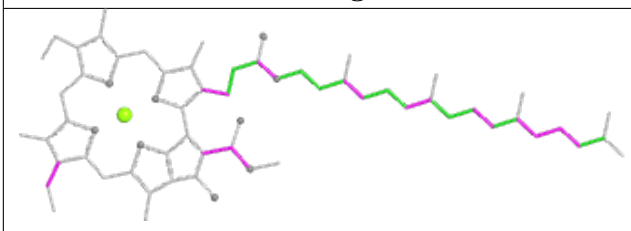
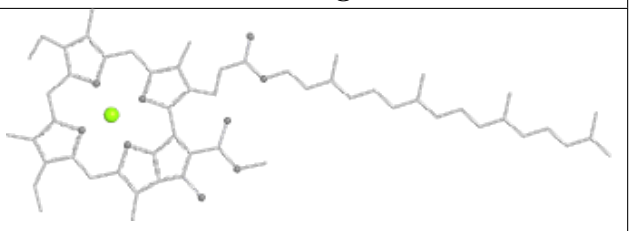
Ligand CLA AA 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR KK 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

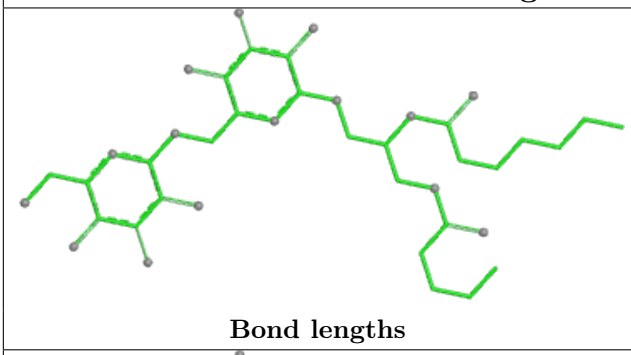
Ligand CLA AA 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B1 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

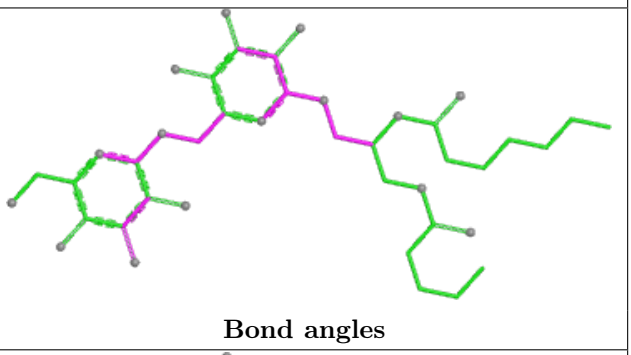
Ligand CLA A2 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

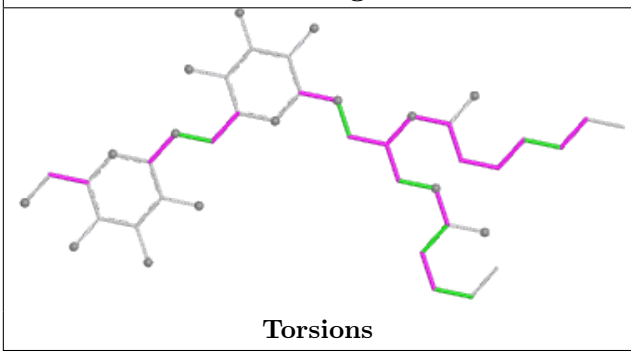
Ligand DGD B 856



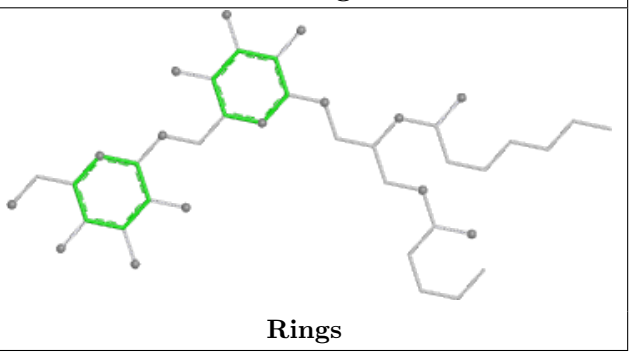
Bond lengths



Bond angles

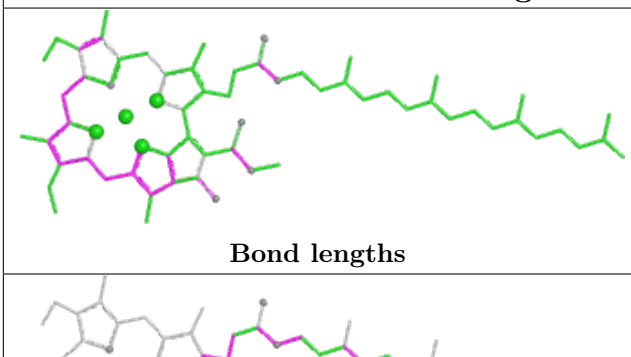


Torsions

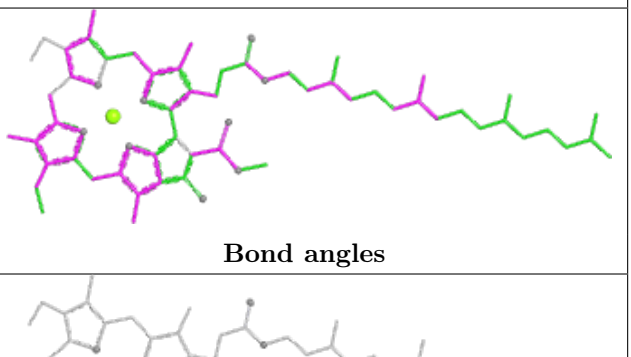


Rings

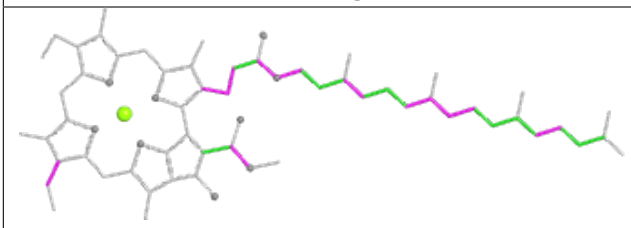
Ligand CL0 AA 803



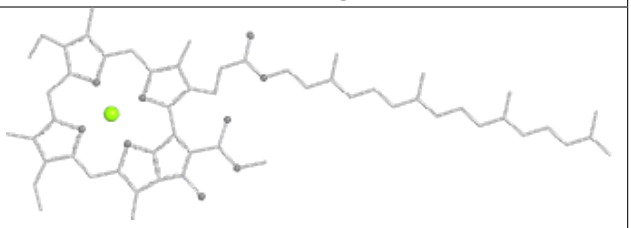
Bond lengths



Bond angles

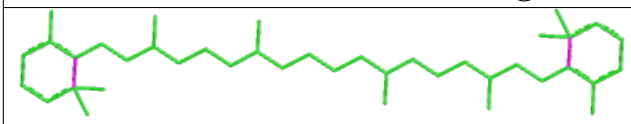


Torsions

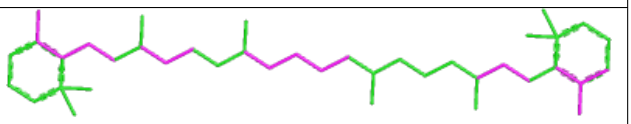


Rings

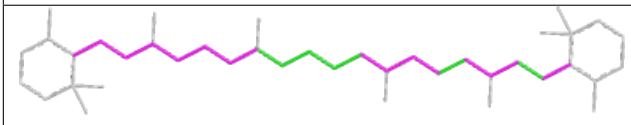
Ligand BCR L2 207



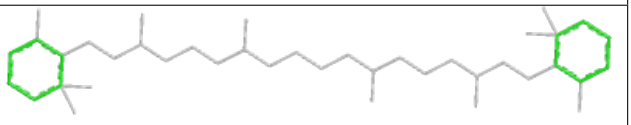
Bond lengths



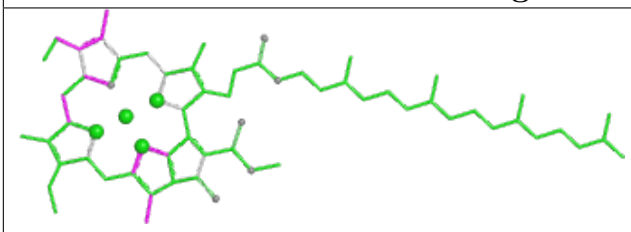
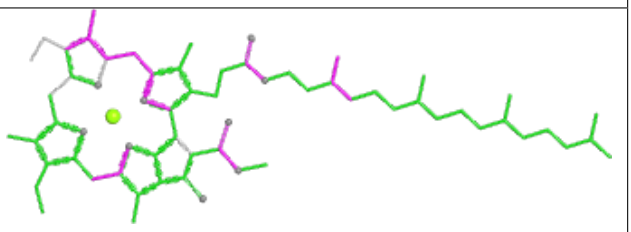
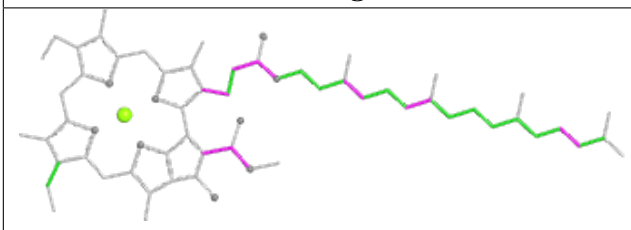
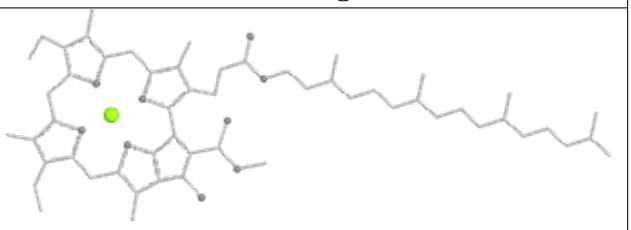
Bond angles



Torsions



Rings

Ligand CLA BB 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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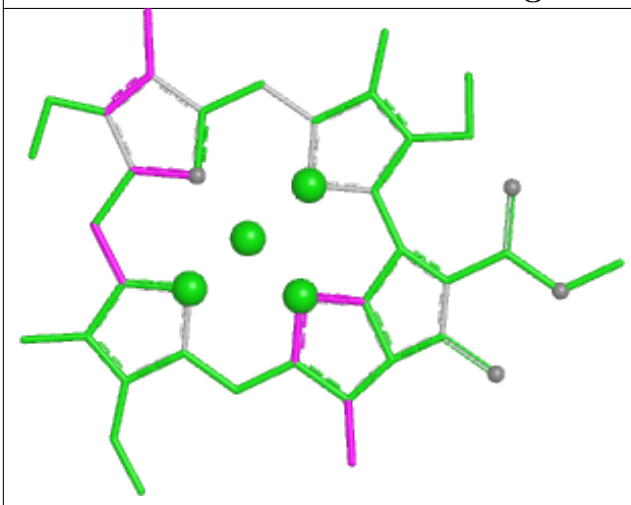
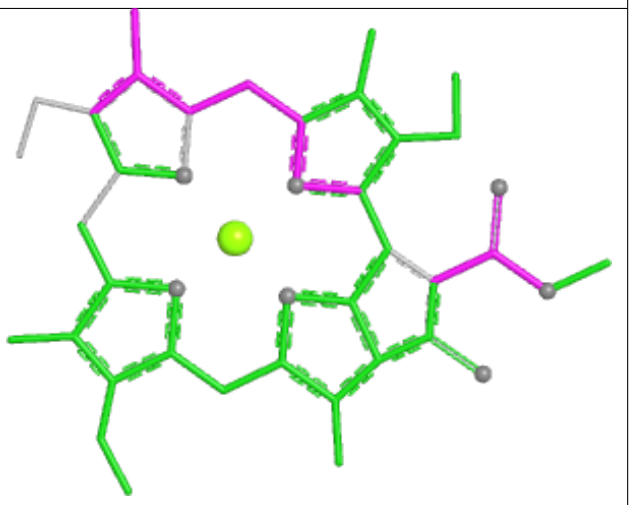
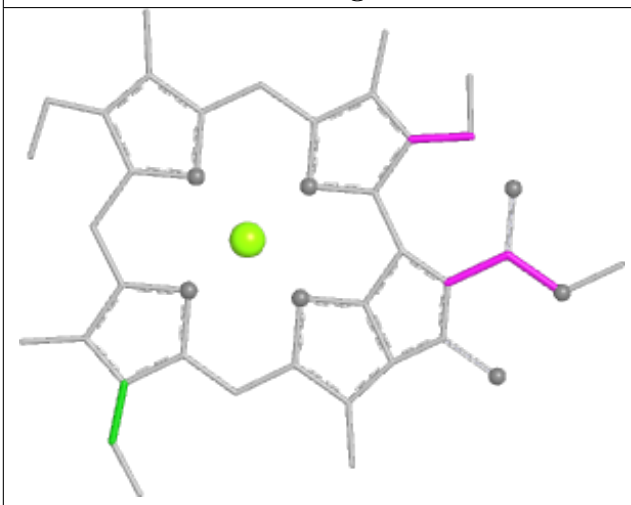
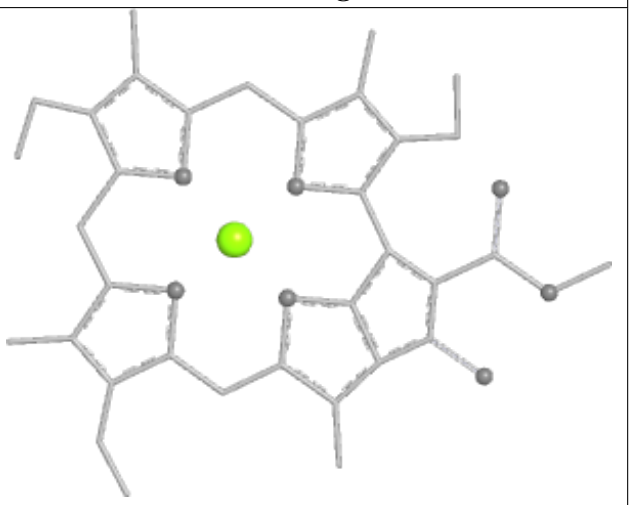
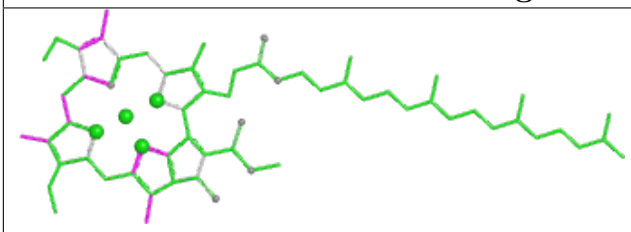
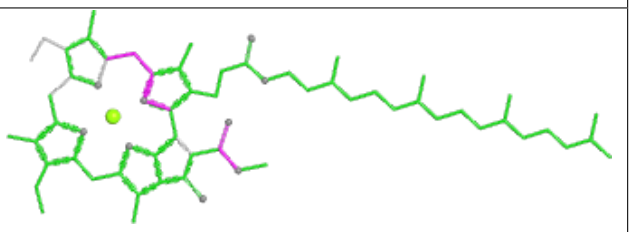
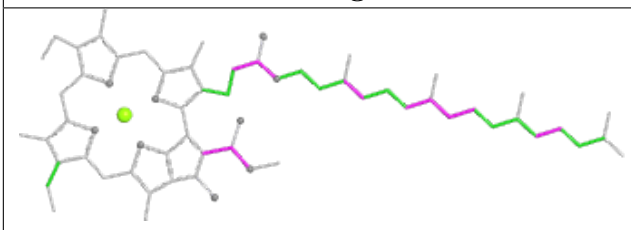
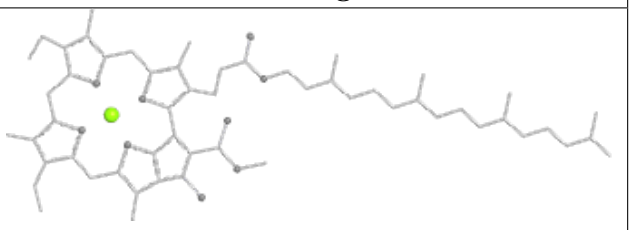
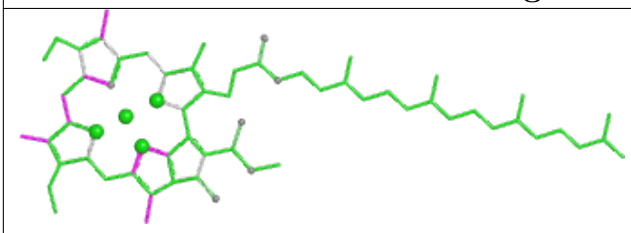
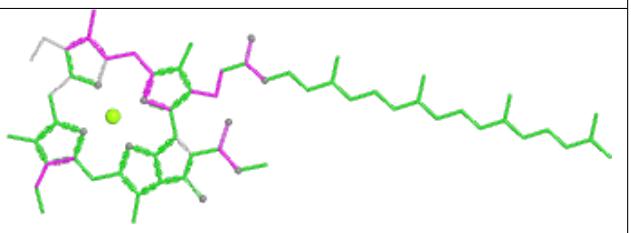
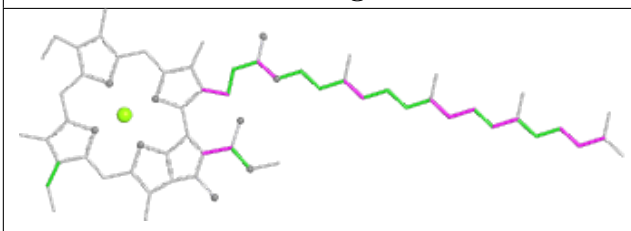
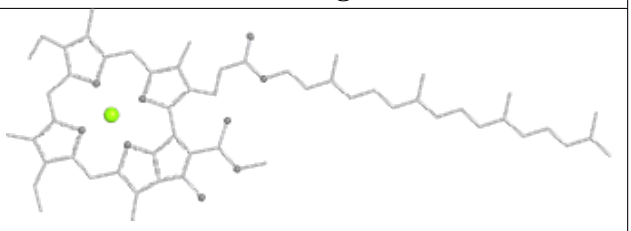
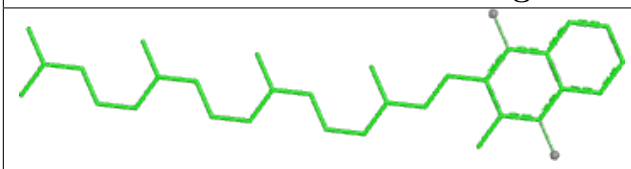
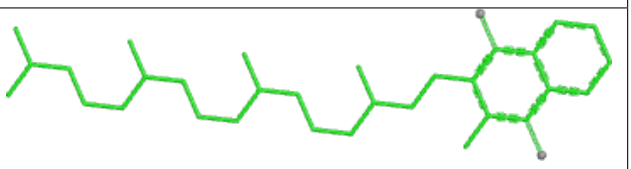
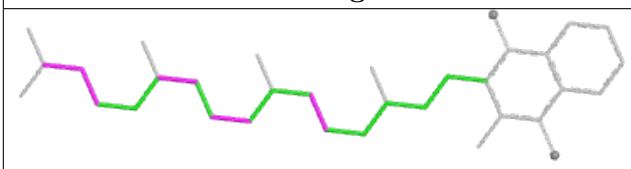
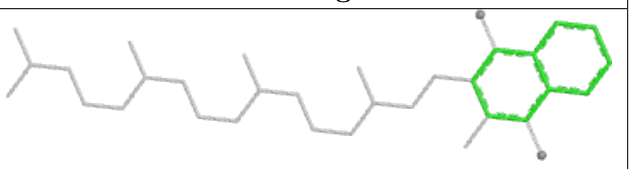
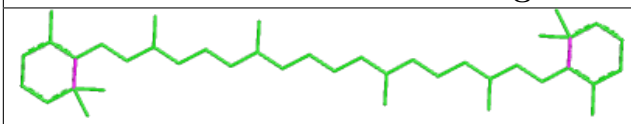
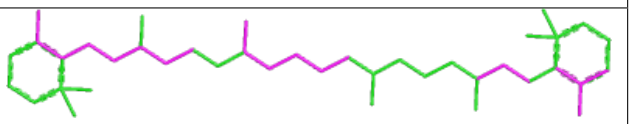
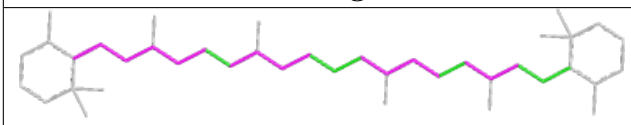
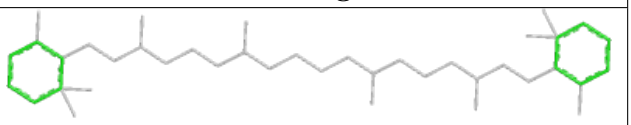
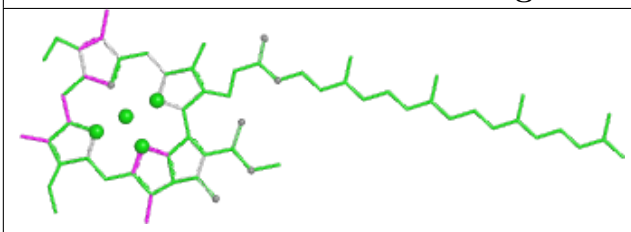
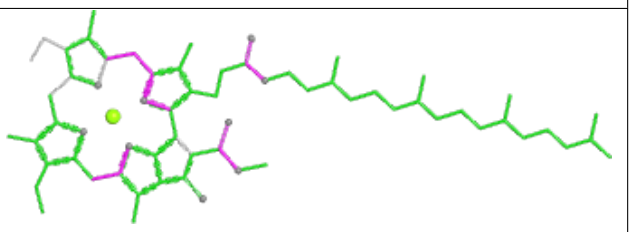
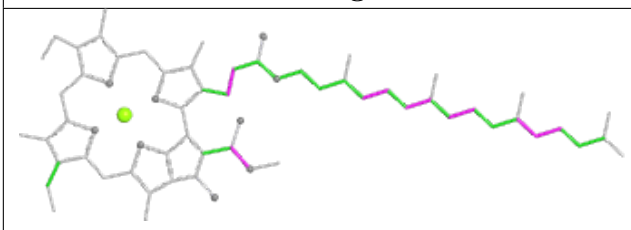
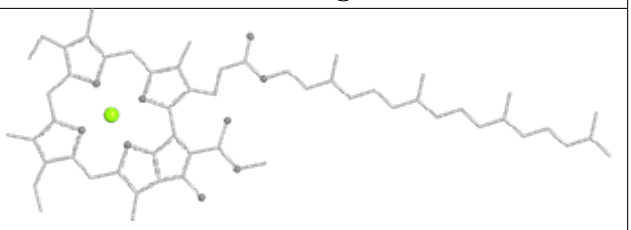
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PQN B2 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B2 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

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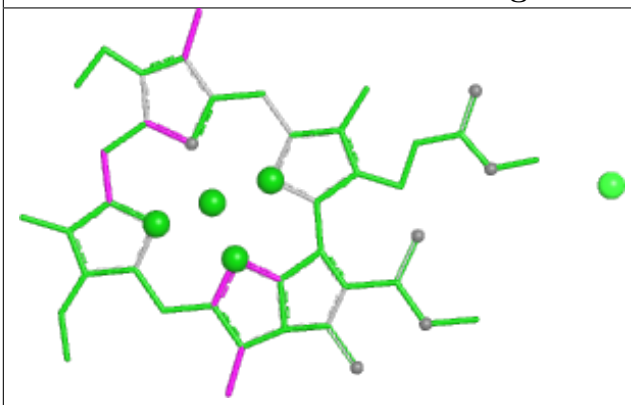
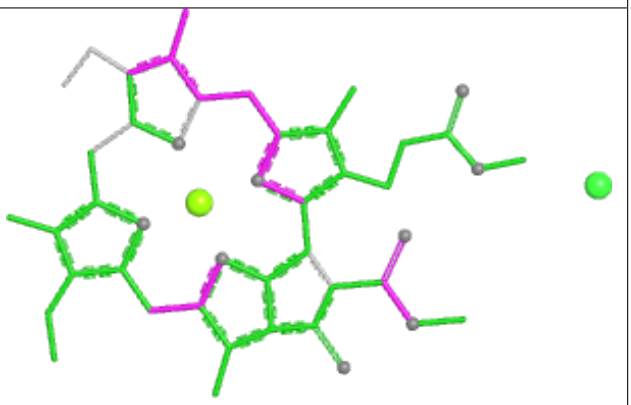
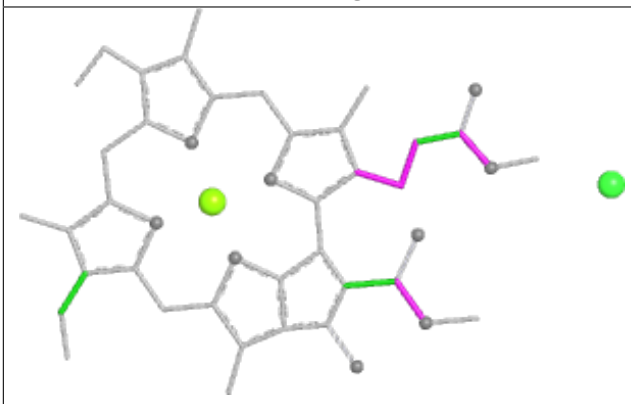
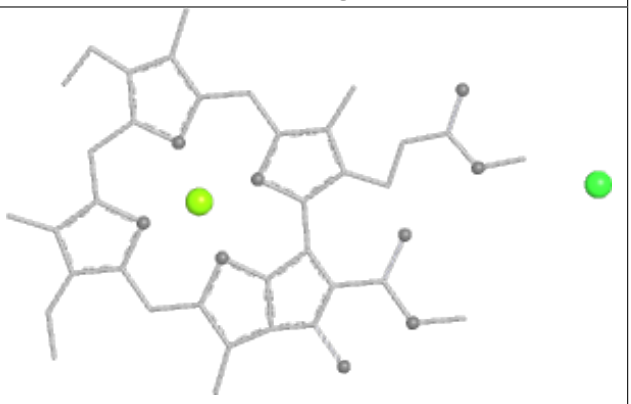
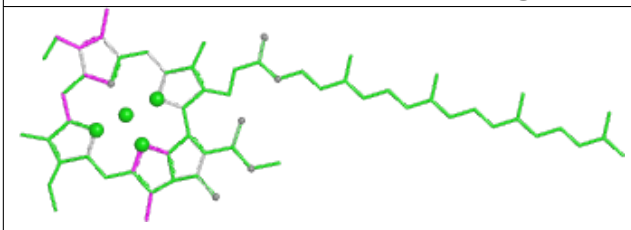
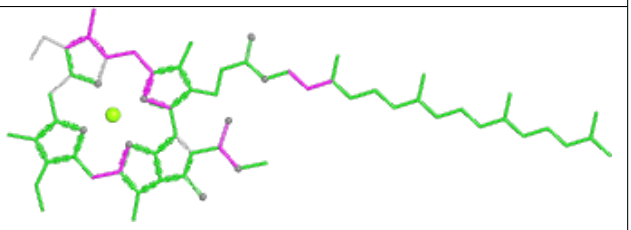
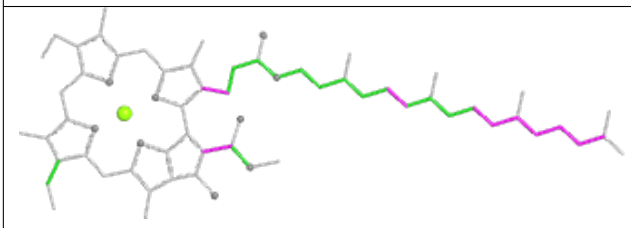
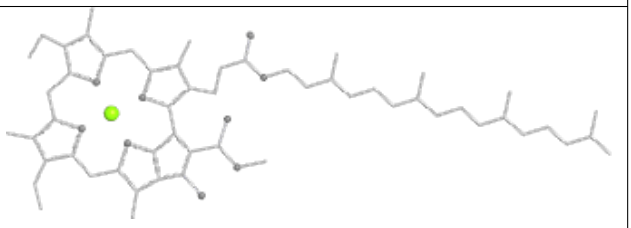
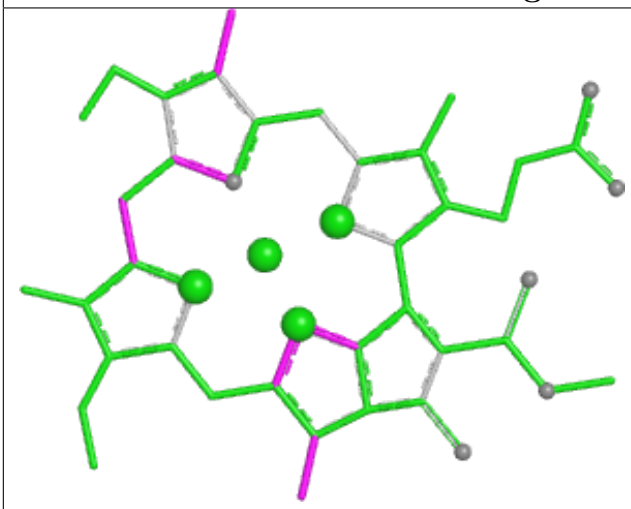
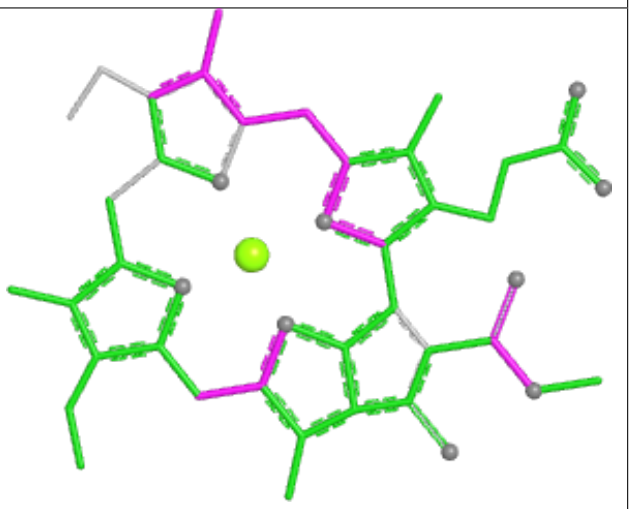
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

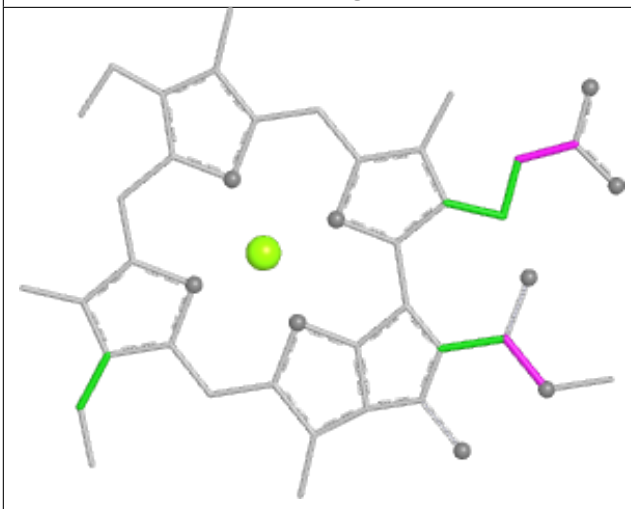
Ligand CLA A 837



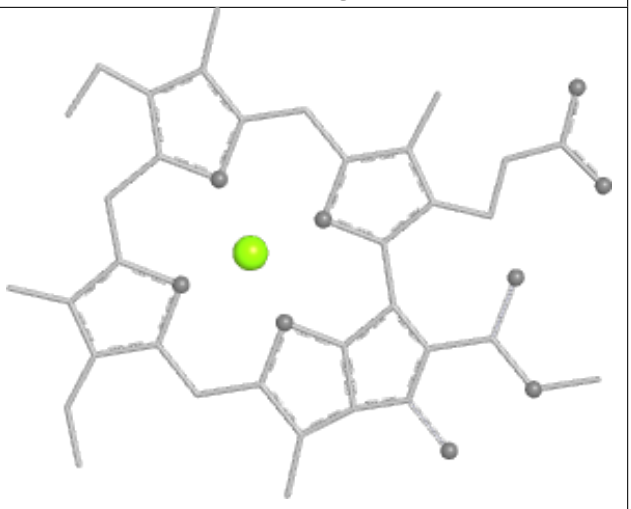
Bond lengths



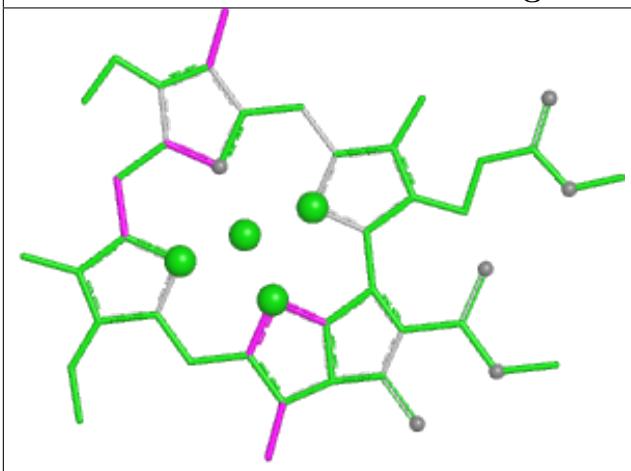
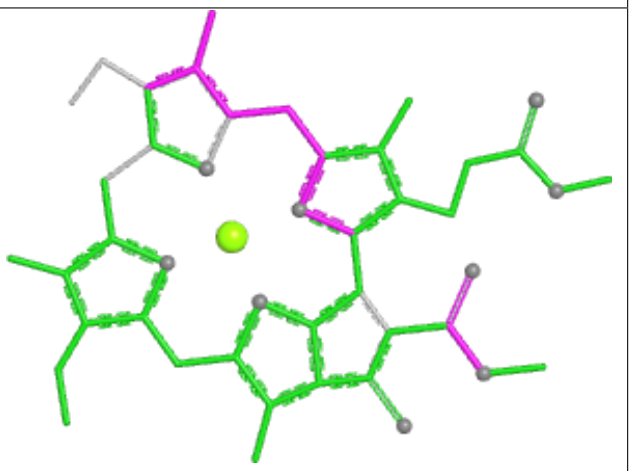
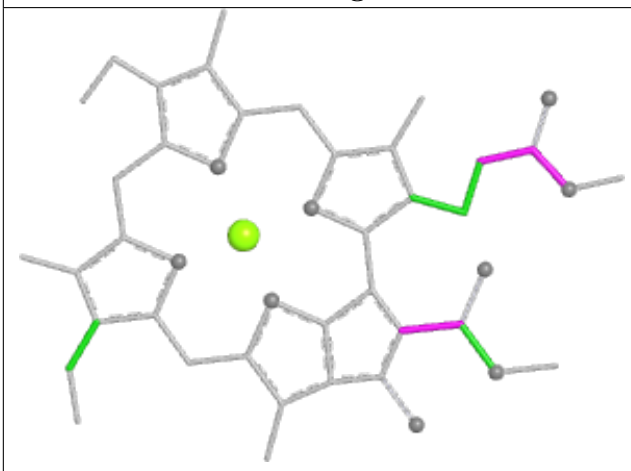
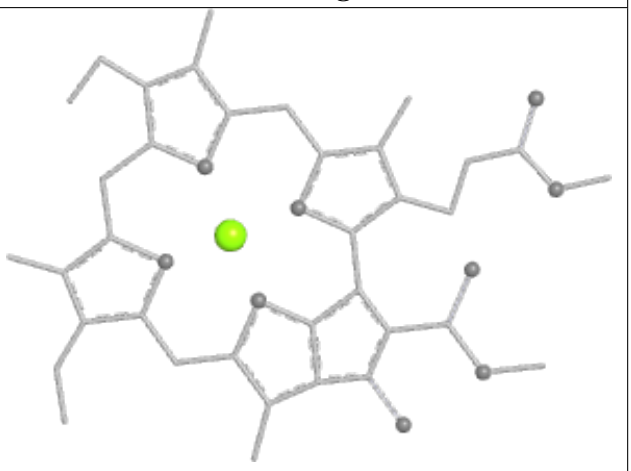
Bond angles

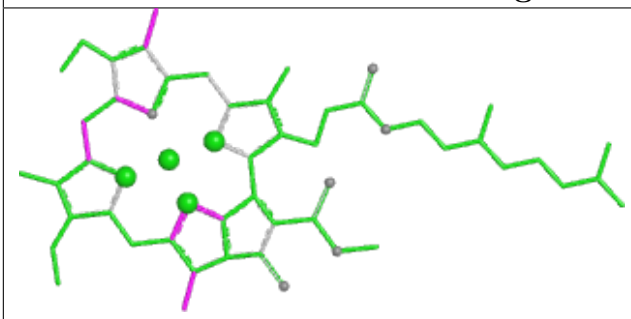
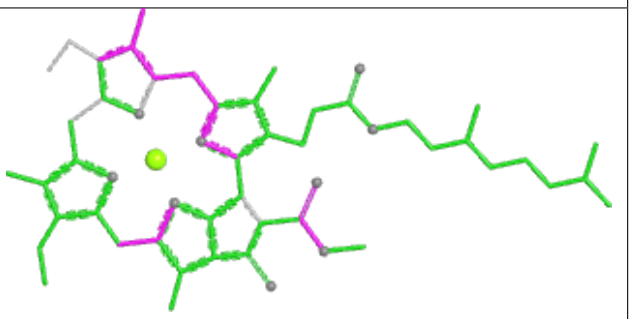
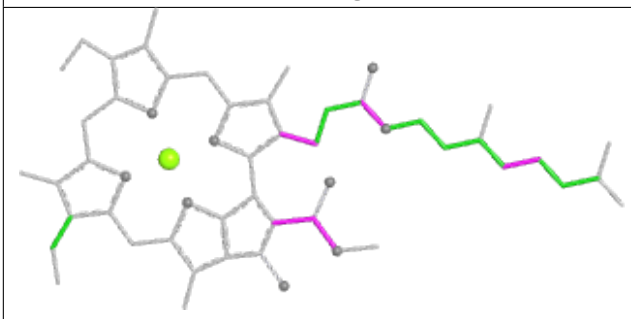
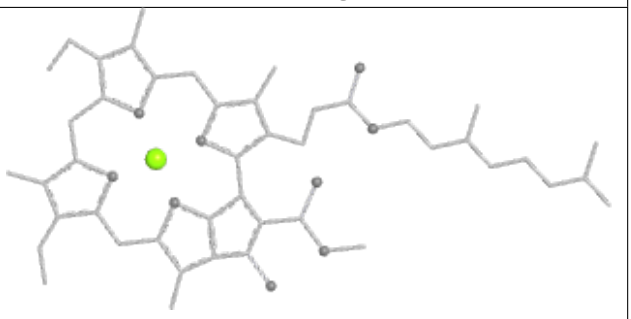


Torsions

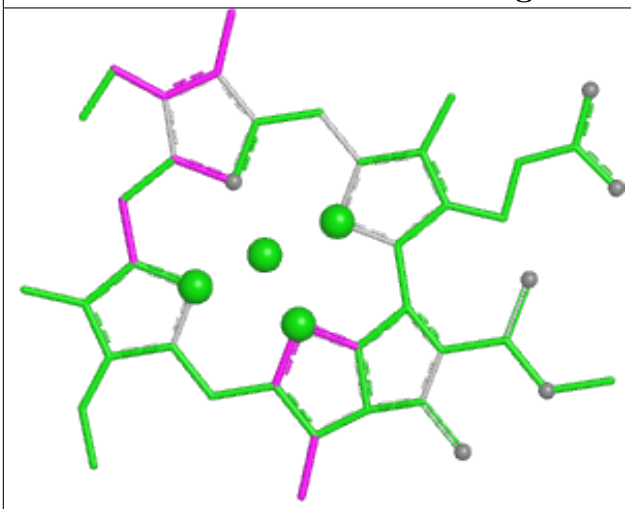


Rings

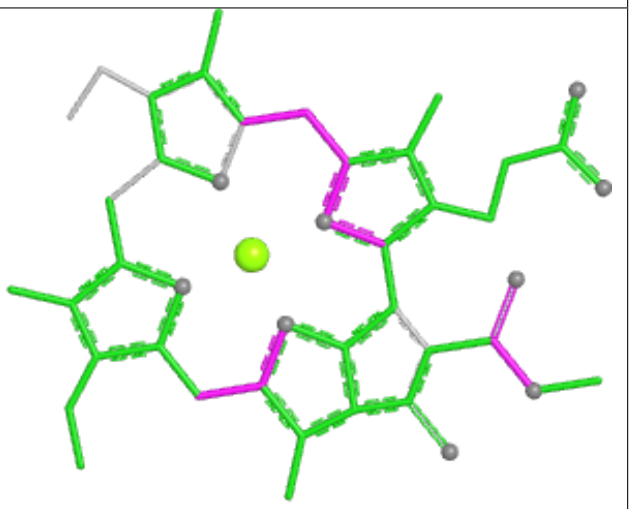
Ligand CLA A 841	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A2 815	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

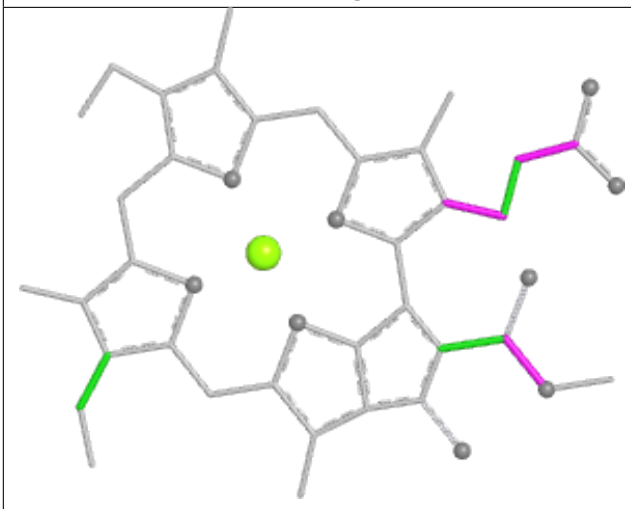
Ligand CLA B1 831



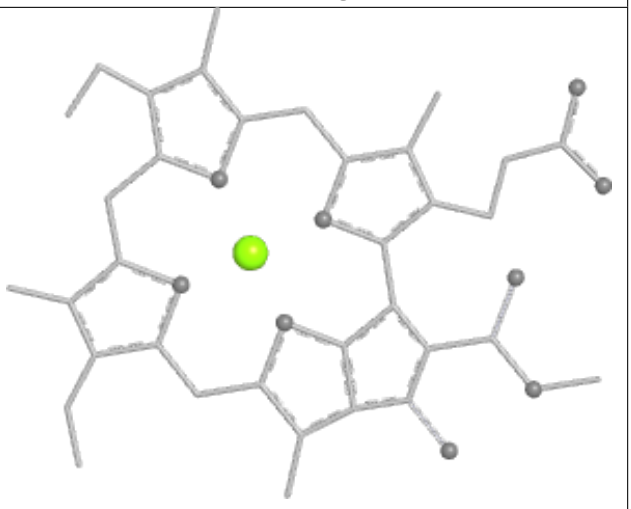
Bond lengths



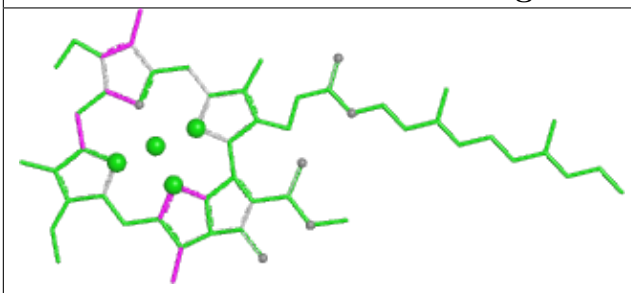
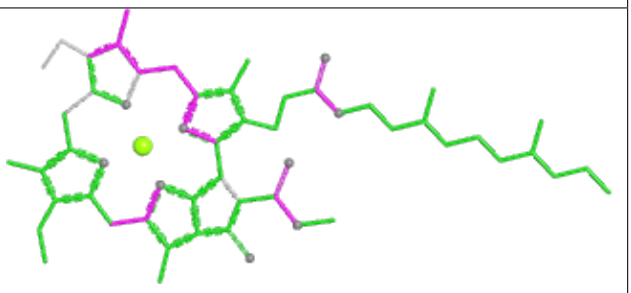
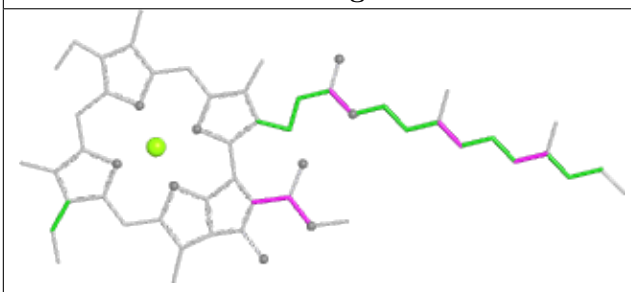
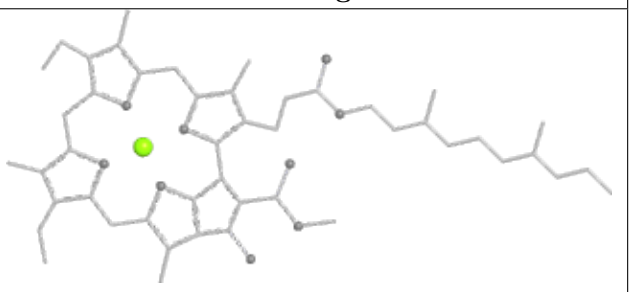
Bond angles



Torsions



Rings

Ligand CLA B1 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

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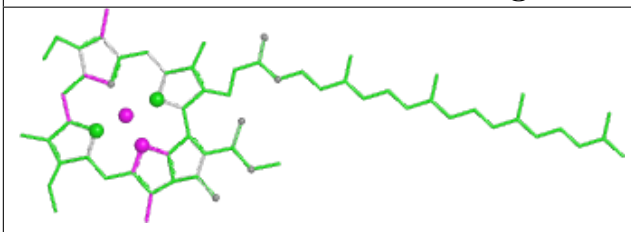
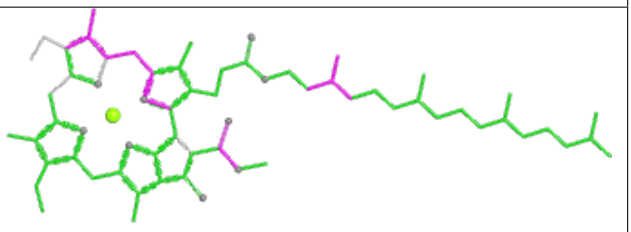
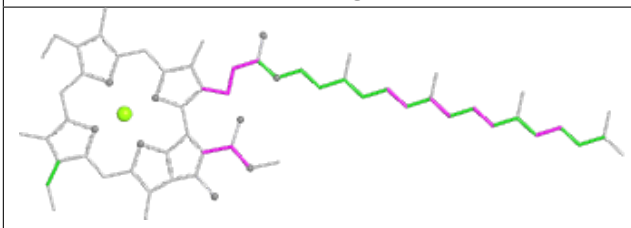
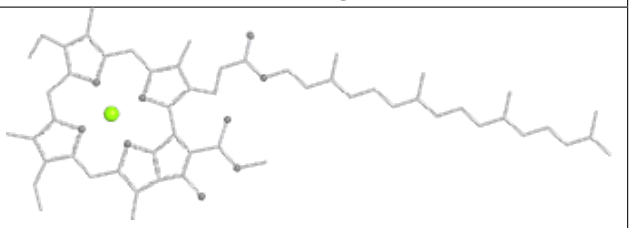
	
Bond lengths	Bond angles
	
Torsions	Rings

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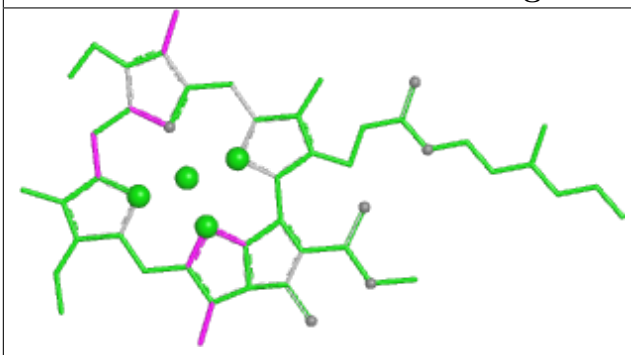
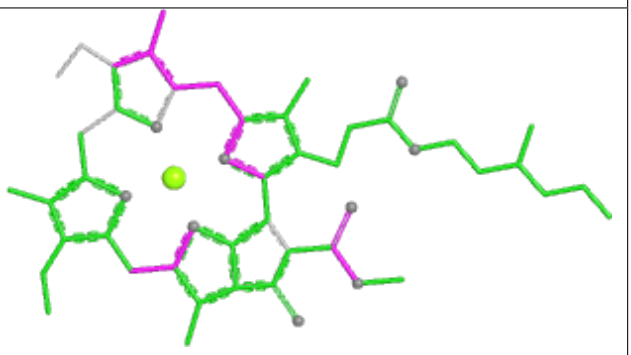
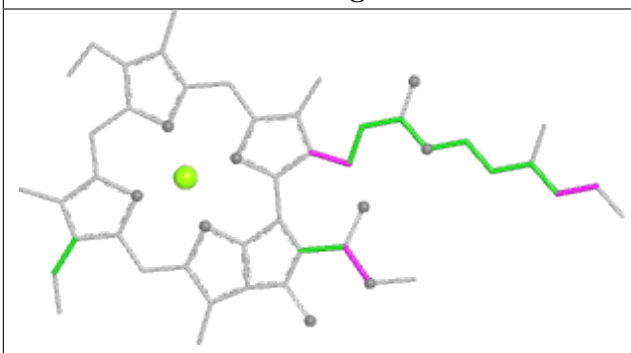
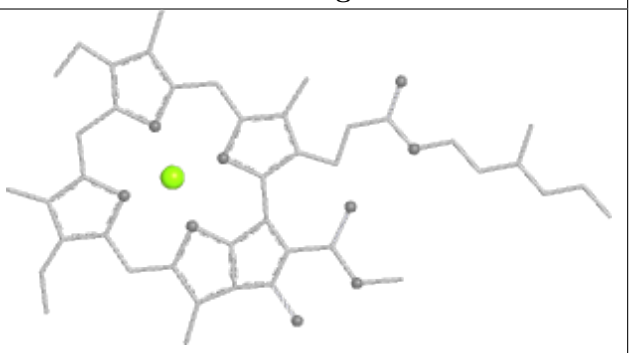
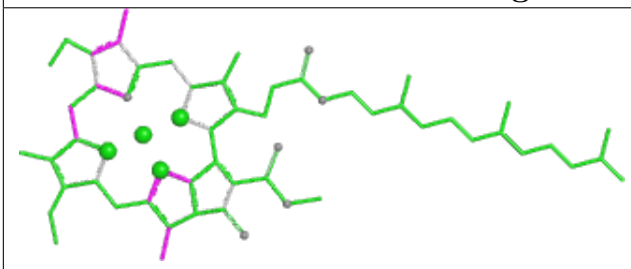
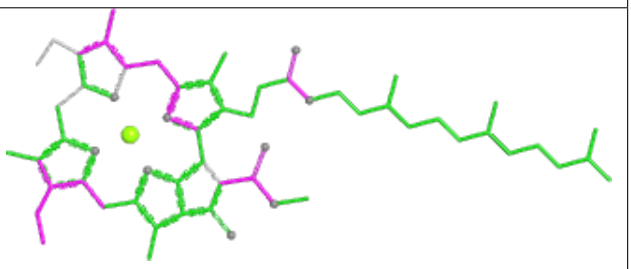
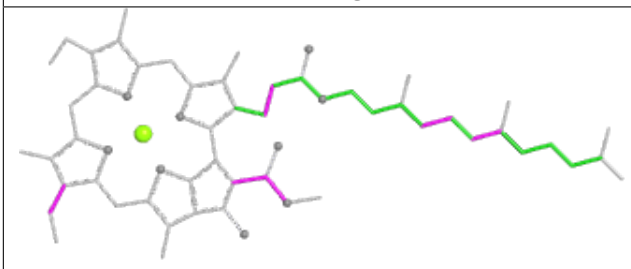
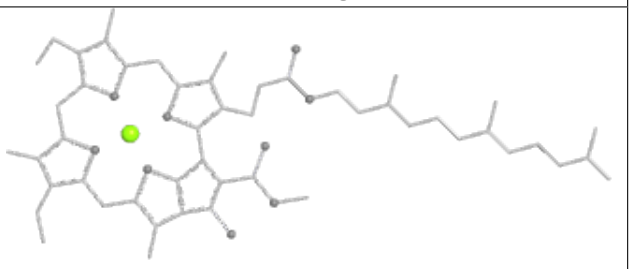
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BB 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

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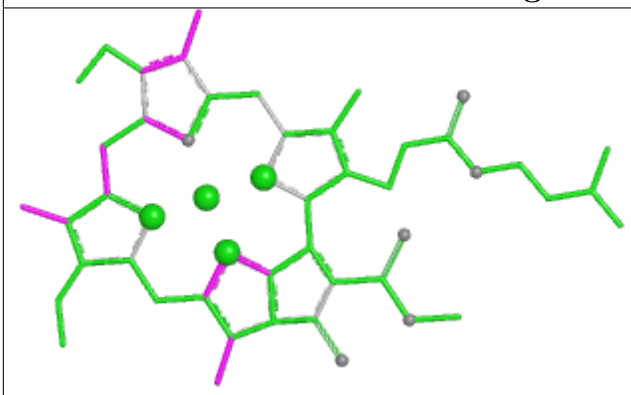
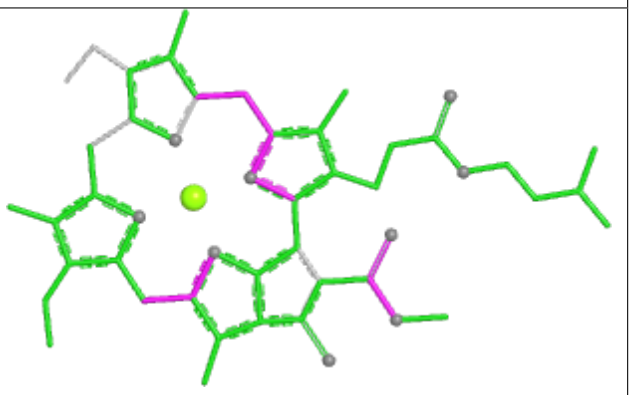
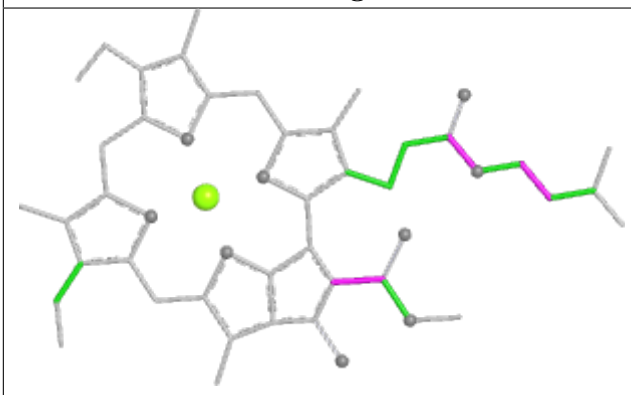
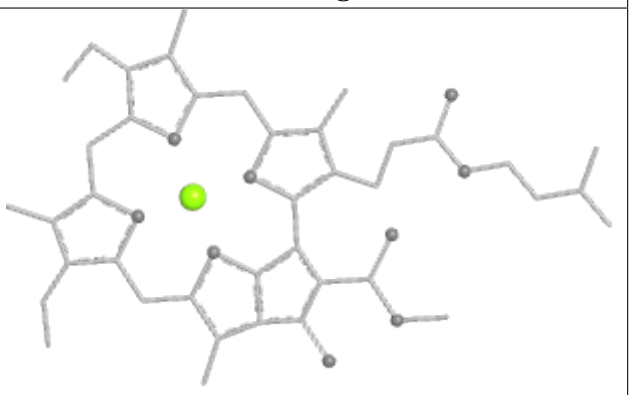
	
Bond lengths	Bond angles
	
Torsions	Rings

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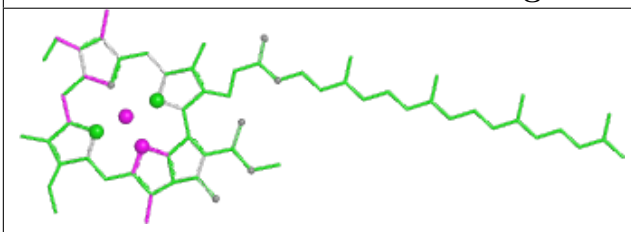
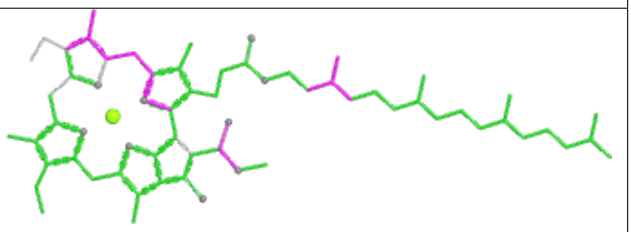
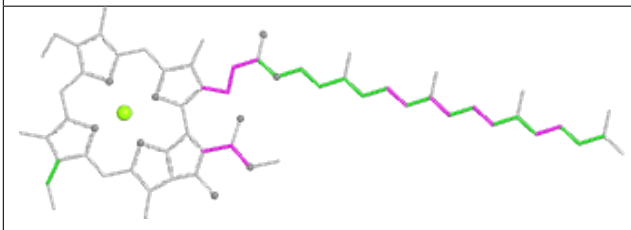
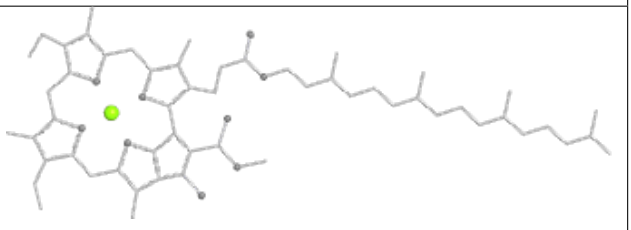
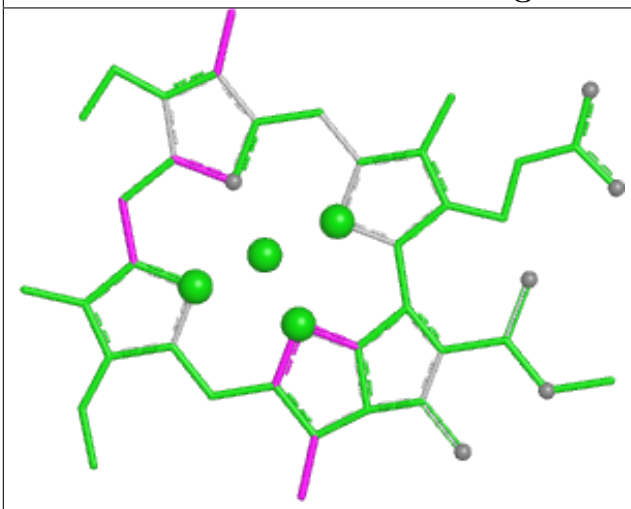
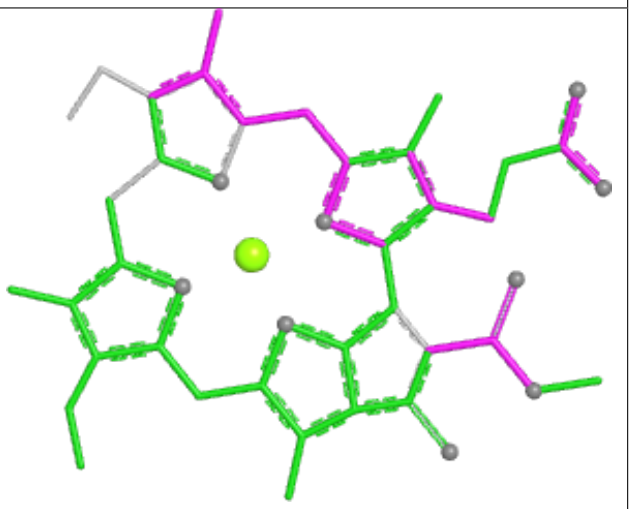
	
Bond lengths	Bond angles
	
Torsions	Rings

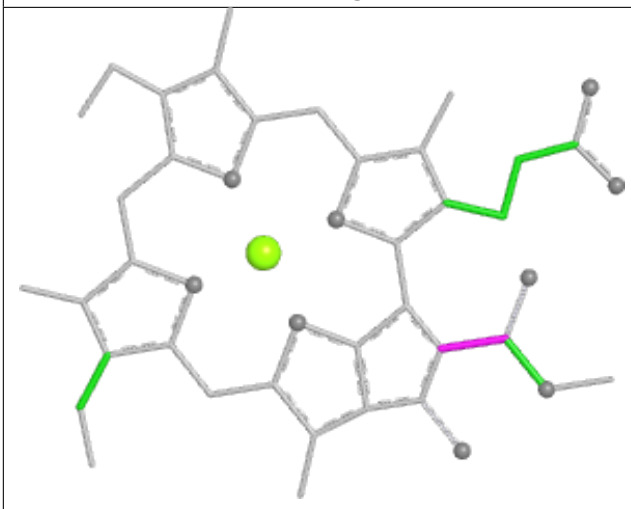
Ligand CLA K2 102



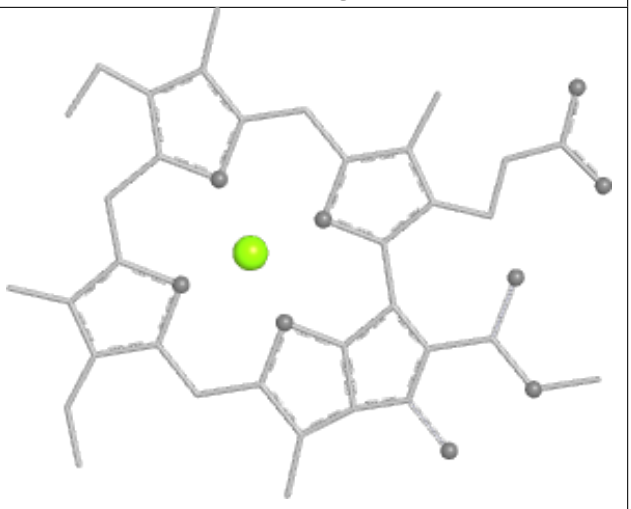
Bond lengths



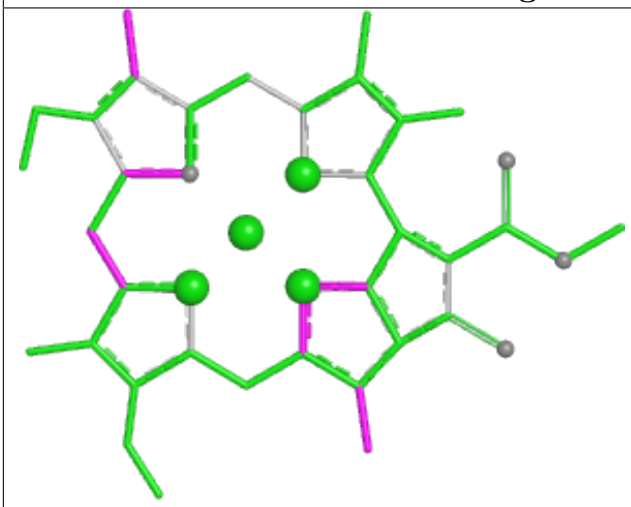
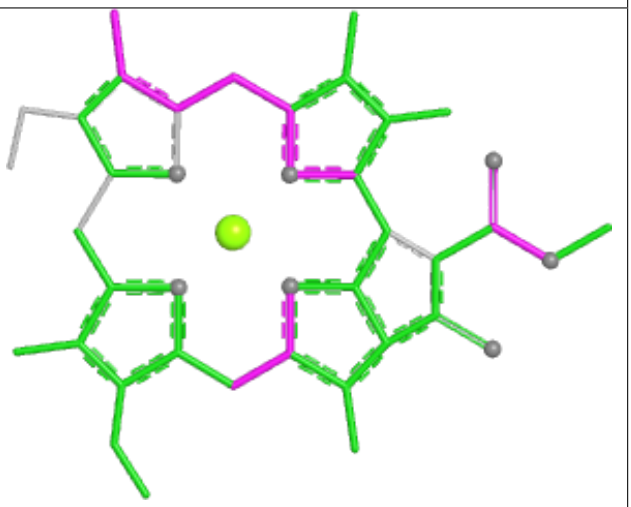
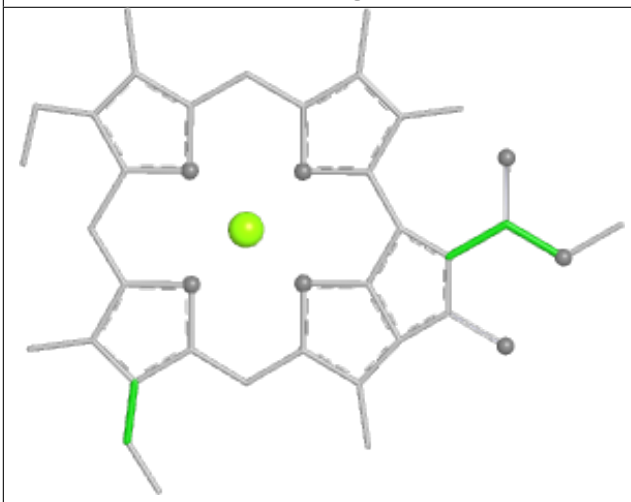
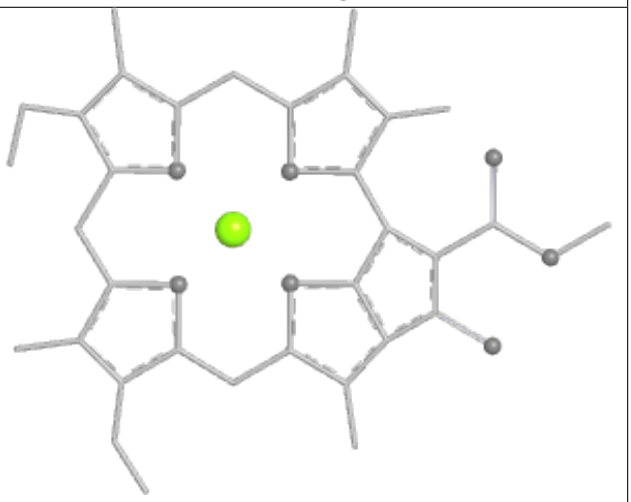
Bond angles

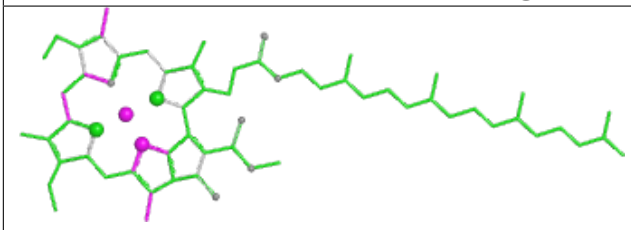
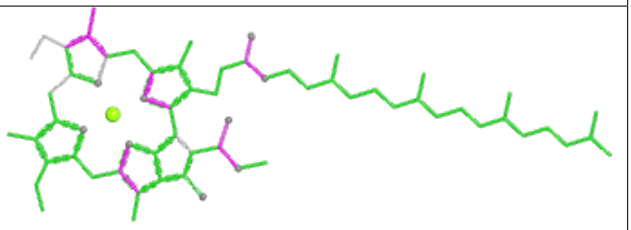
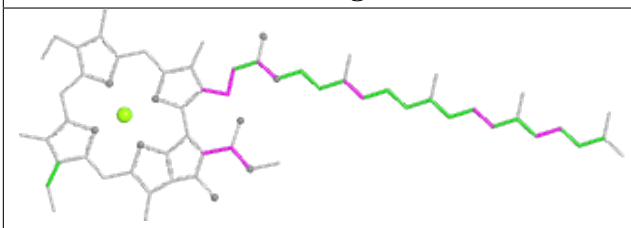
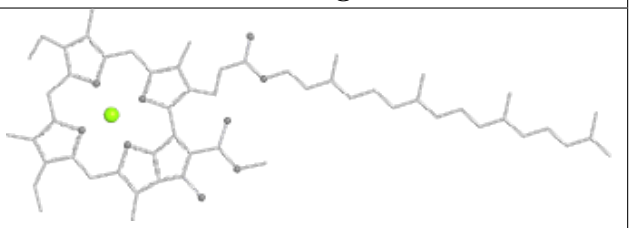


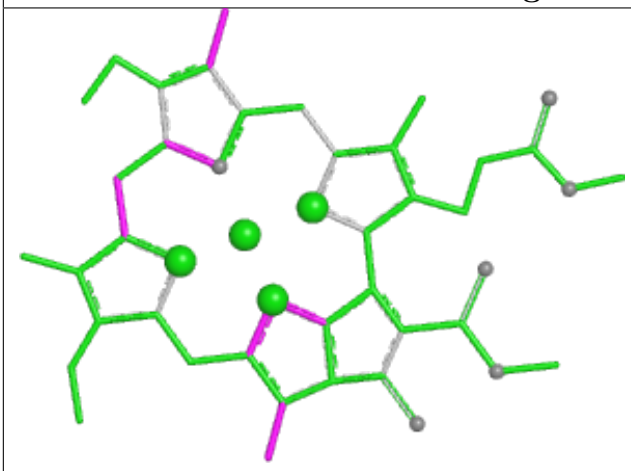
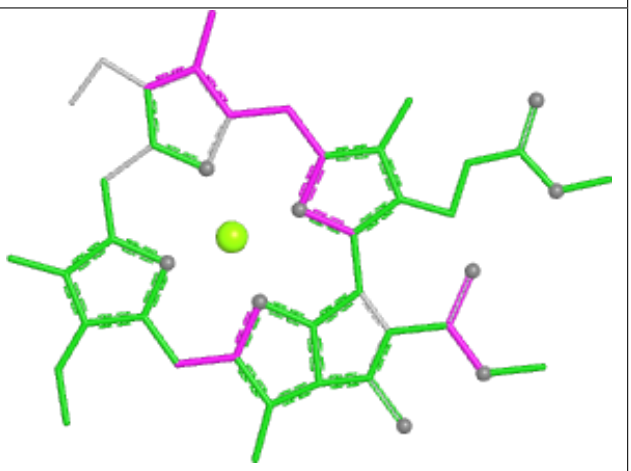
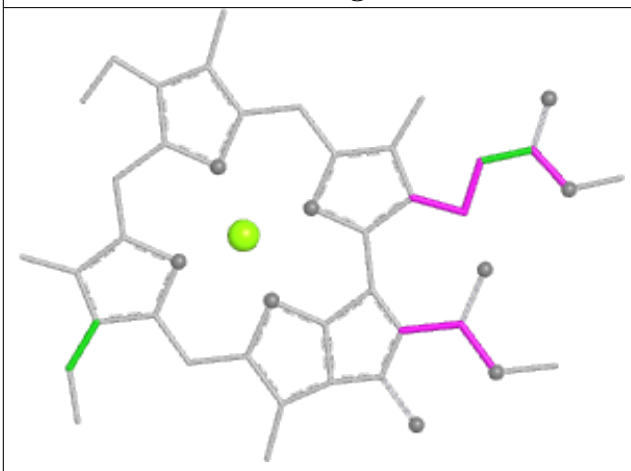
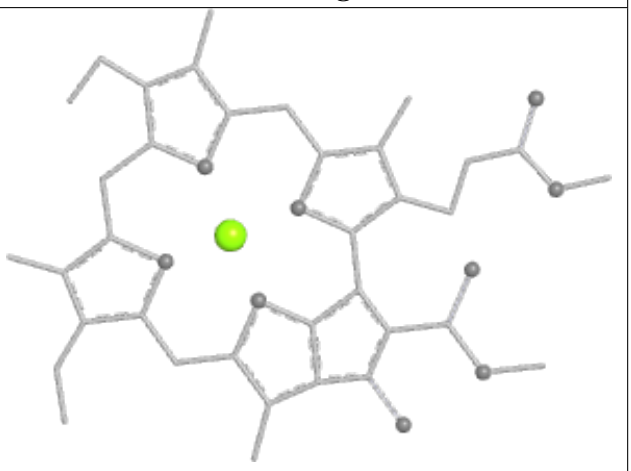
Torsions

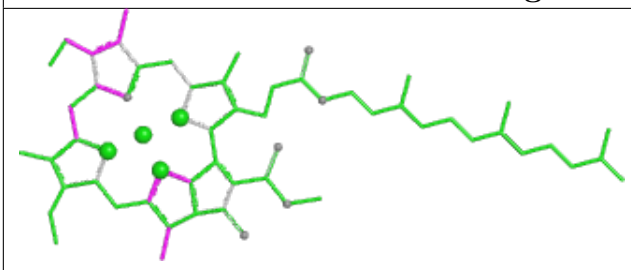
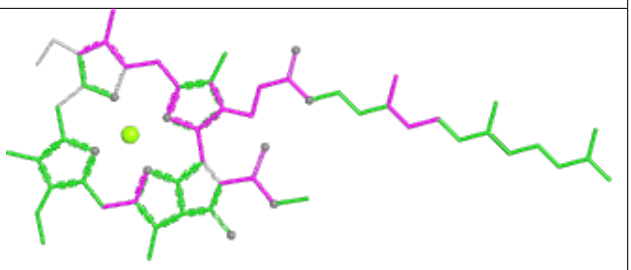
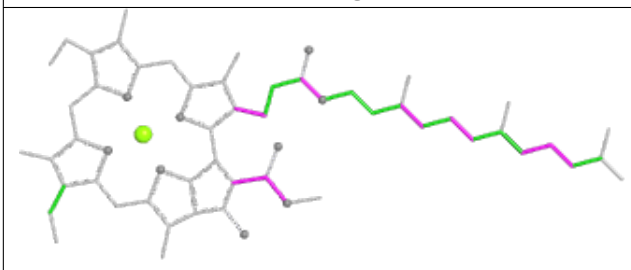
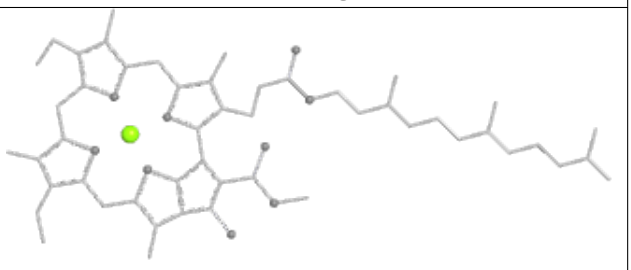


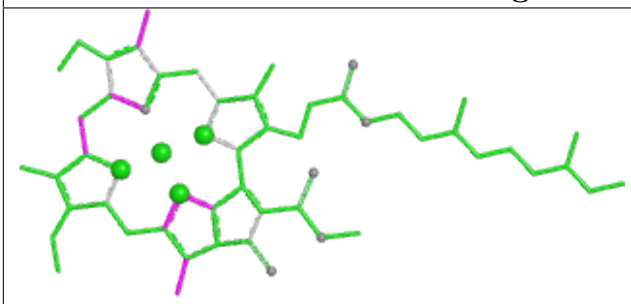
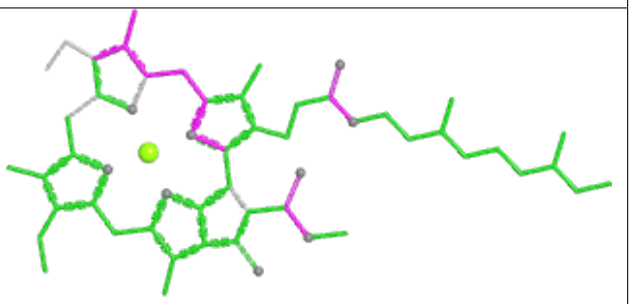
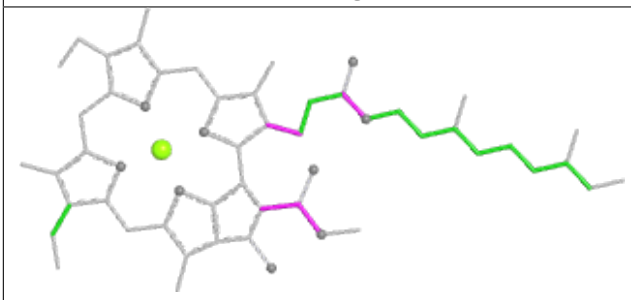
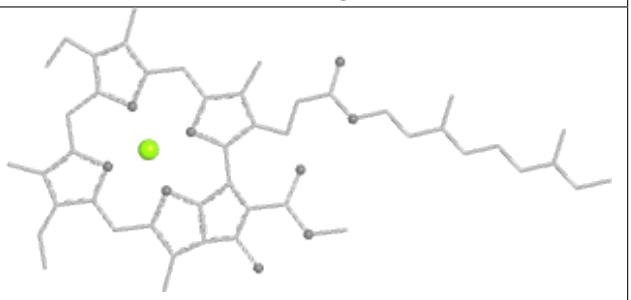
Rings

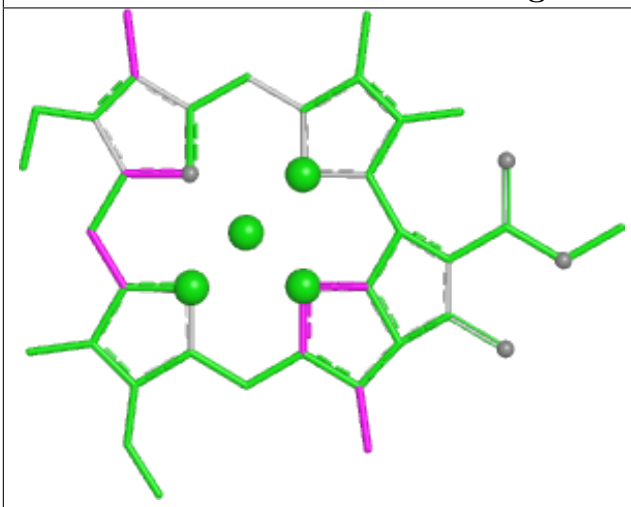
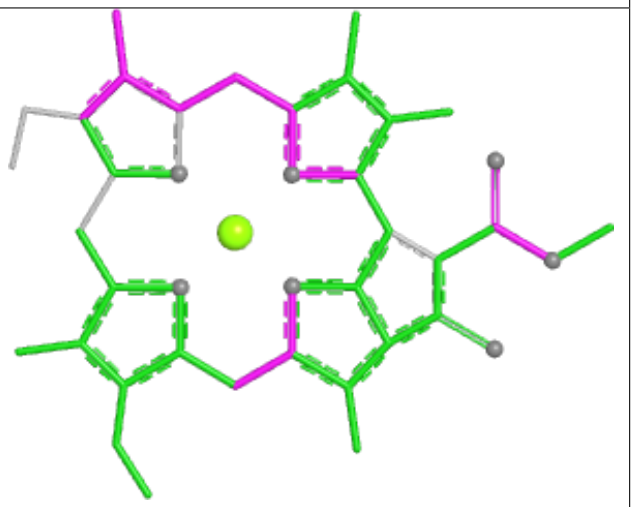
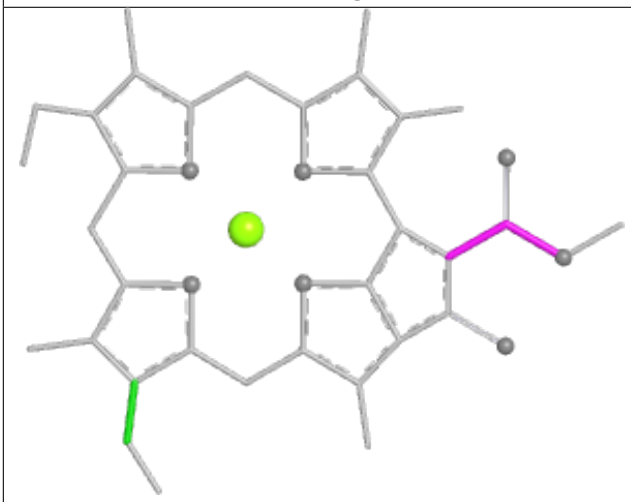
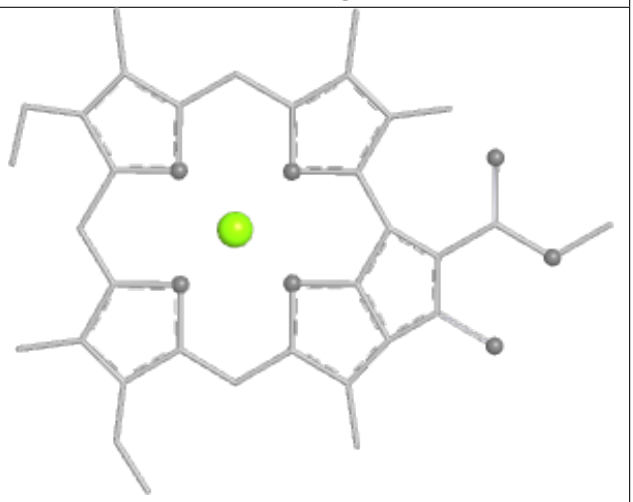
Ligand CLA J1 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

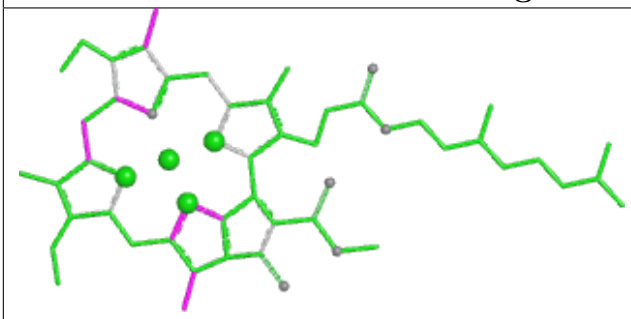
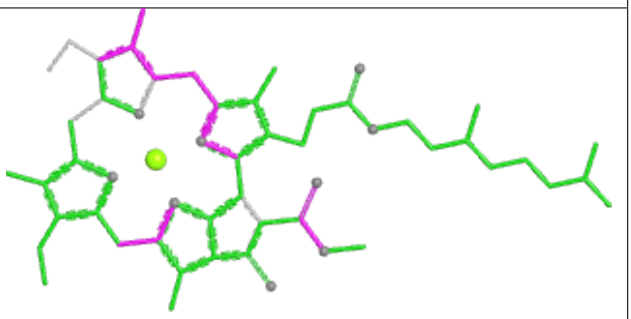
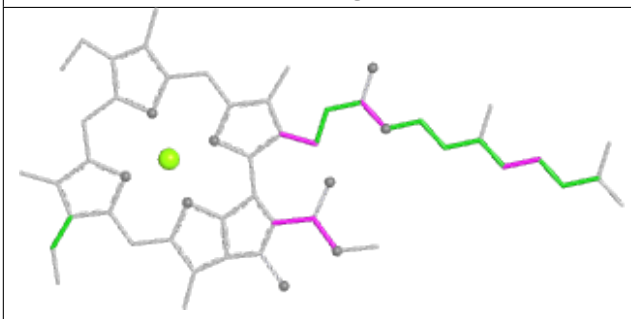
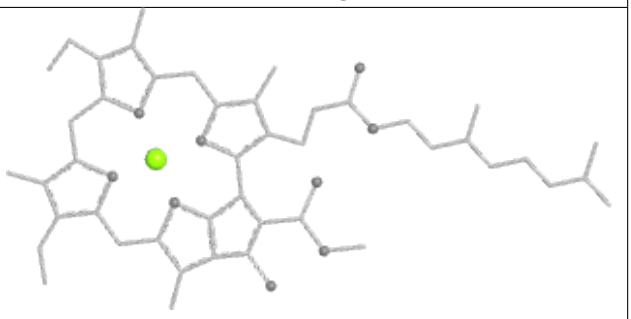
Ligand CLA L1 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

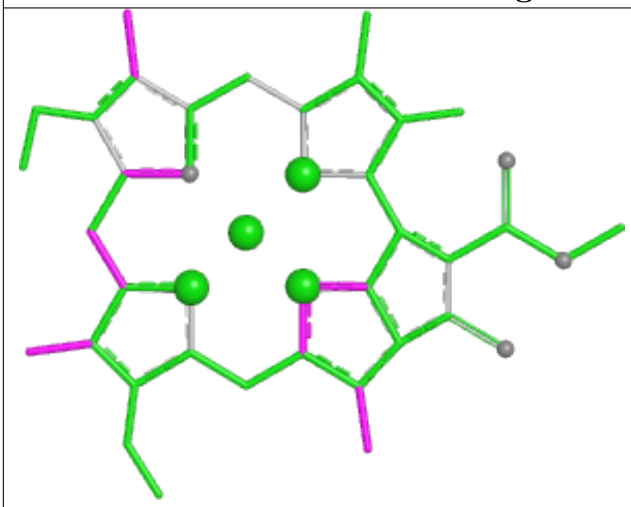
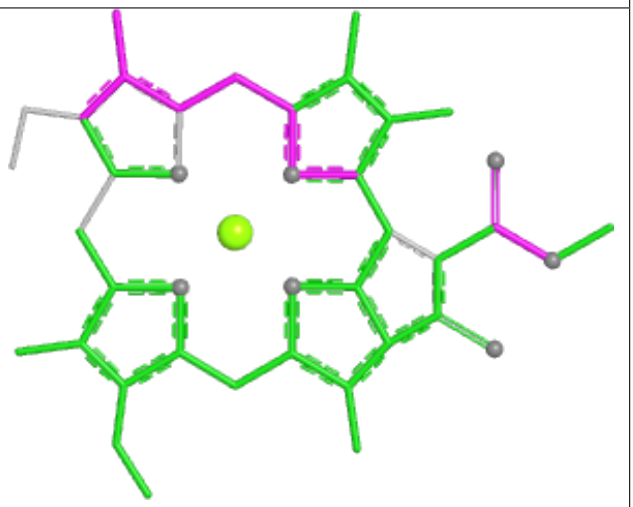
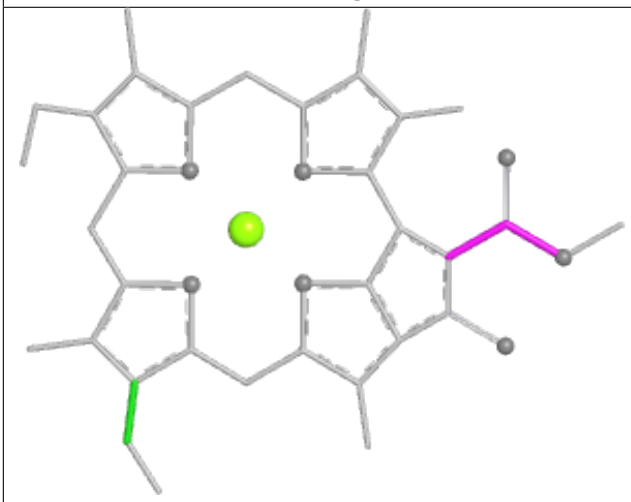
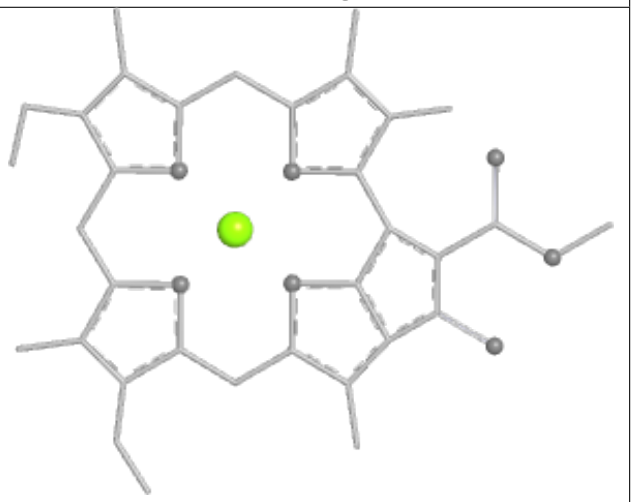
Ligand CLA K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 859	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 830	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA J 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A1 814	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B2 819	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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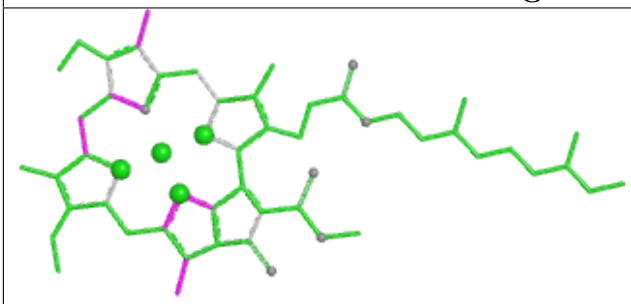
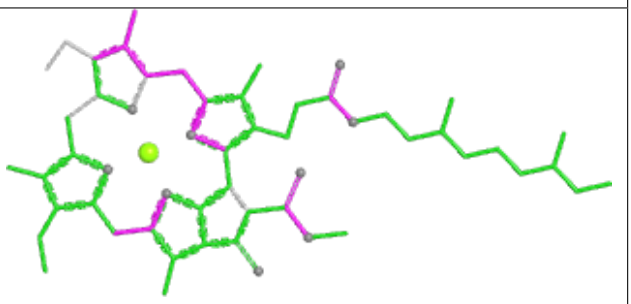
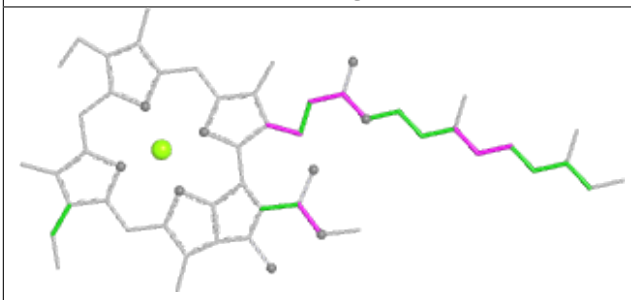
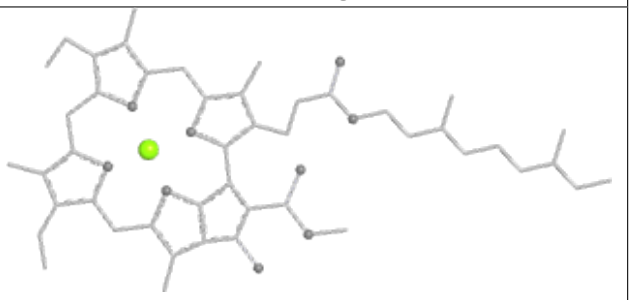
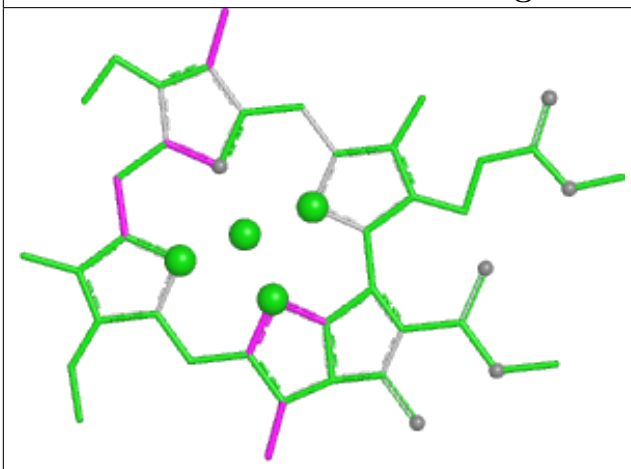
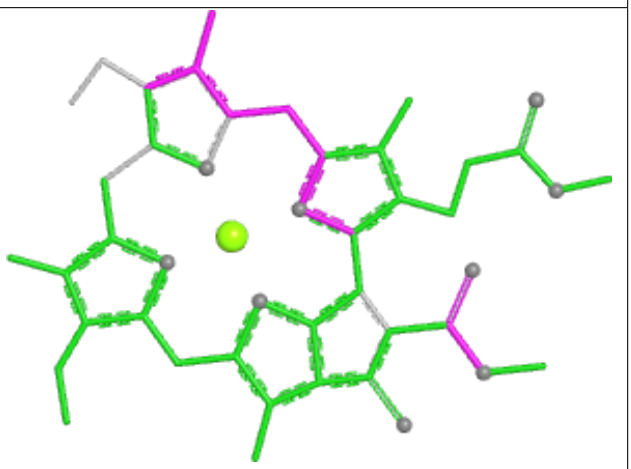
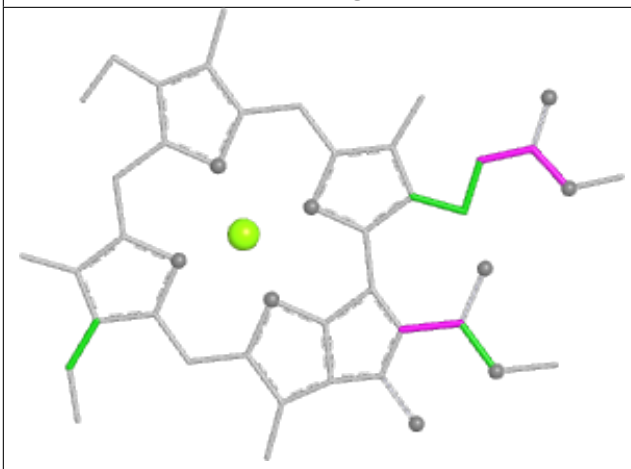
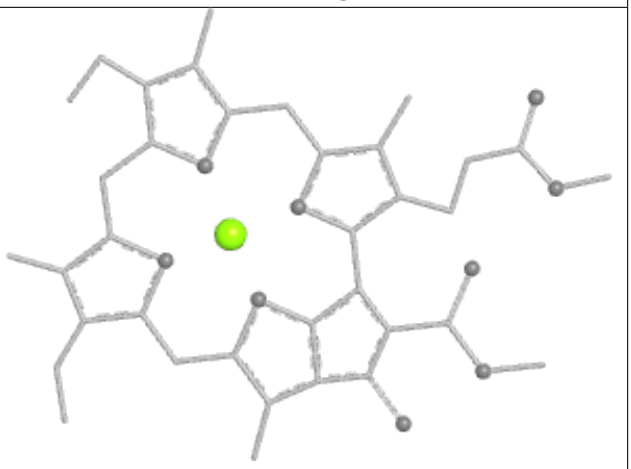
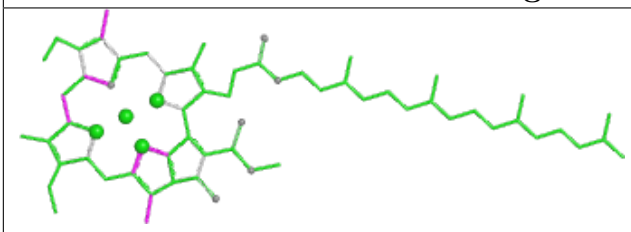
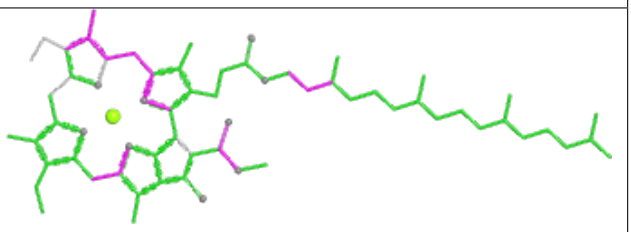
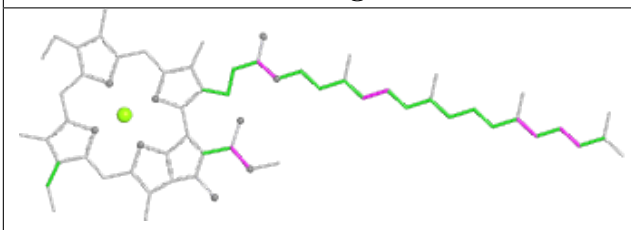
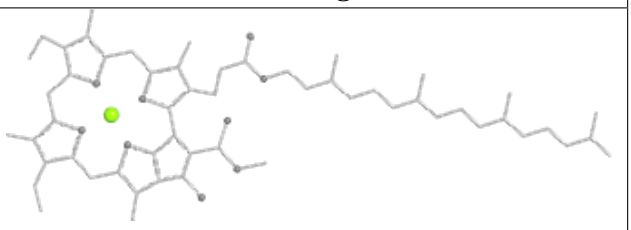
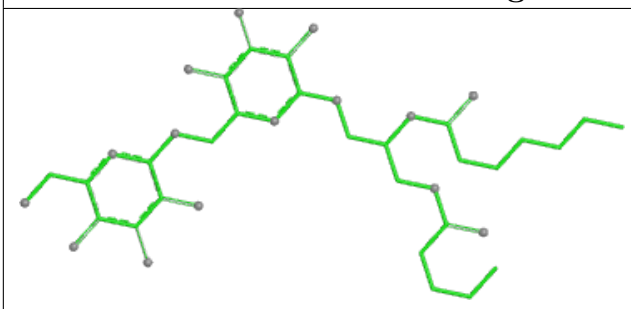
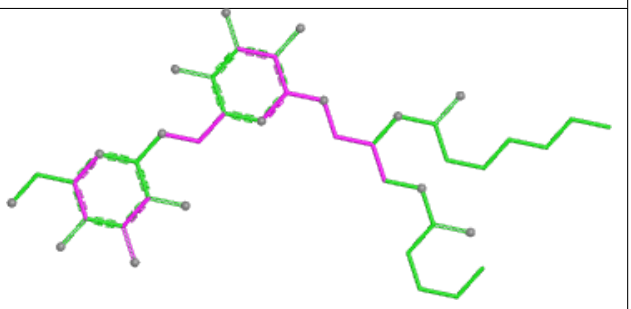
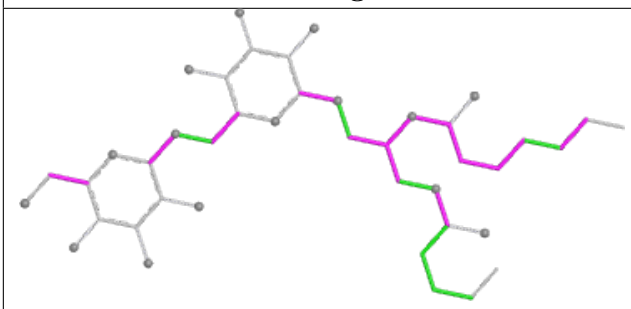
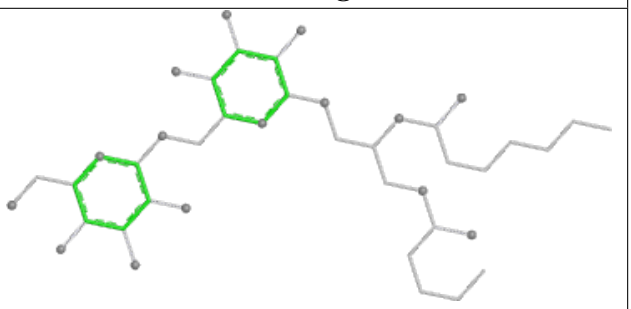
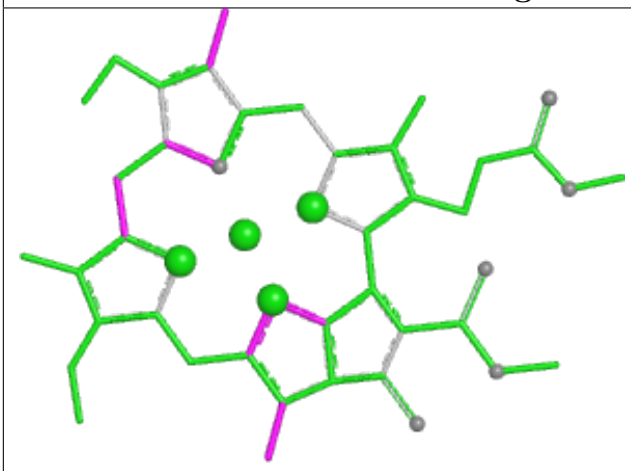
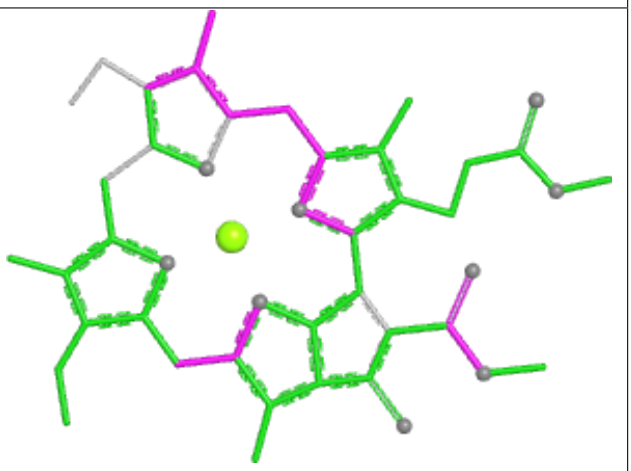
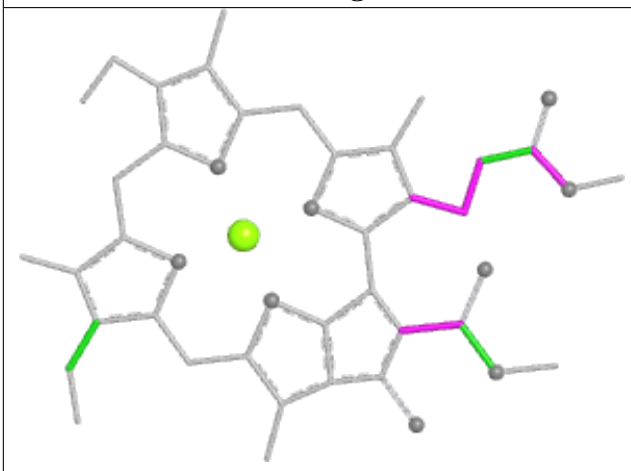
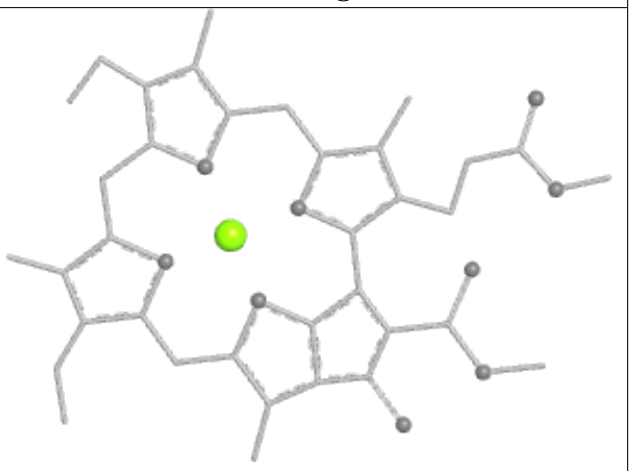
	
Bond lengths	Bond angles
	
Torsions	Rings

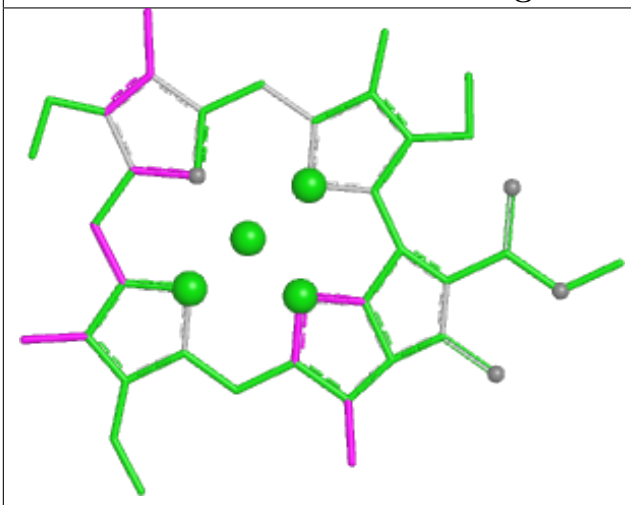
Ligand CLA A2 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

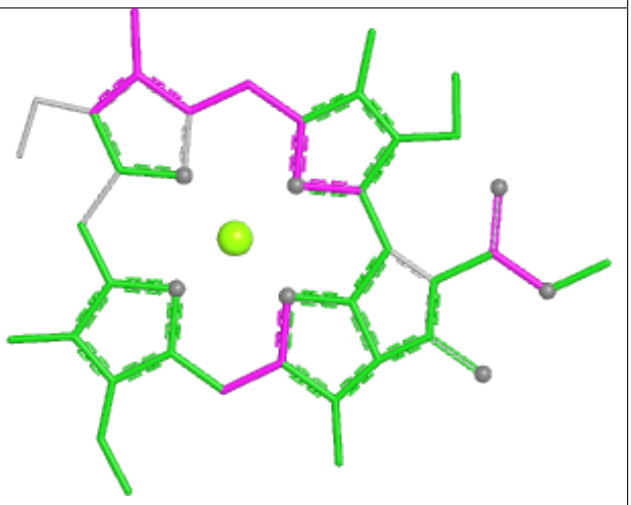
Ligand DGD BB 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K1 103	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

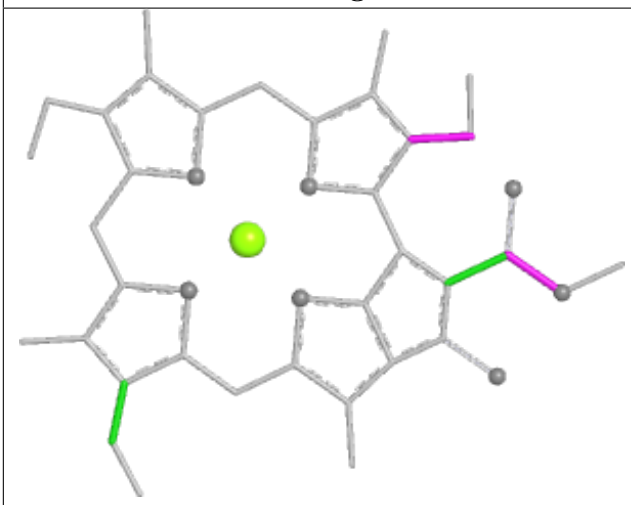
Ligand CLA A2 825



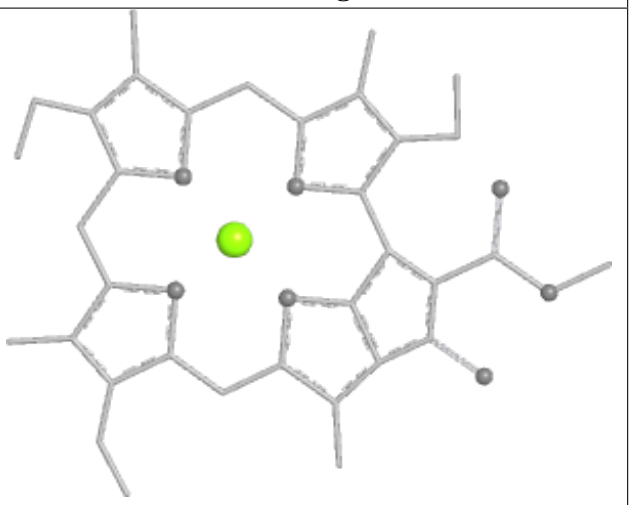
Bond lengths



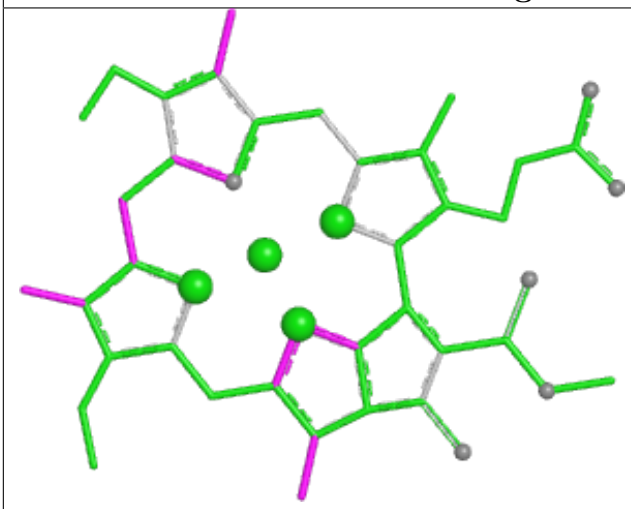
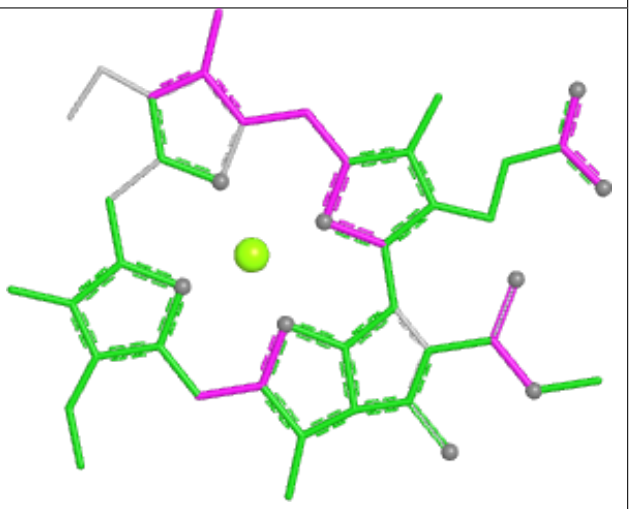
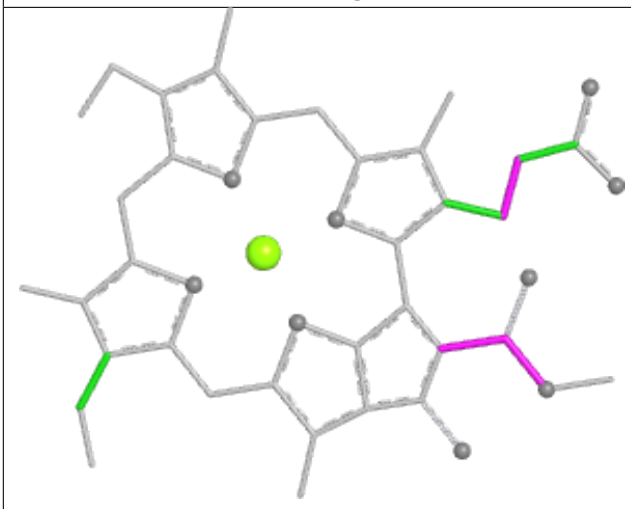
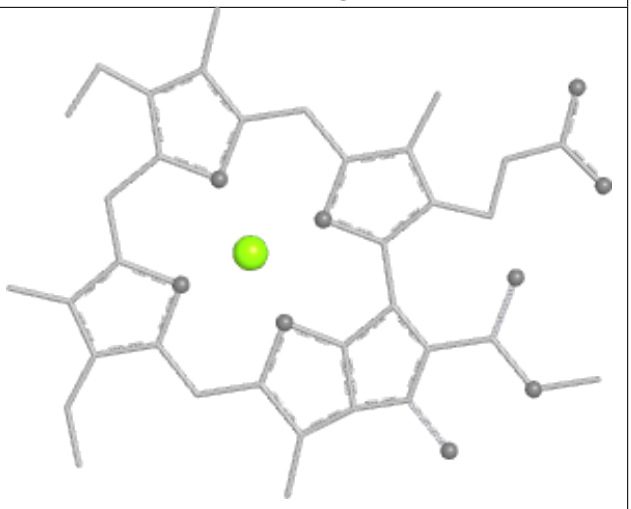
Bond angles



Torsions



Rings

Ligand CLA A1 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

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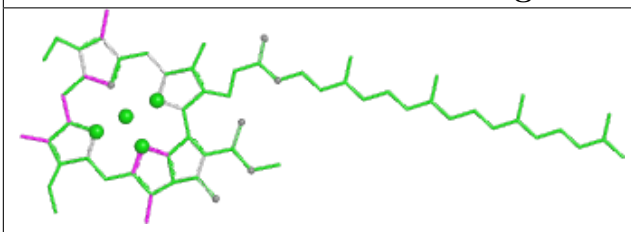
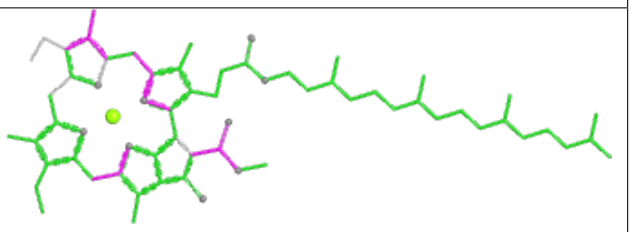
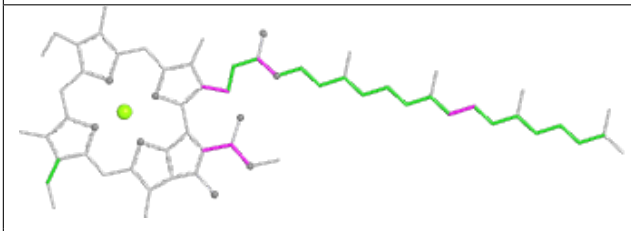
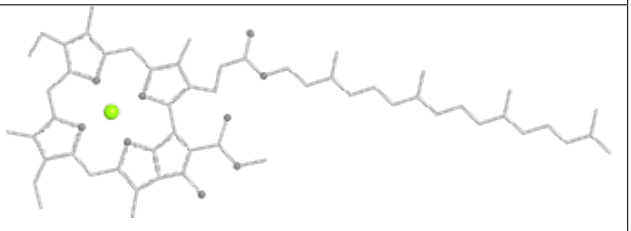
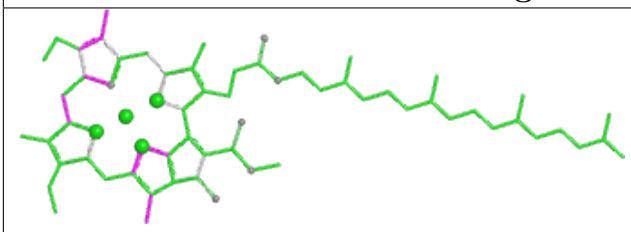
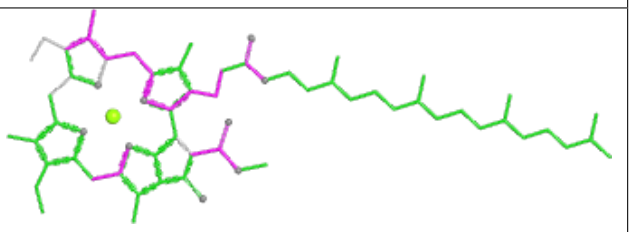
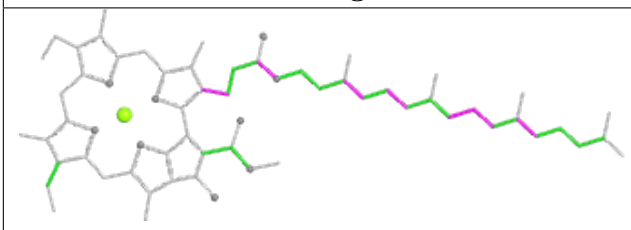
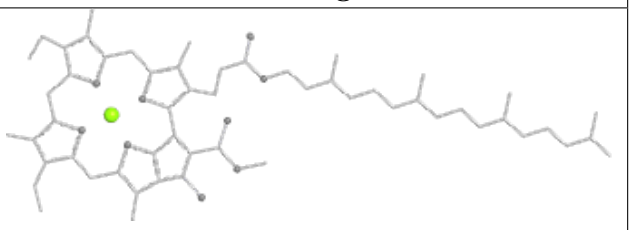
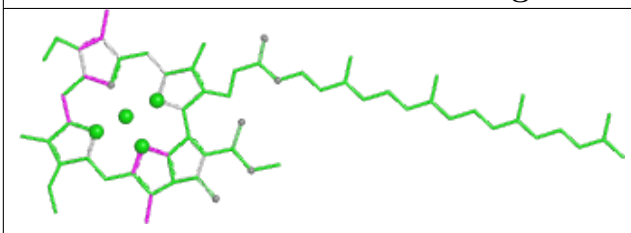
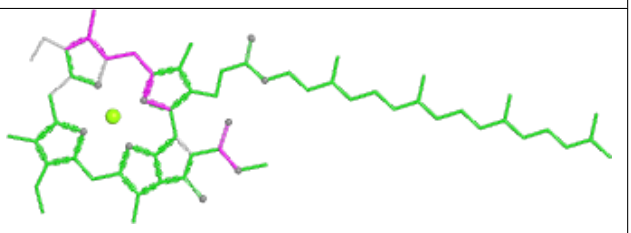
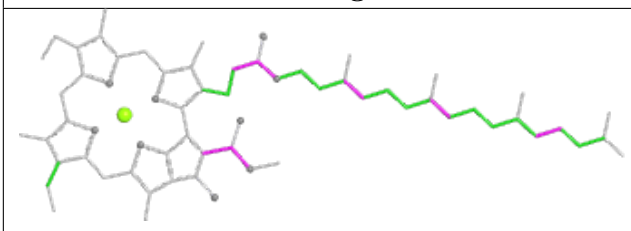
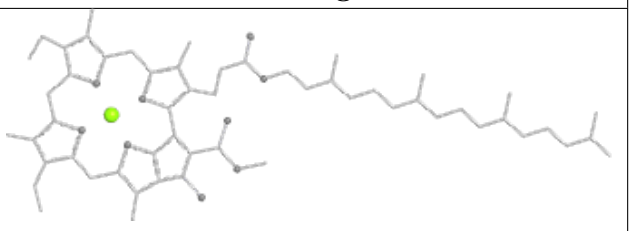
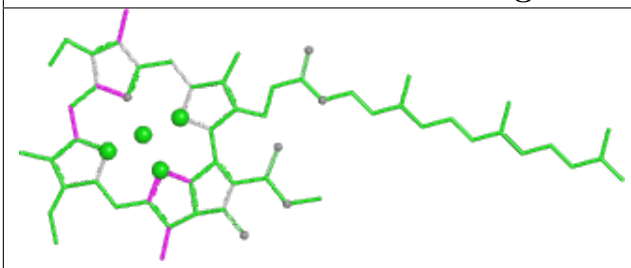
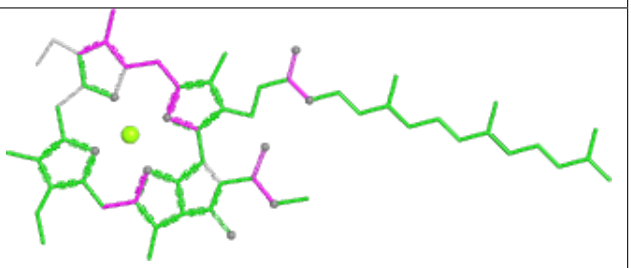
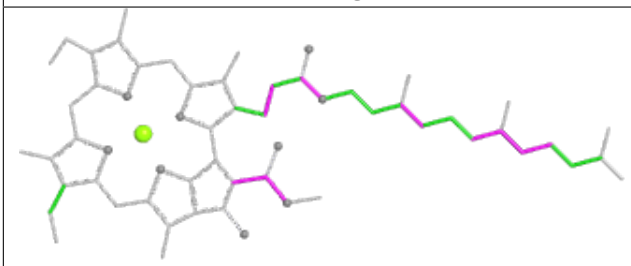
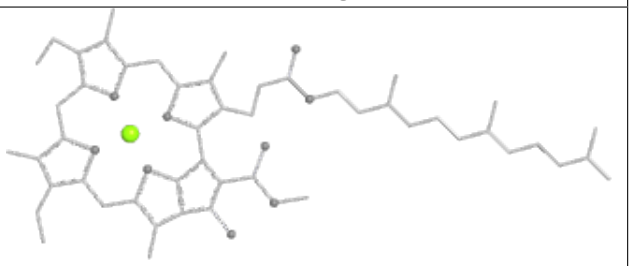
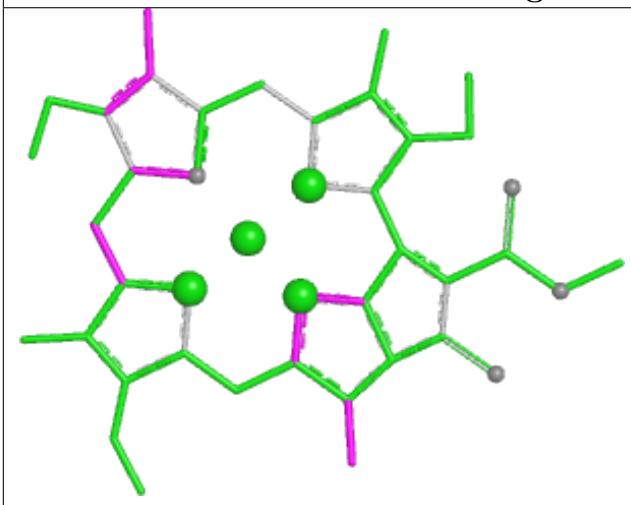
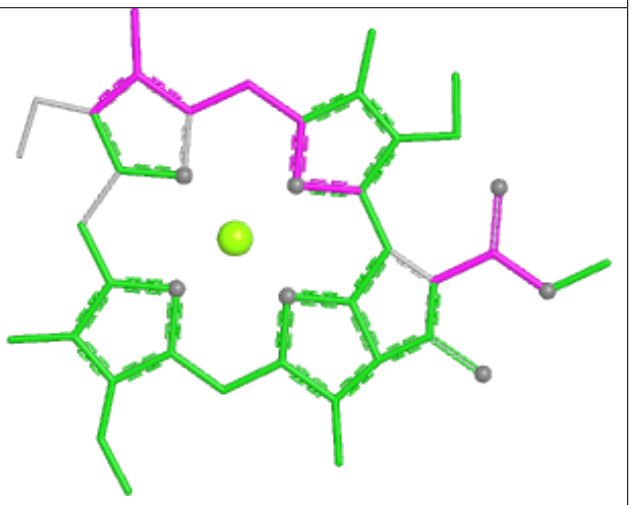
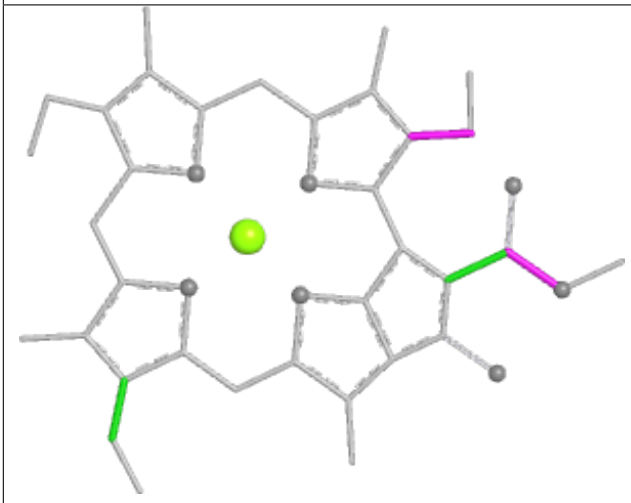
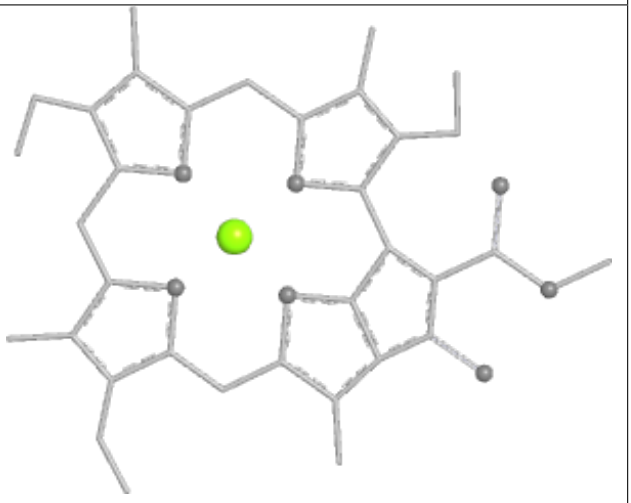
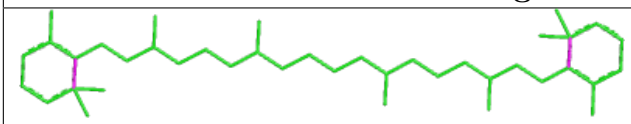
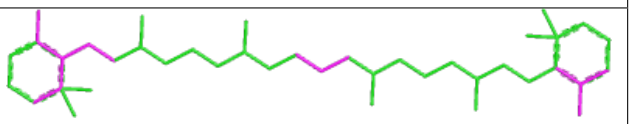
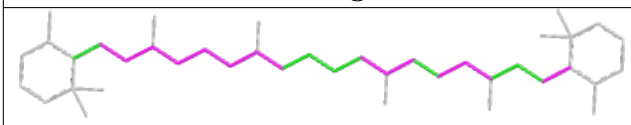
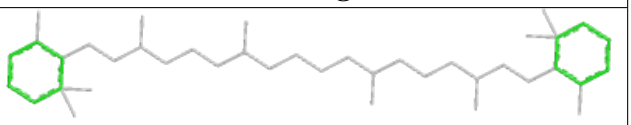
	
Bond lengths	Bond angles
	
Torsions	Rings

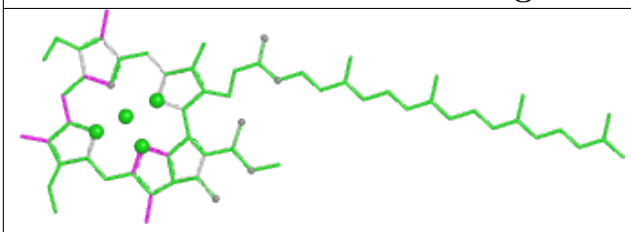
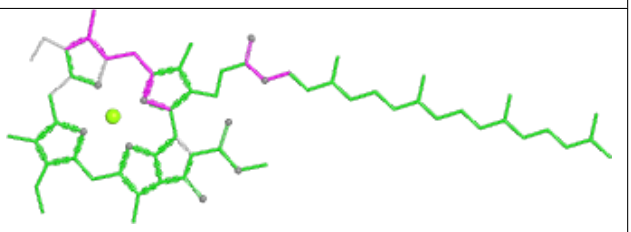
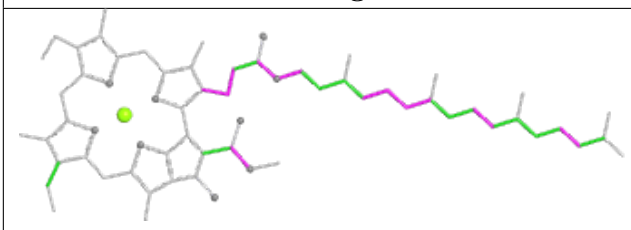
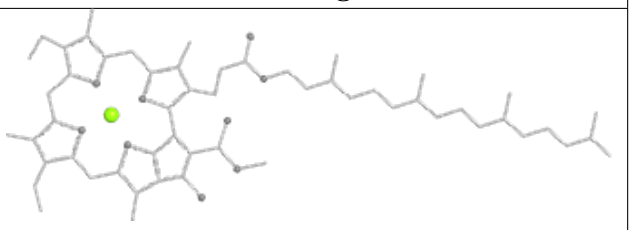
Ligand CLA A2 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BB 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B2 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

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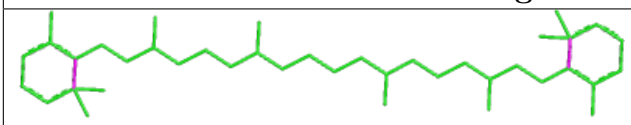
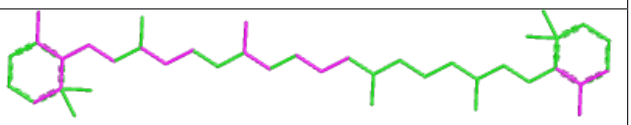
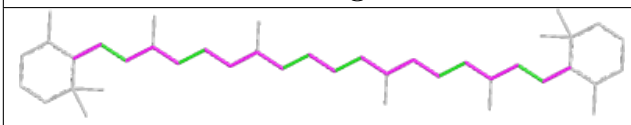
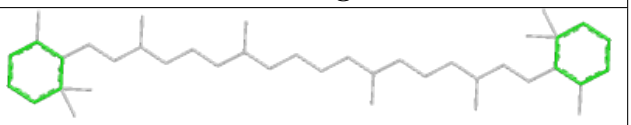
 Bond lengths	 Bond angles
 Torsions	 Rings

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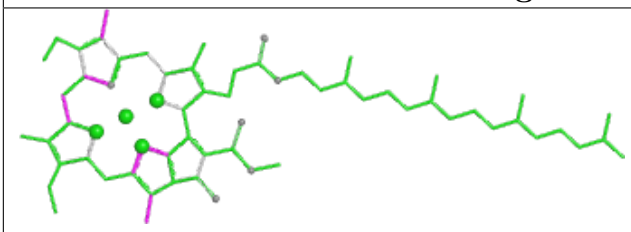
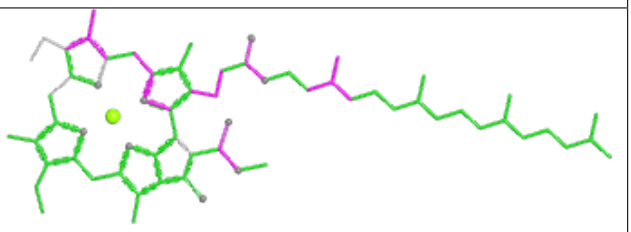
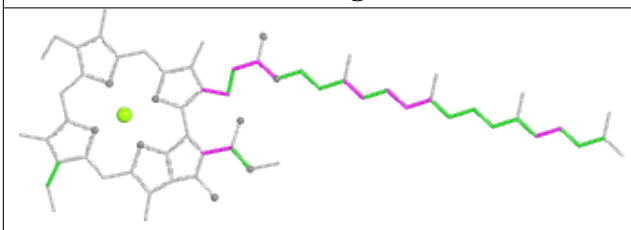
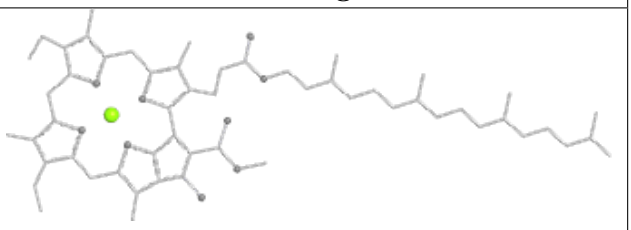
 Bond lengths	 Bond angles
 Torsions	 Rings

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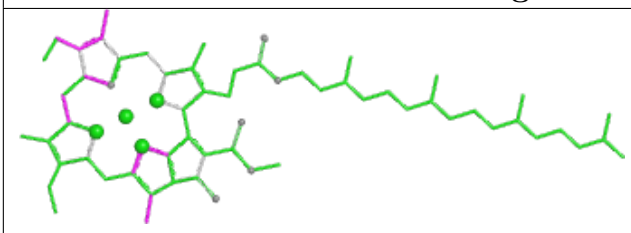
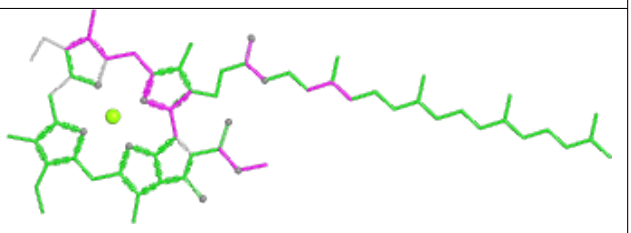
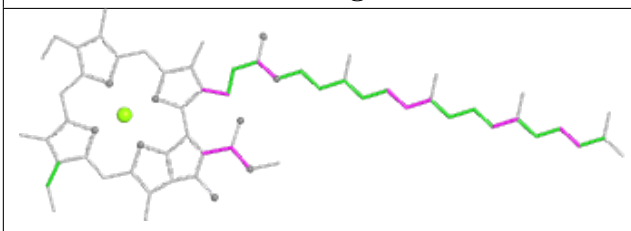
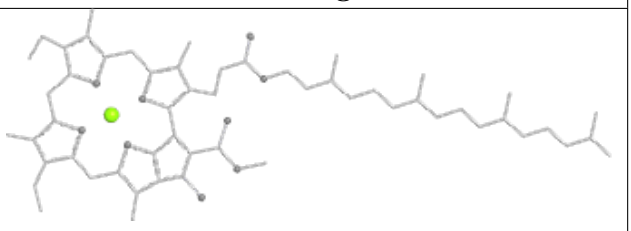
 Bond lengths	 Bond angles
 Torsions	 Rings

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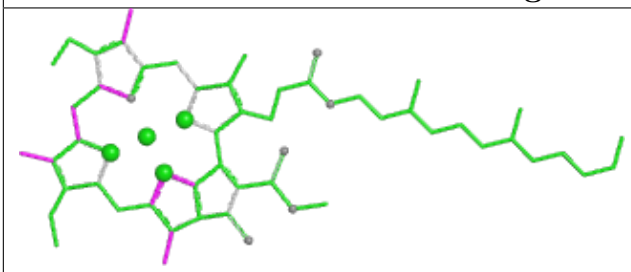
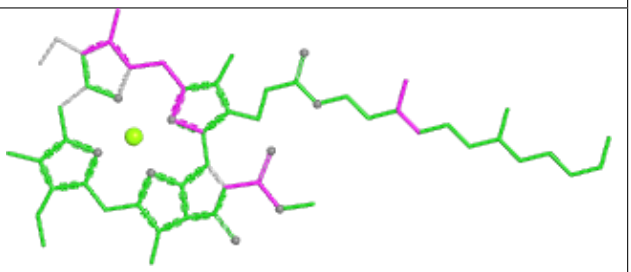
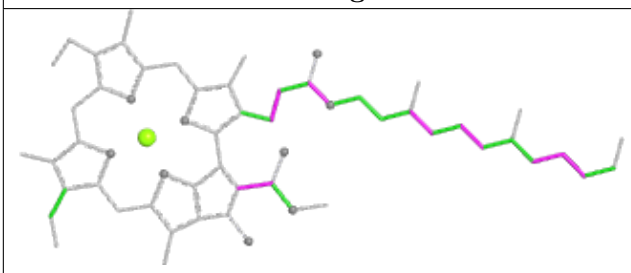
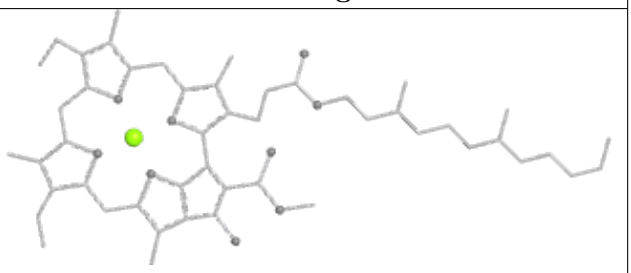
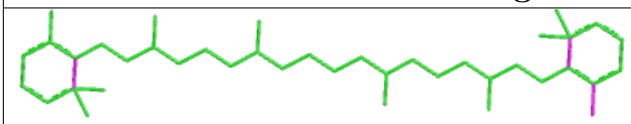
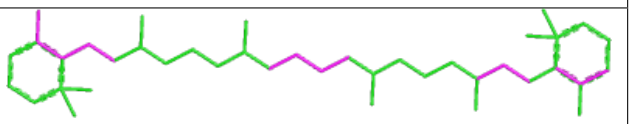
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B1 843	
	
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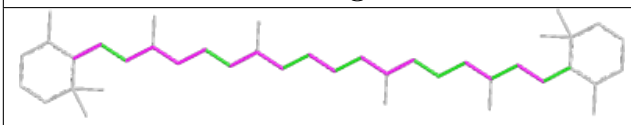	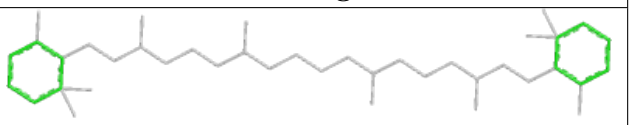
Torsions	Rings

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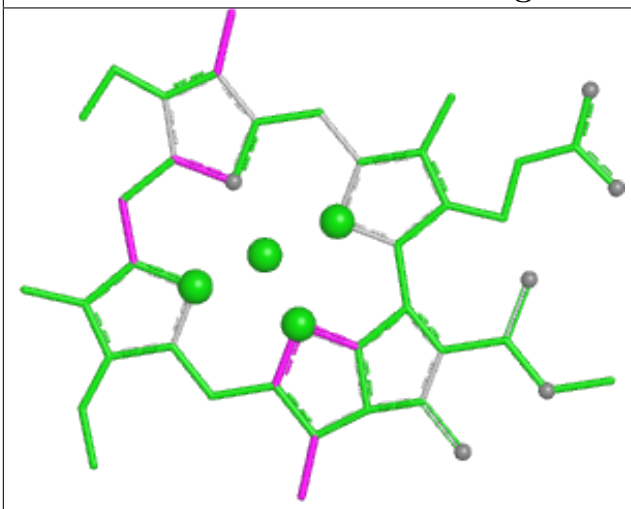
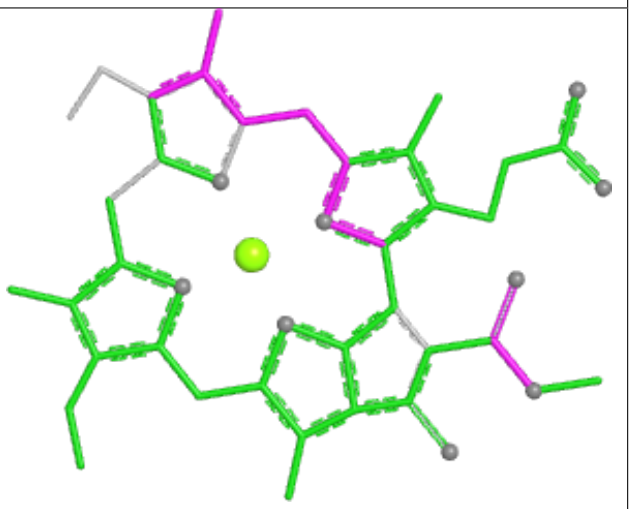
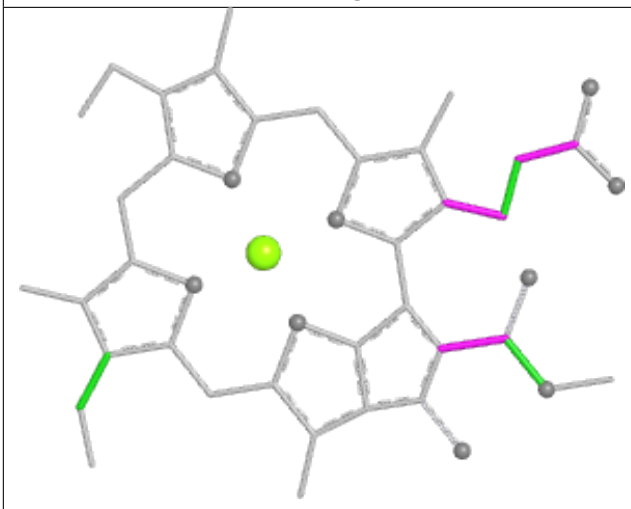
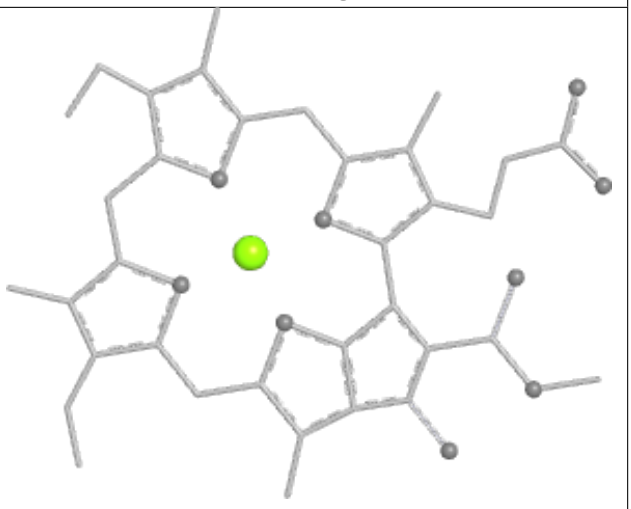
 Bond lengths	 Bond angles
 Torsions	 Rings

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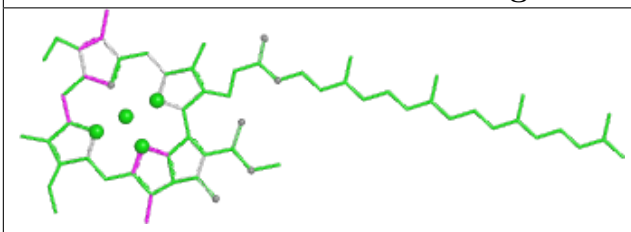
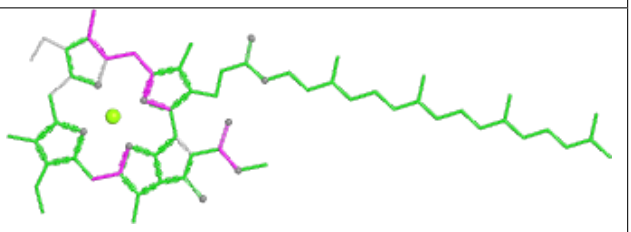
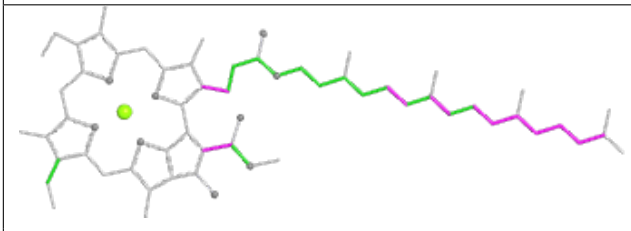
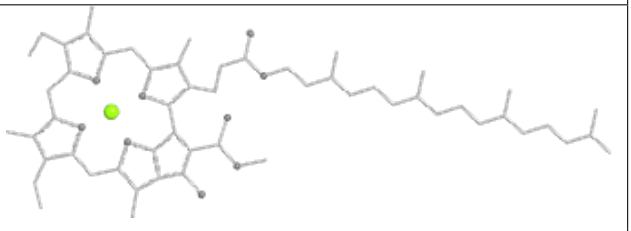
 Bond lengths	 Bond angles
 Torsions	 Rings

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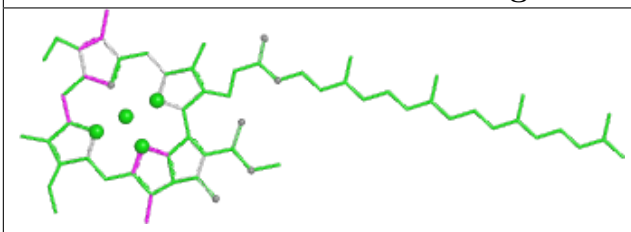
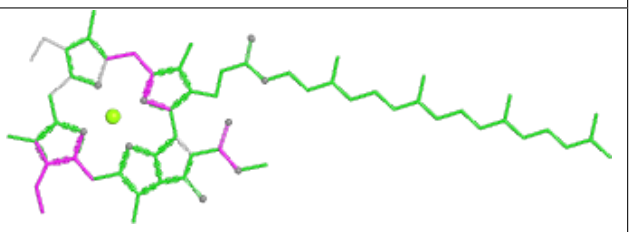
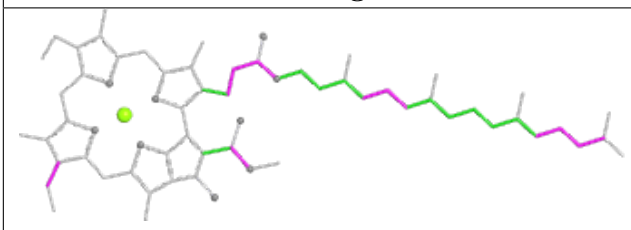
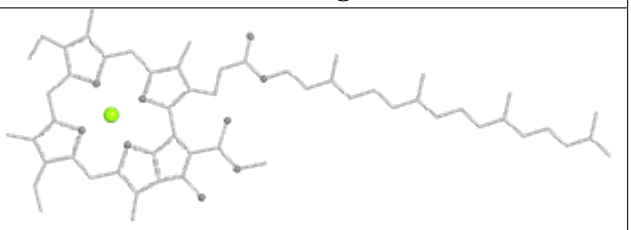
 Bond lengths	 Bond angles
 Torsions	 Rings

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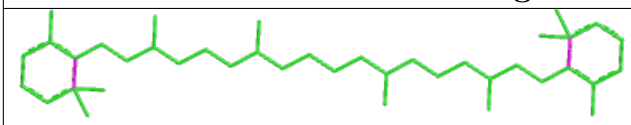
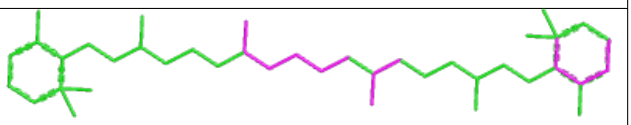
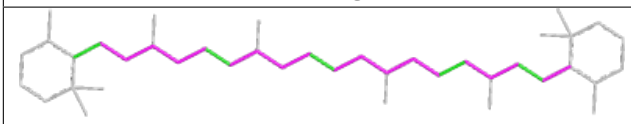
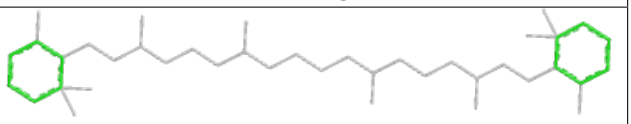
 Bond lengths	 Bond angles
 Torsions	 Rings

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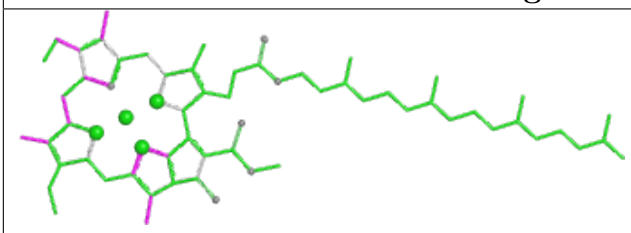
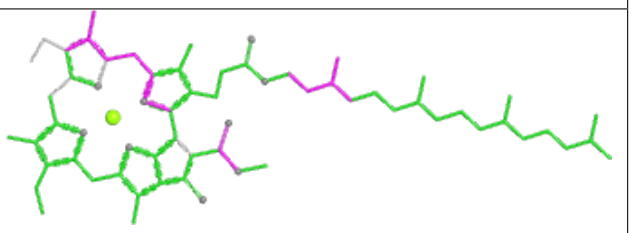
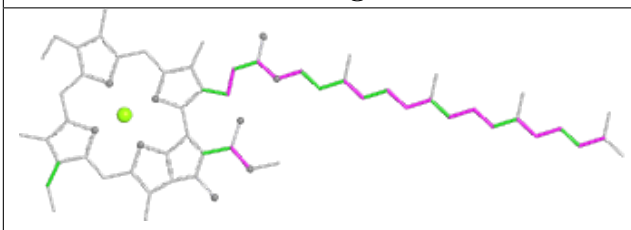
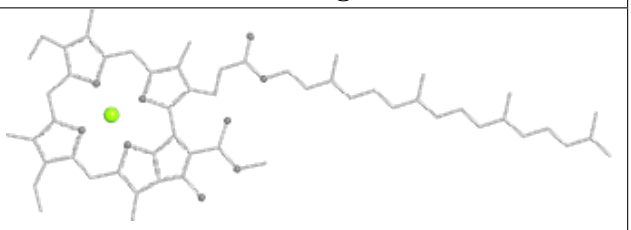
 Bond lengths	 Bond angles
 Torsions	 Rings

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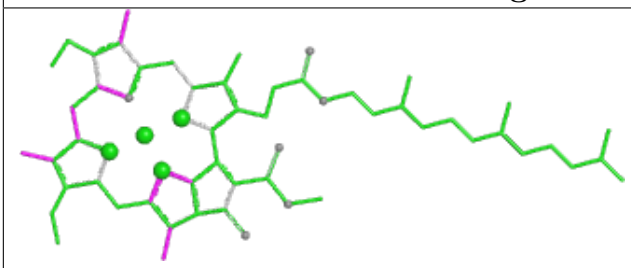
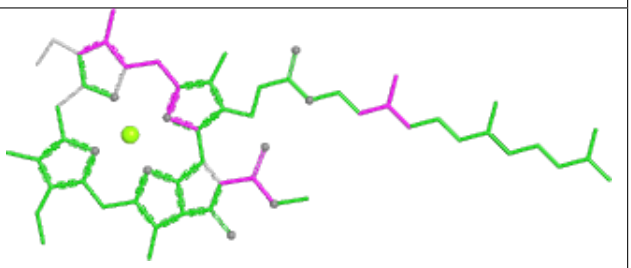
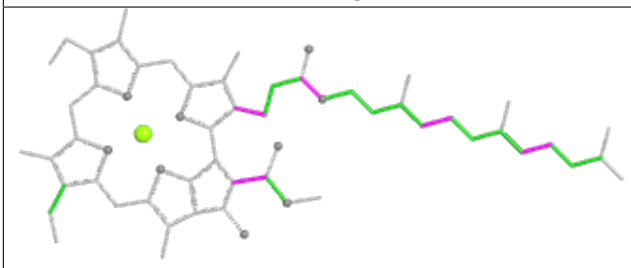
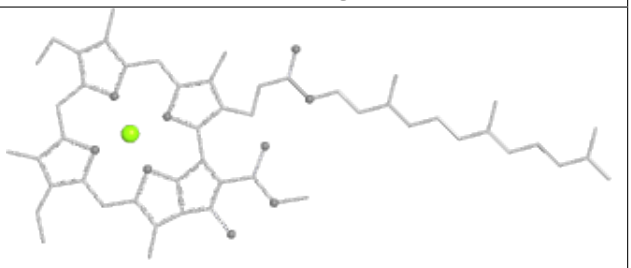
 Bond lengths	 Bond angles
 Torsions	 Rings

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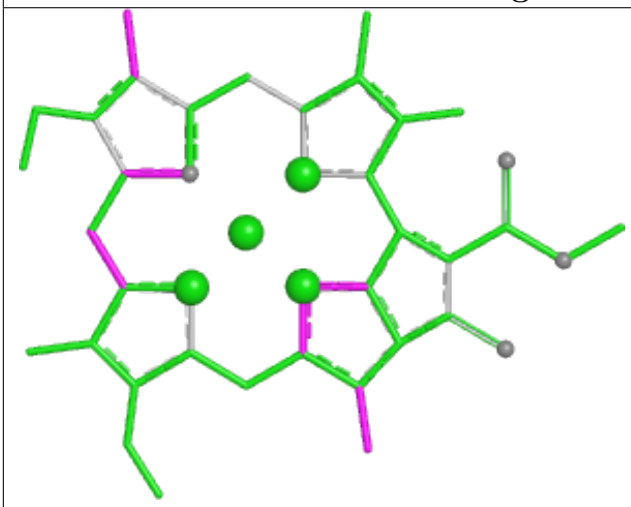
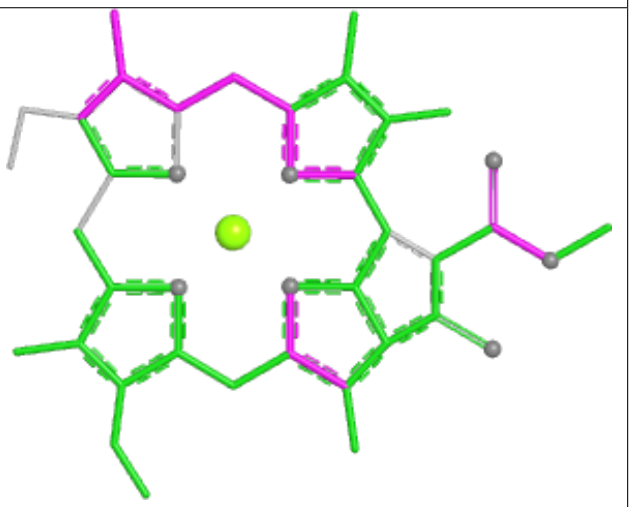
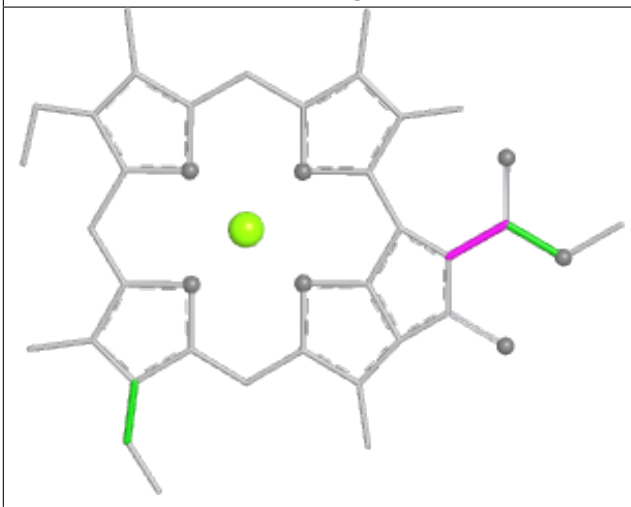
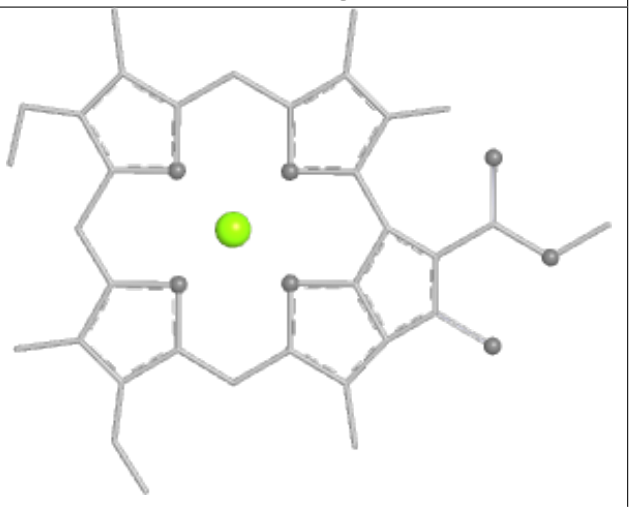
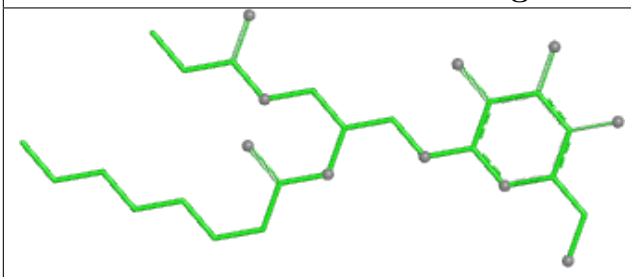
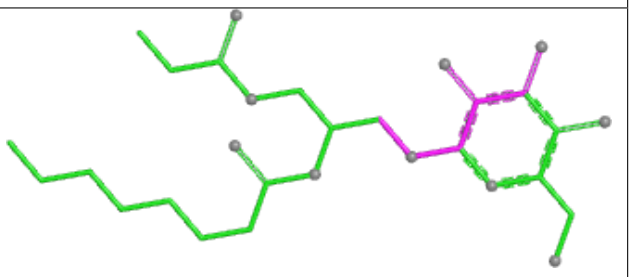
 Bond lengths	 Bond angles
 Torsions	 Rings

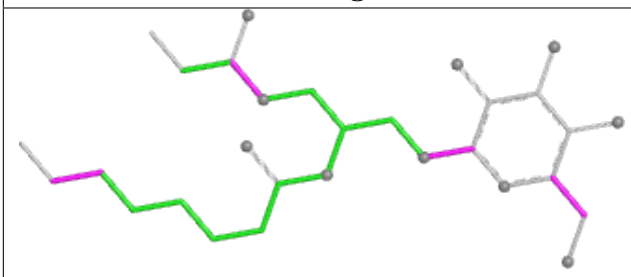
Ligand LMG B1 852



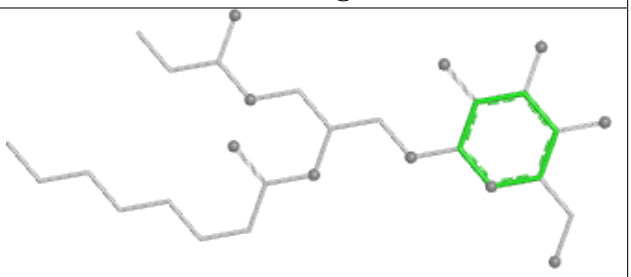
Bond lengths



Bond angles

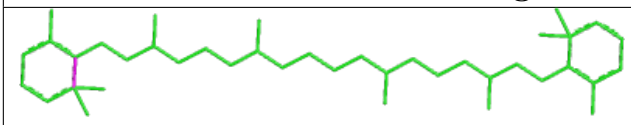


Torsions



Rings

Ligand BCR A1 851



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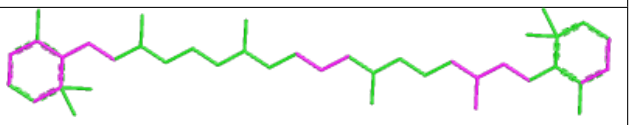
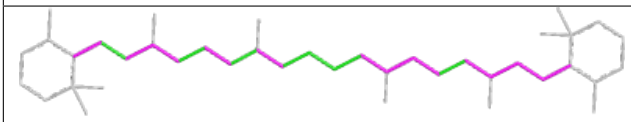


Bond angles



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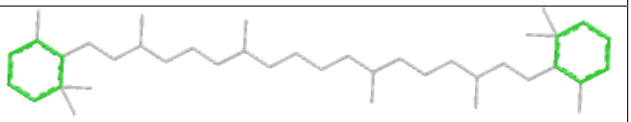
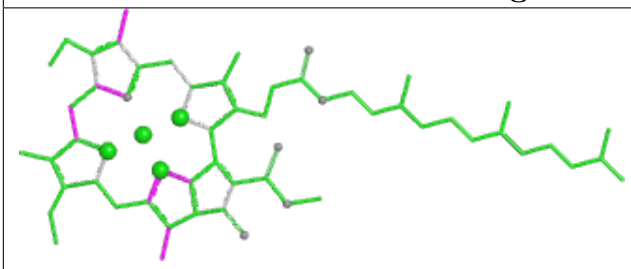
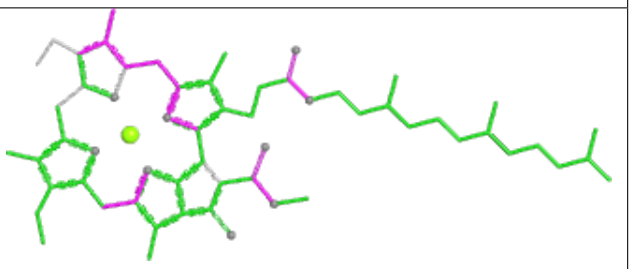


Rings

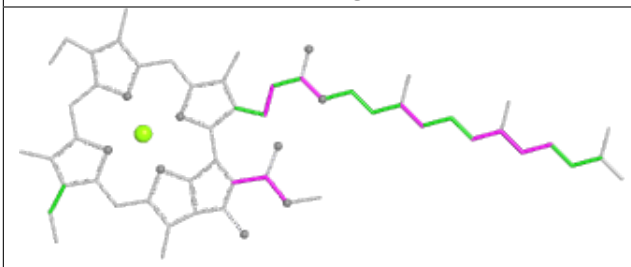
Ligand CLA AA 819



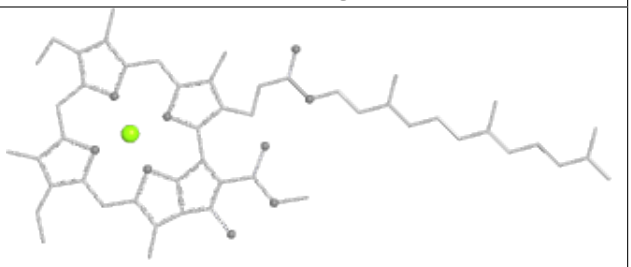
Bond lengths



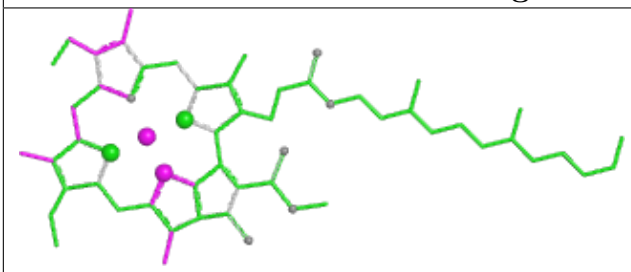
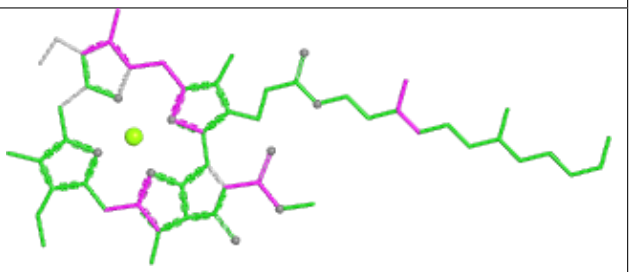
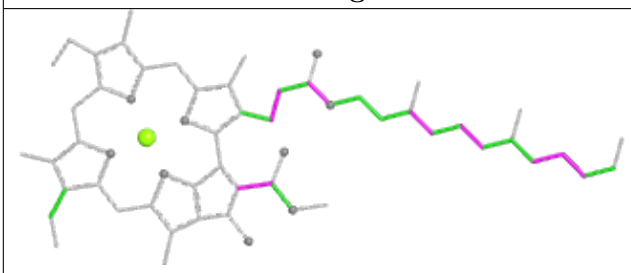
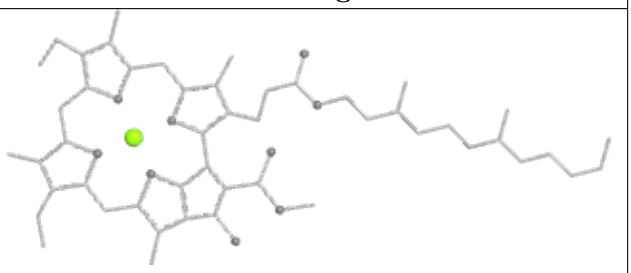
Bond angles

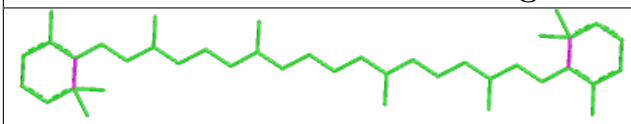
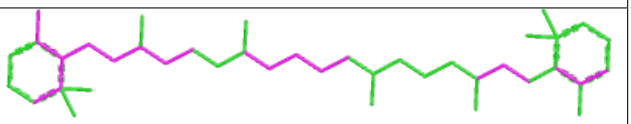
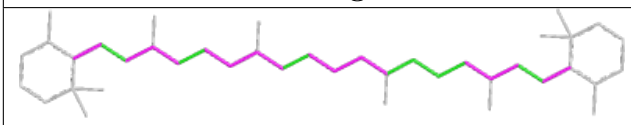
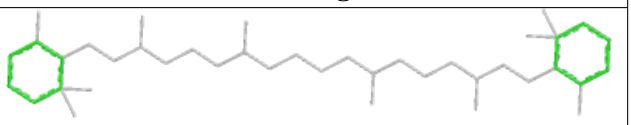


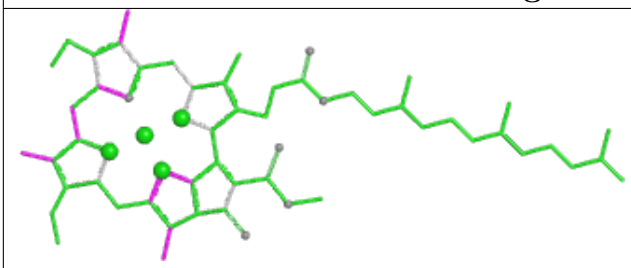
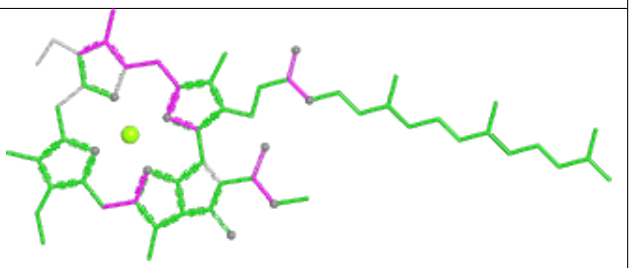
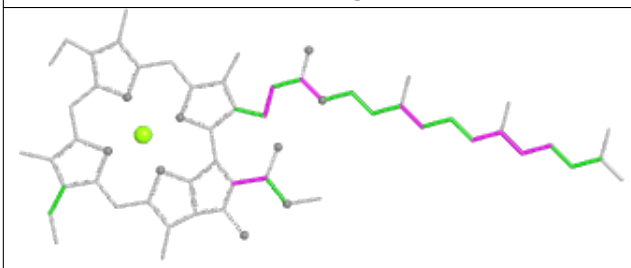
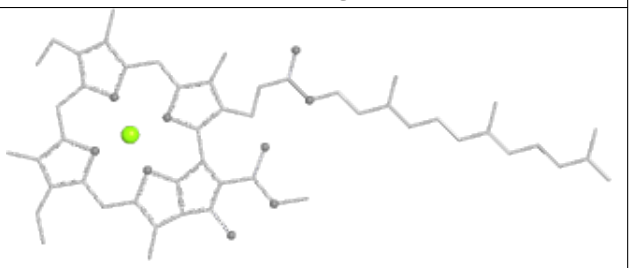
Torsions

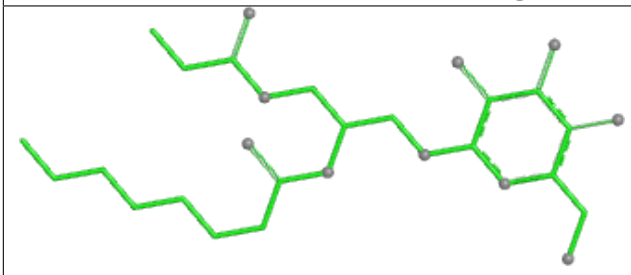
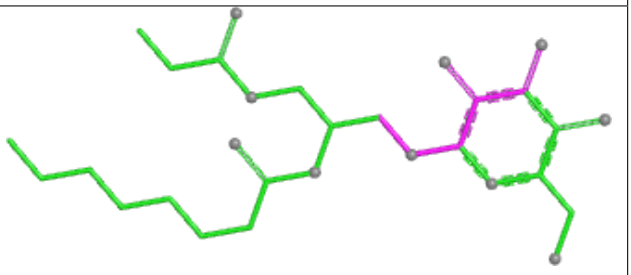
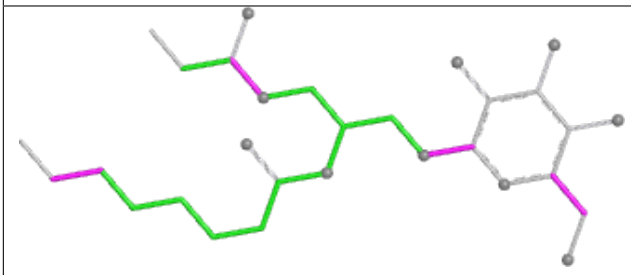
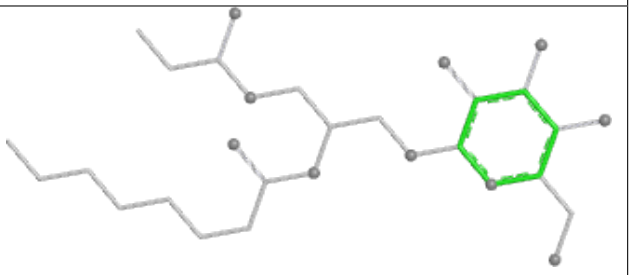


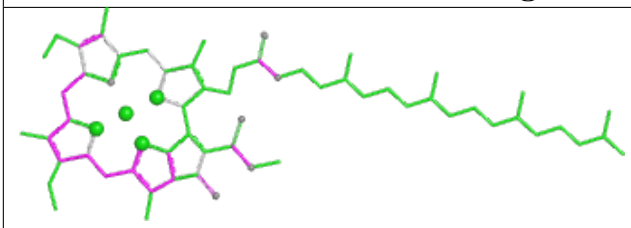
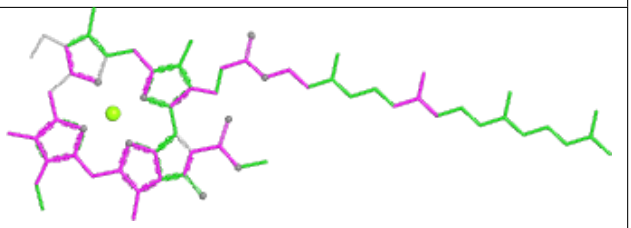
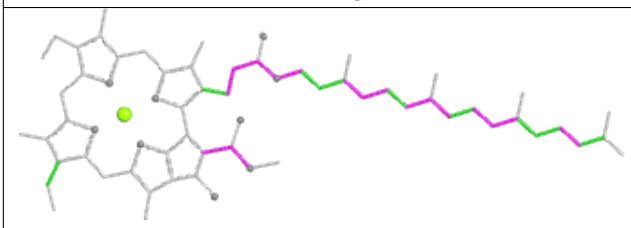
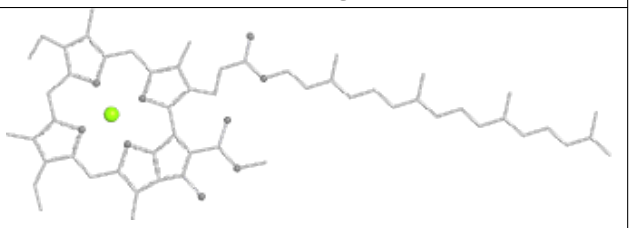
Rings

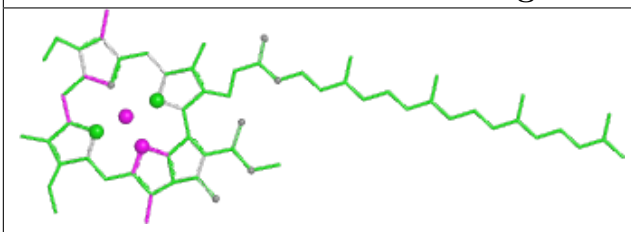
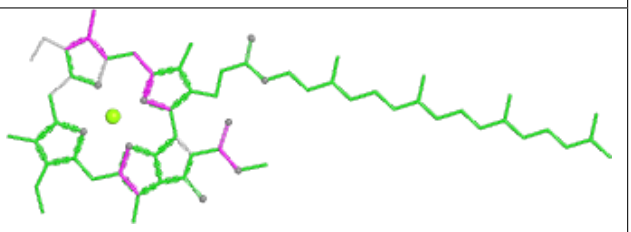
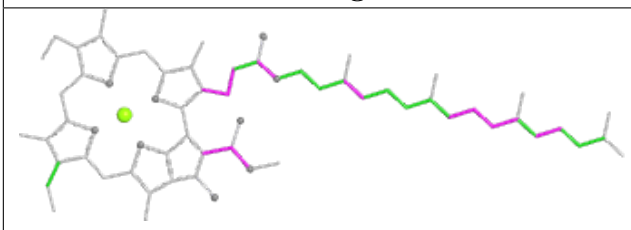
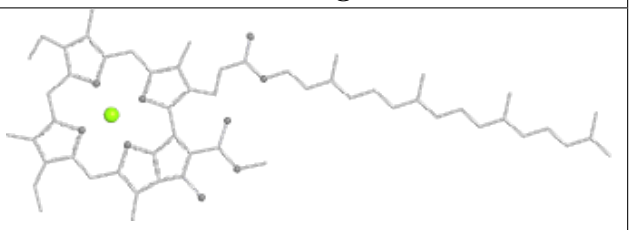
Ligand CLA BB 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

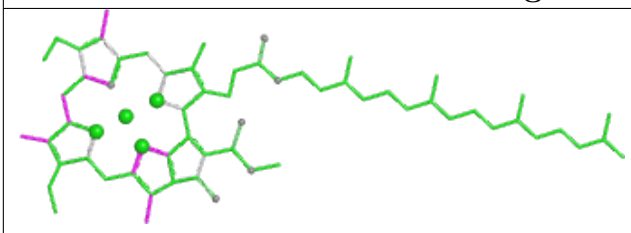
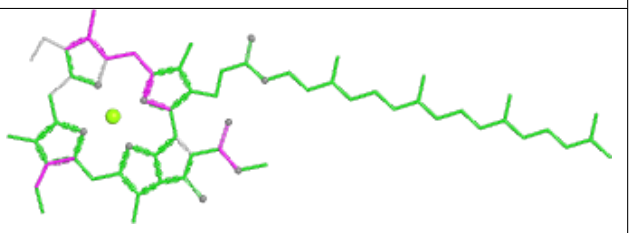
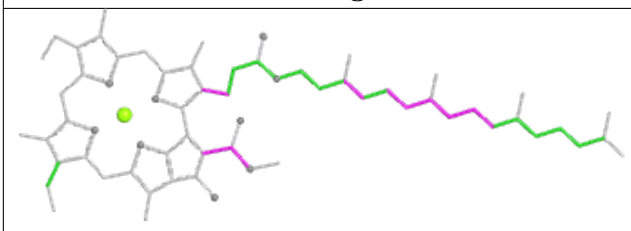
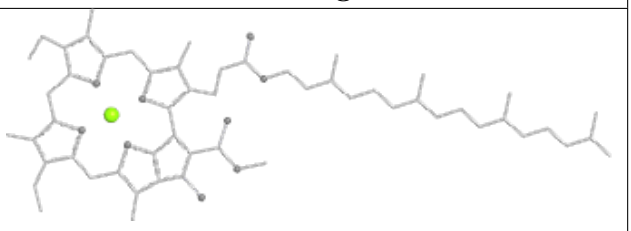
Ligand BCR I2 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

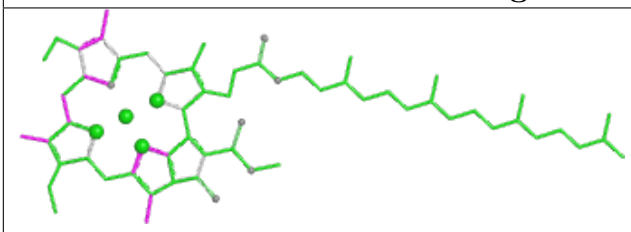
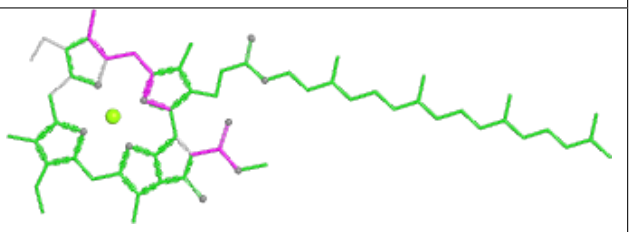
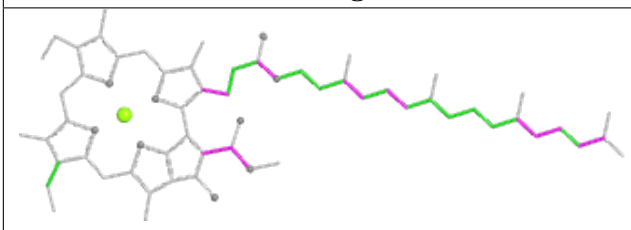
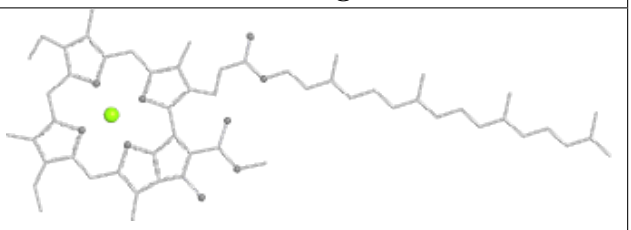
Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG B2 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL0 A2 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L2 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

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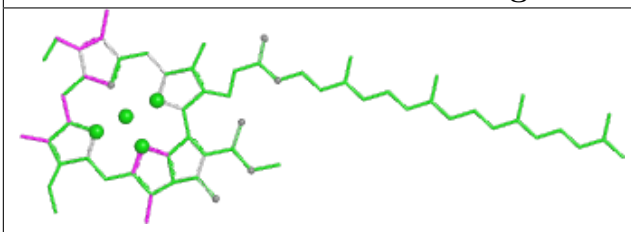
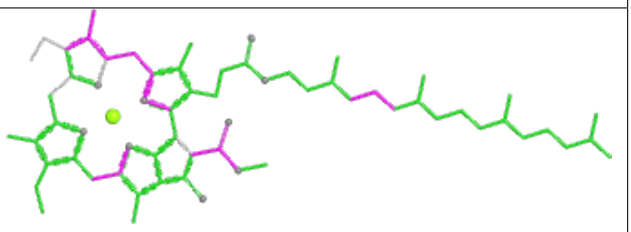
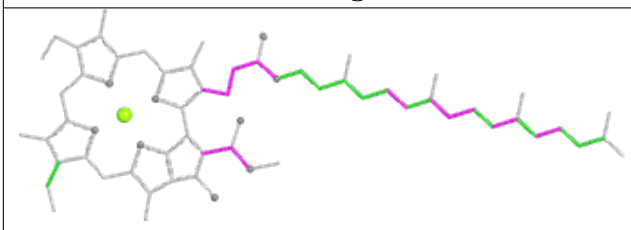
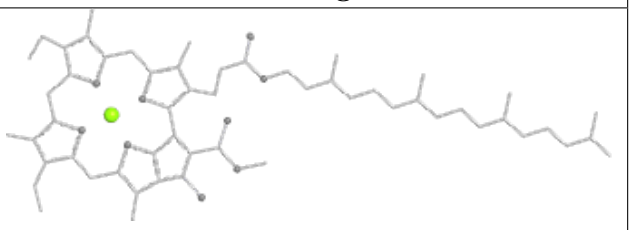
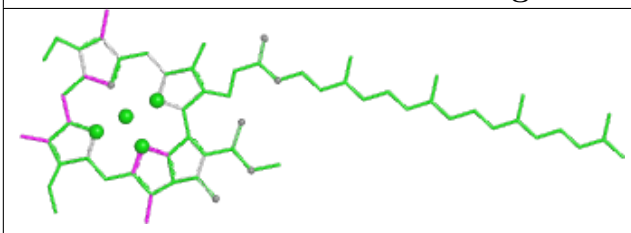
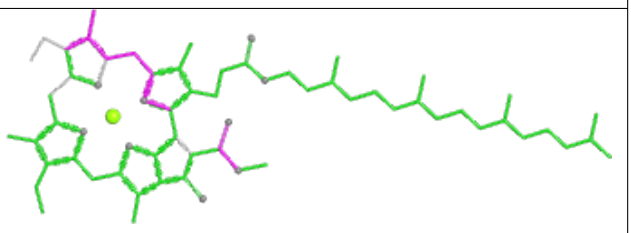
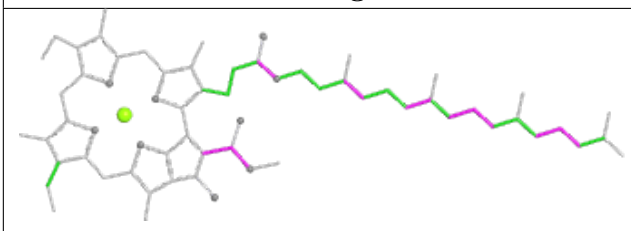
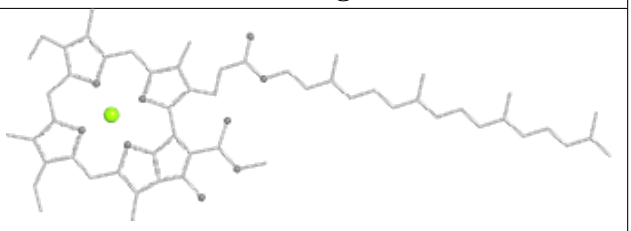
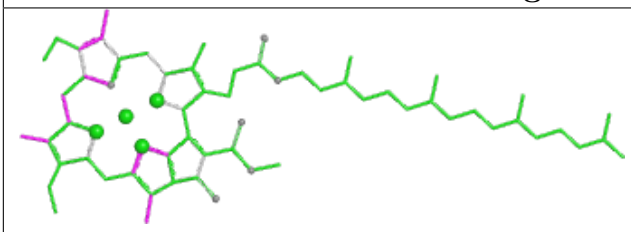
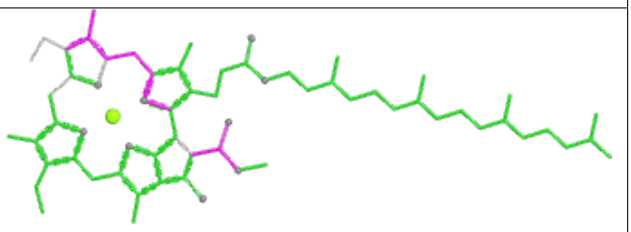
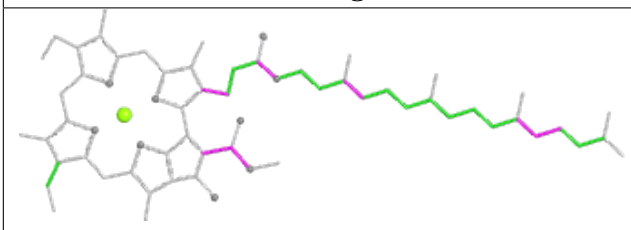
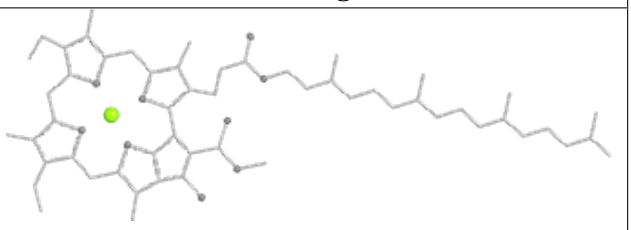
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

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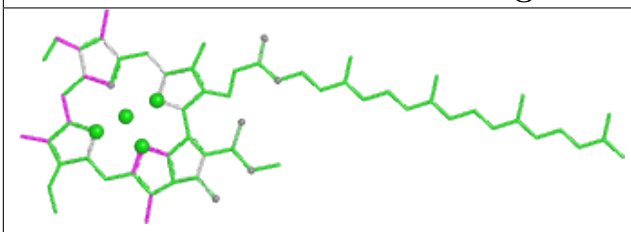
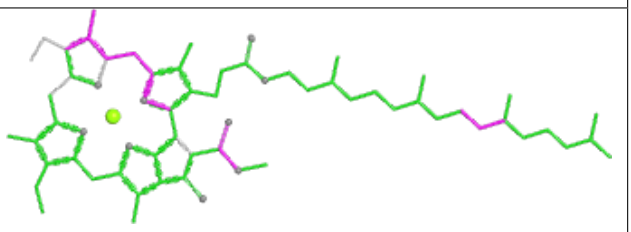
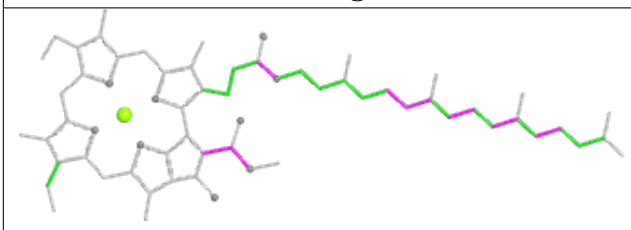
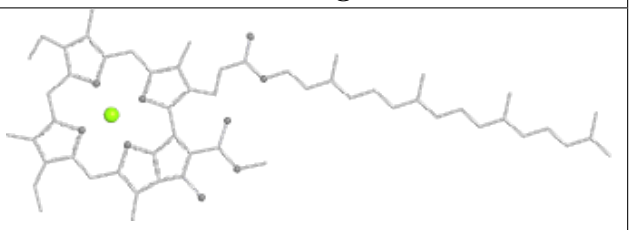
 Bond lengths	 Bond angles
 Torsions	 Rings

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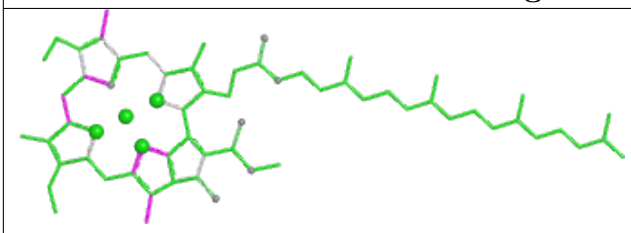
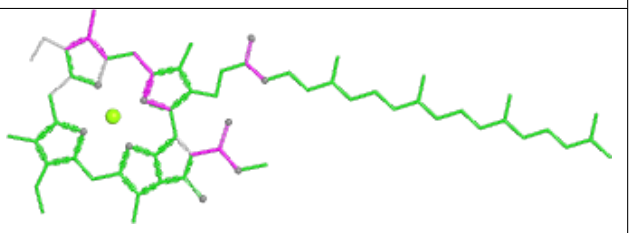
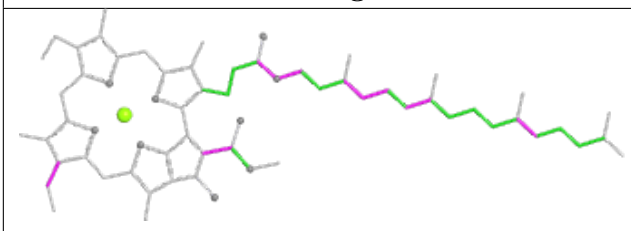
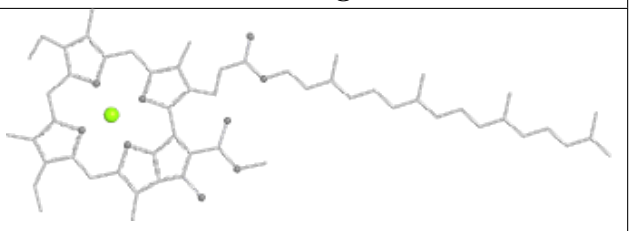
 Bond lengths	 Bond angles
 Torsions	 Rings

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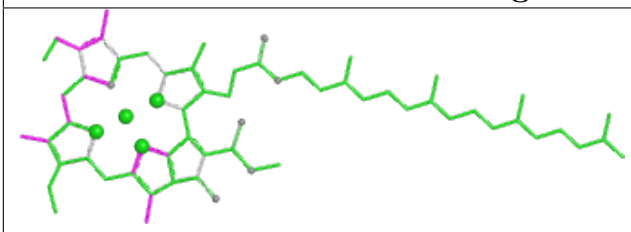
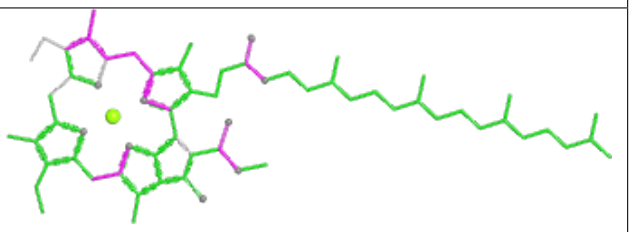
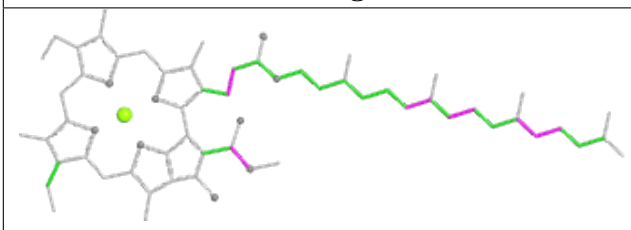
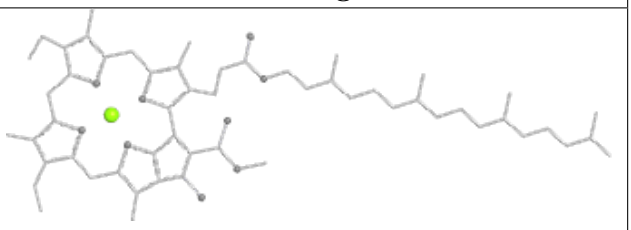
 Bond lengths	 Bond angles
 Torsions	 Rings

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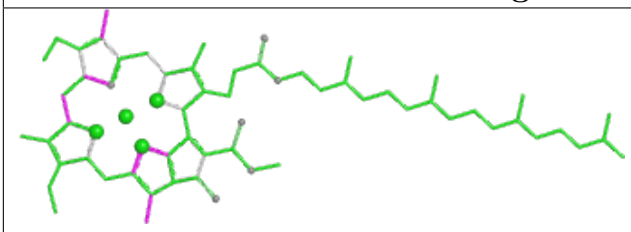
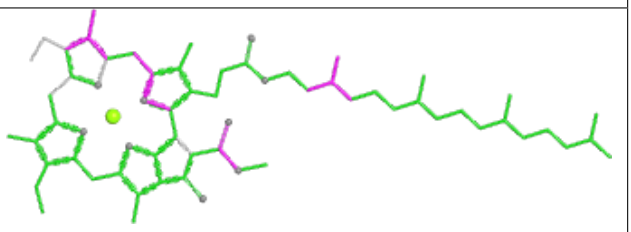
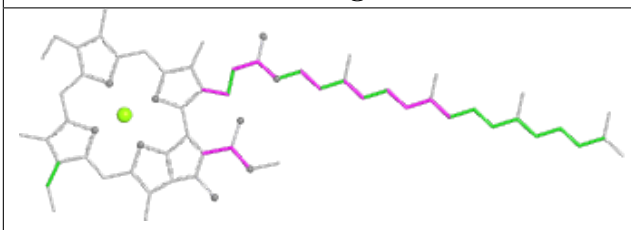
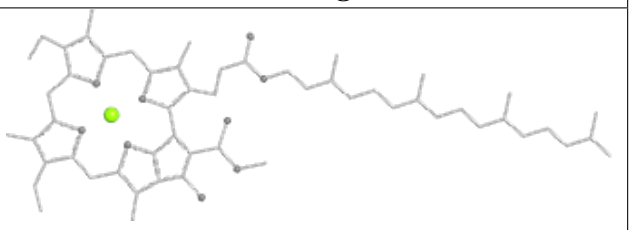
 Bond lengths	 Bond angles
 Torsions	 Rings

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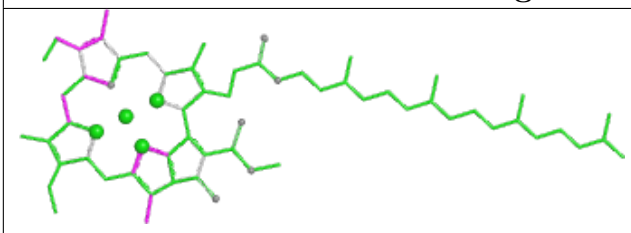
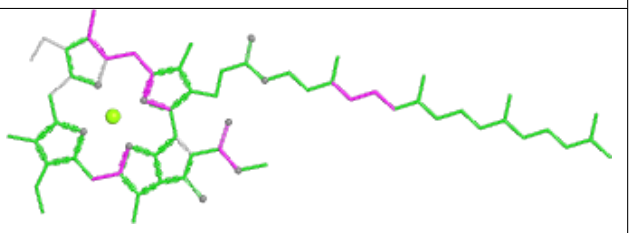
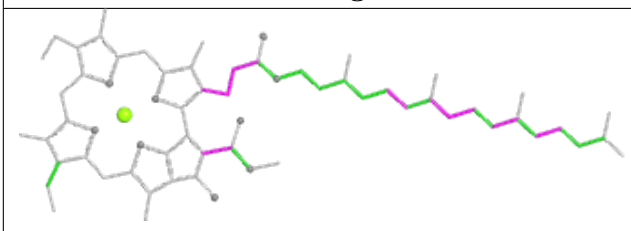
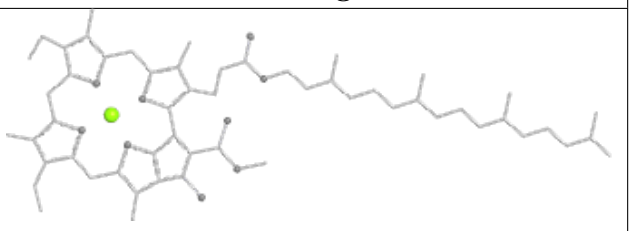
 Bond lengths	 Bond angles
 Torsions	 Rings

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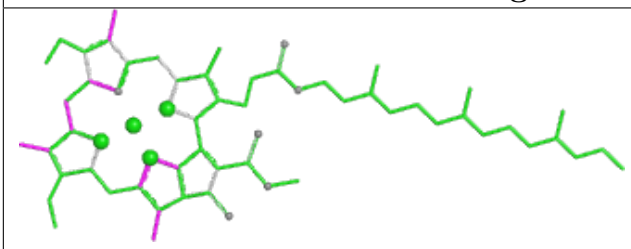
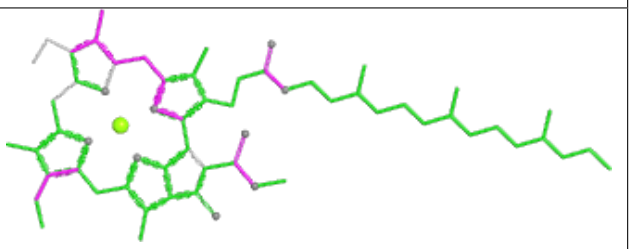
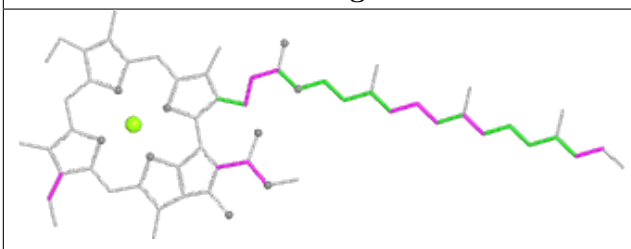
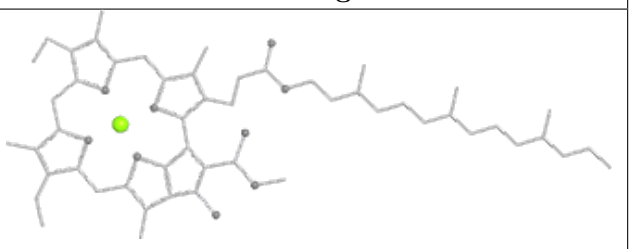
 Bond lengths	 Bond angles
 Torsions	 Rings

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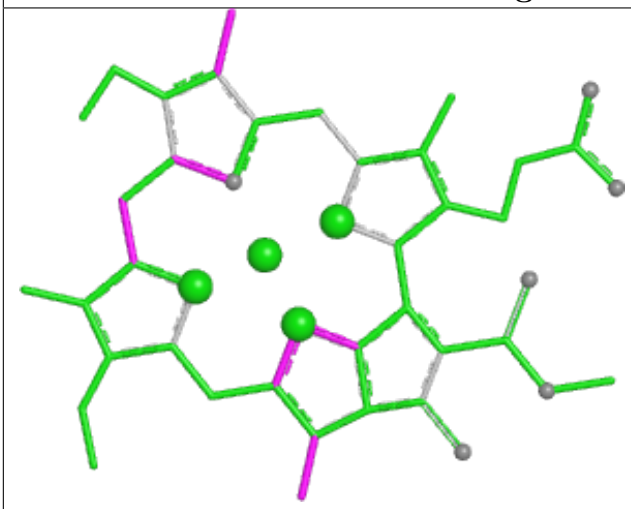
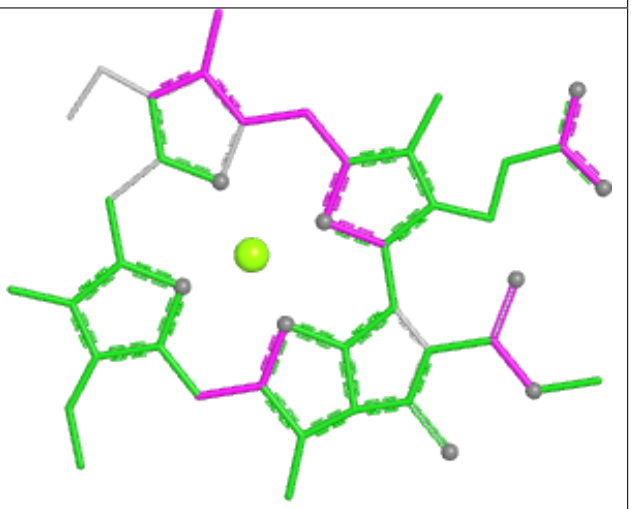
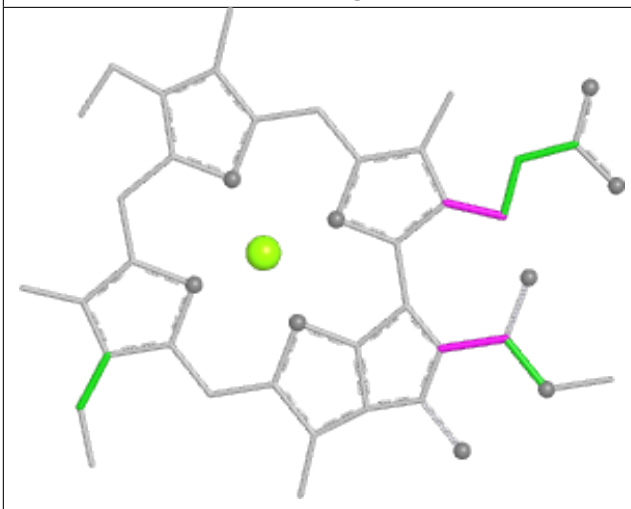
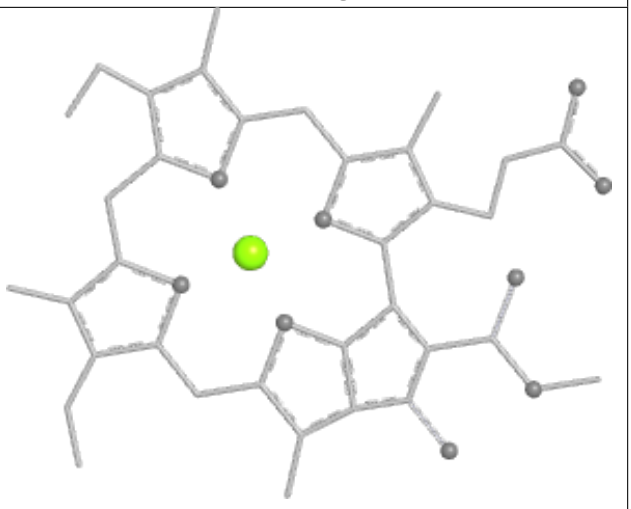
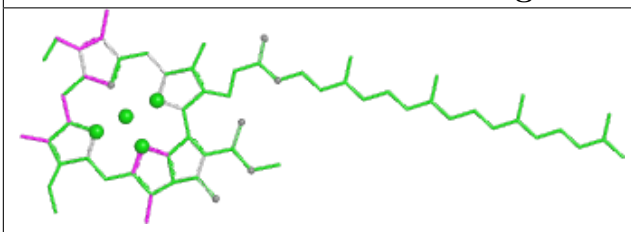
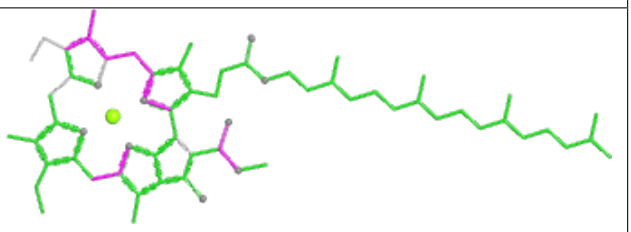
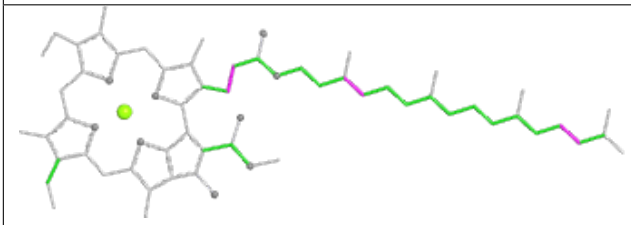
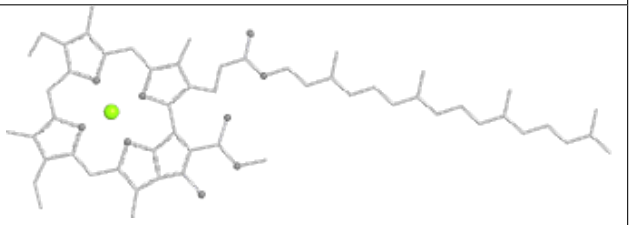
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

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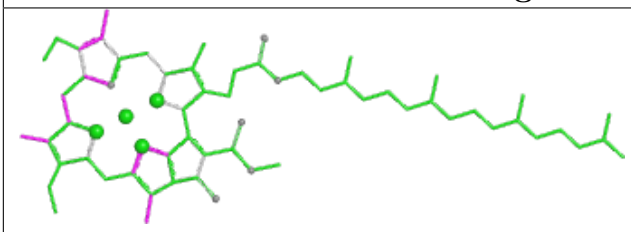
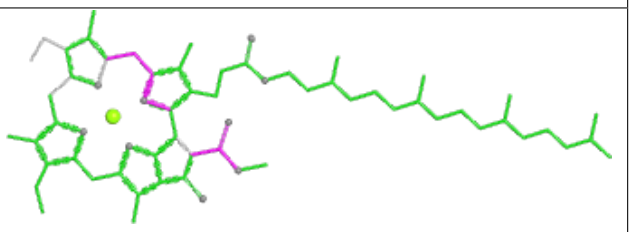
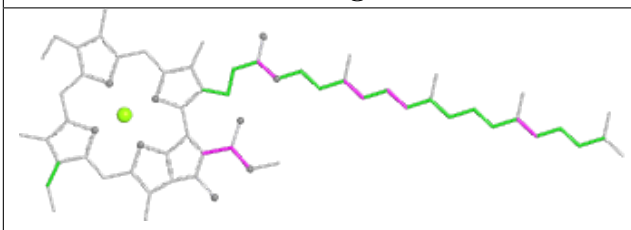
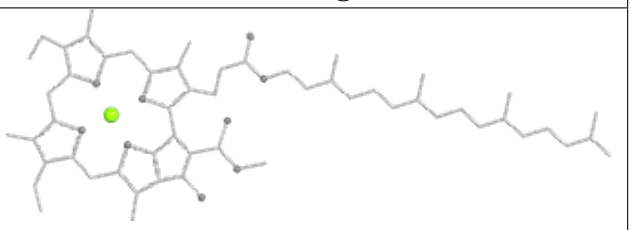
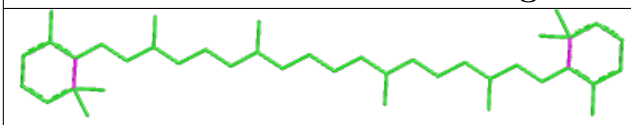
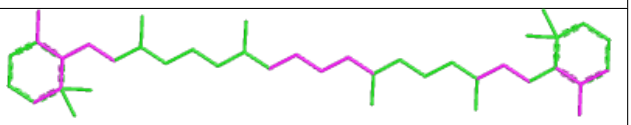
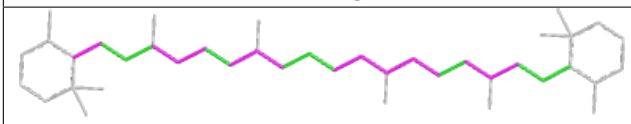
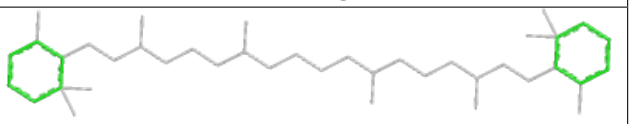
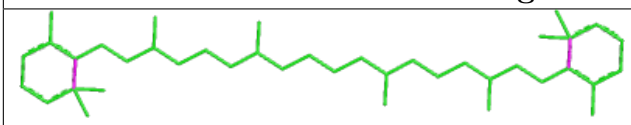
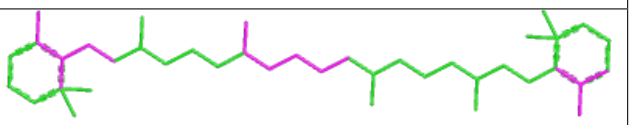
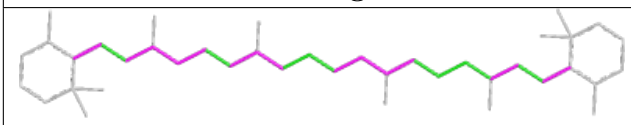
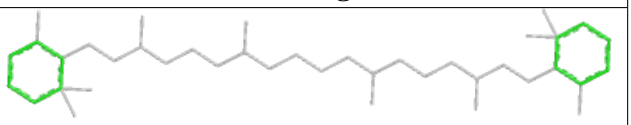
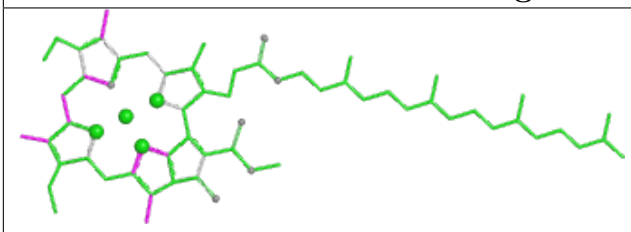
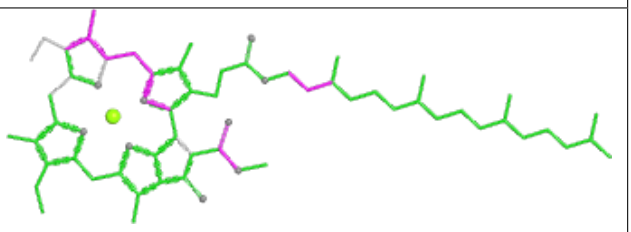
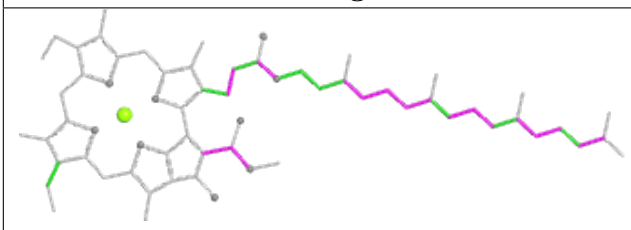
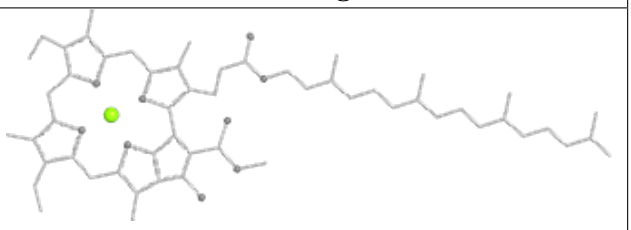
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR I2 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J2 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

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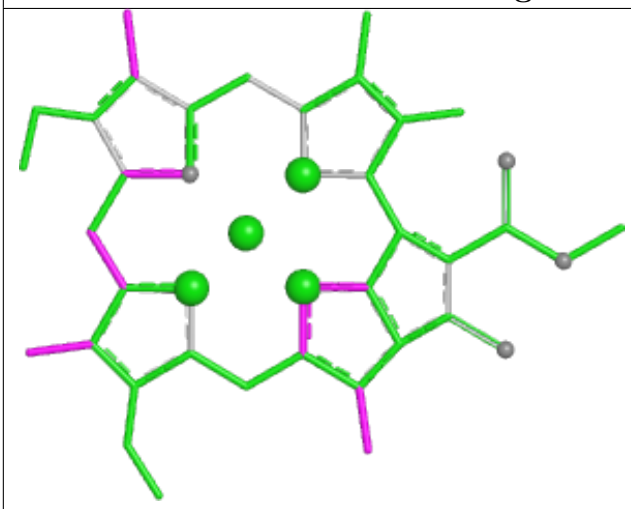
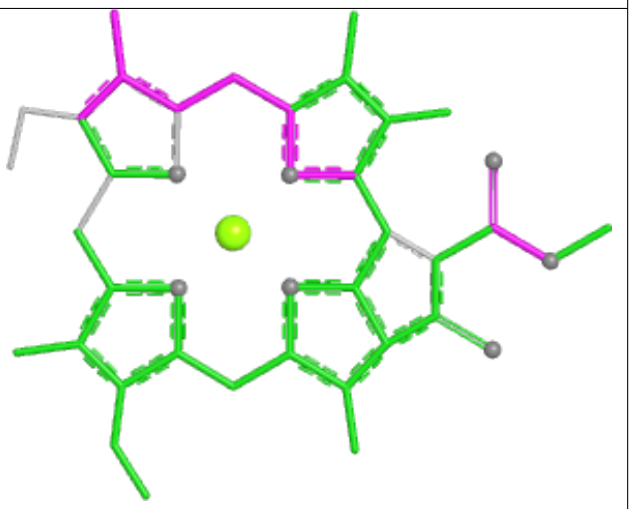
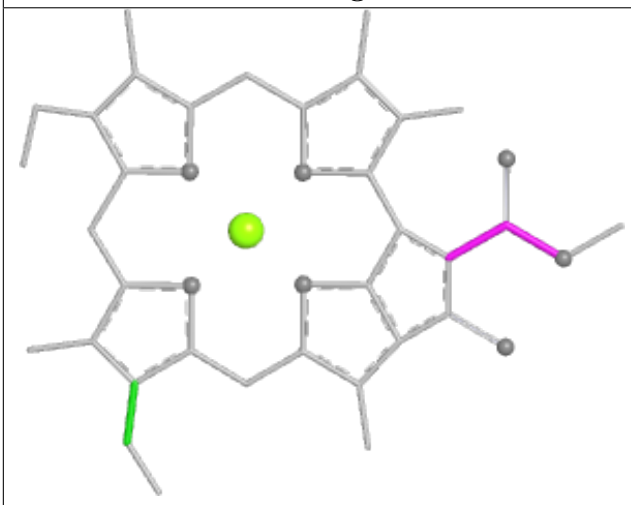
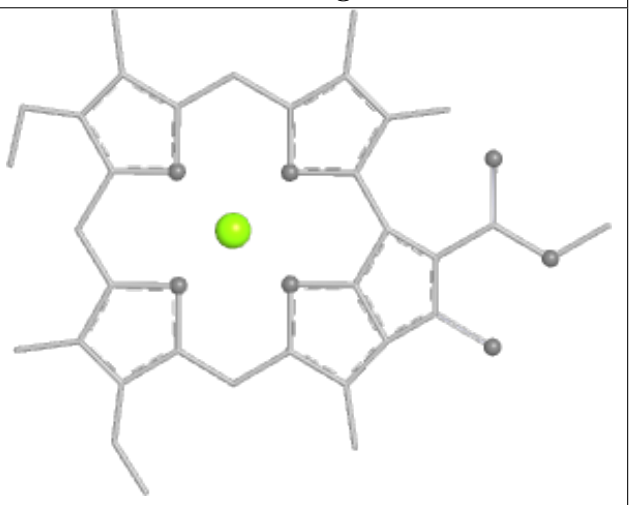
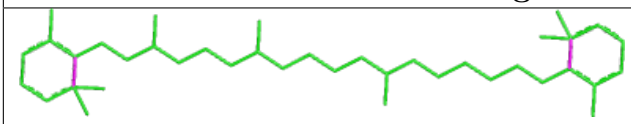
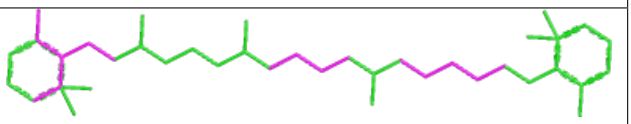
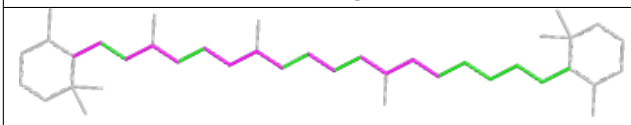
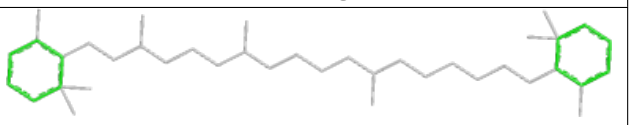
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A2 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

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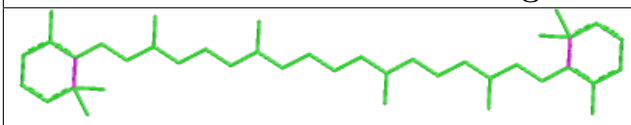
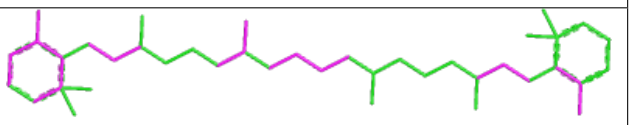
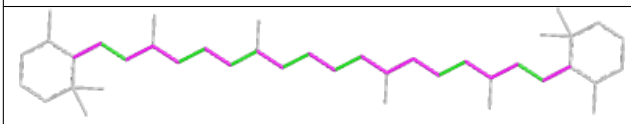
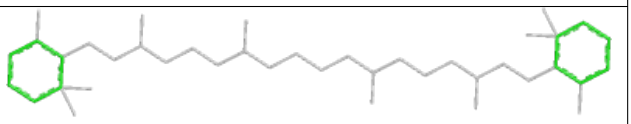
 Bond lengths	 Bond angles
 Torsions	 Rings

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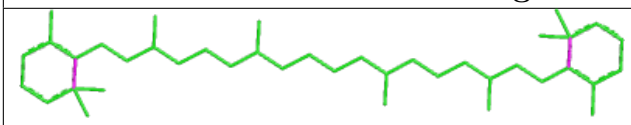
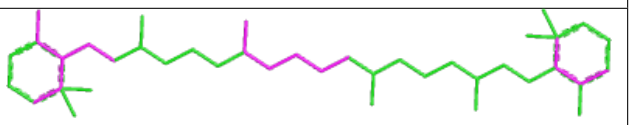
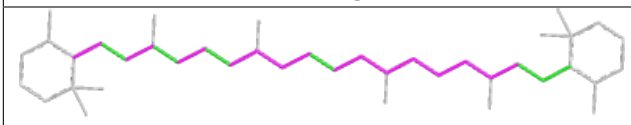
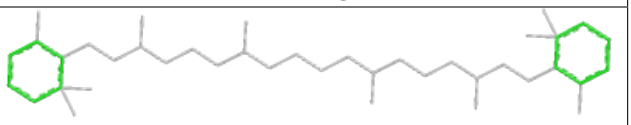
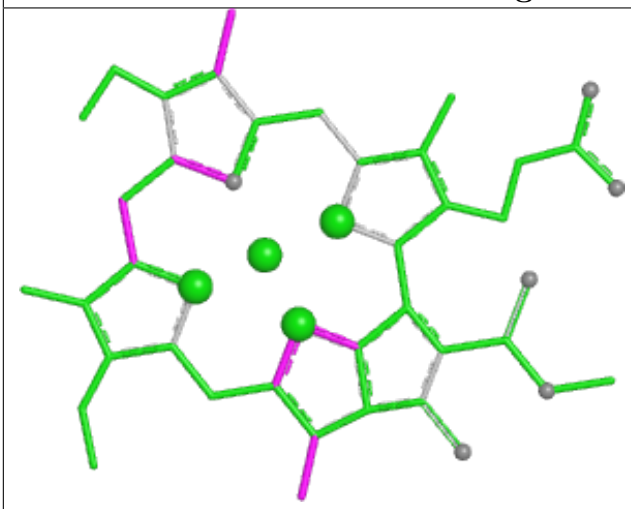
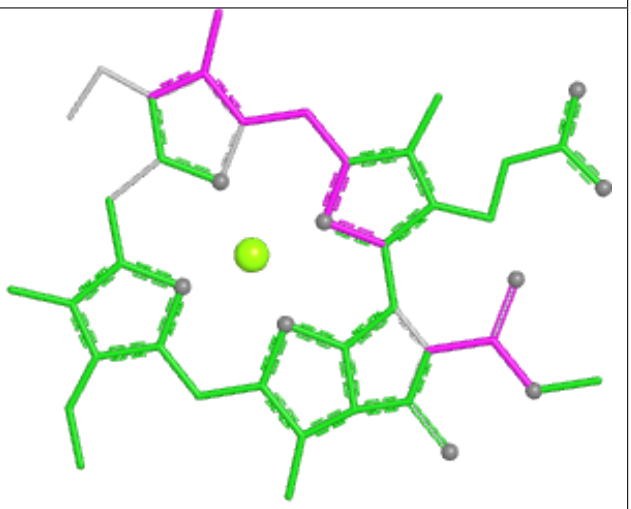
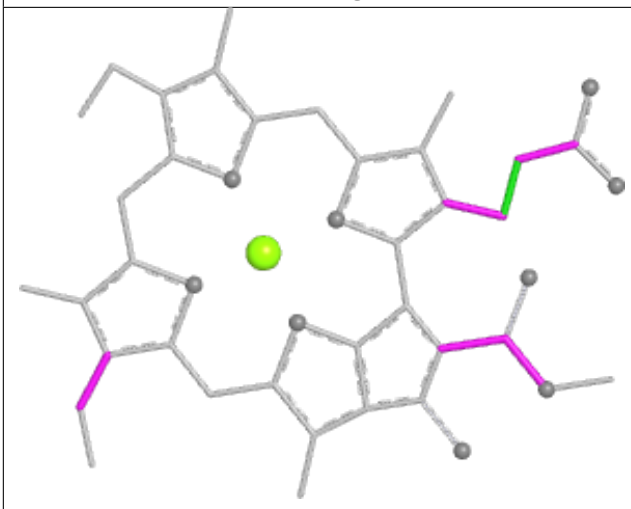
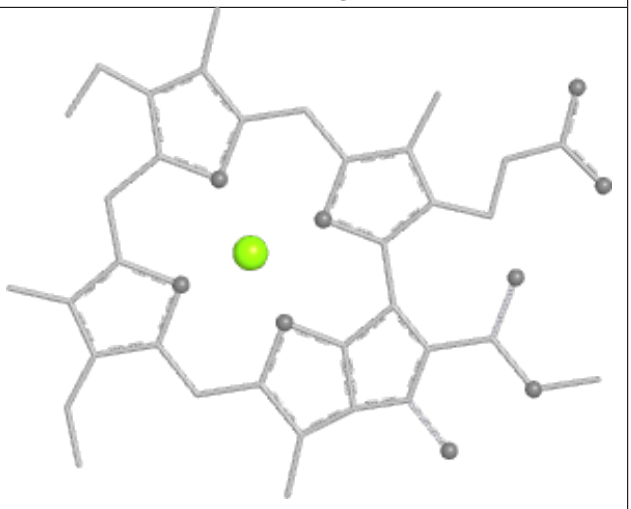
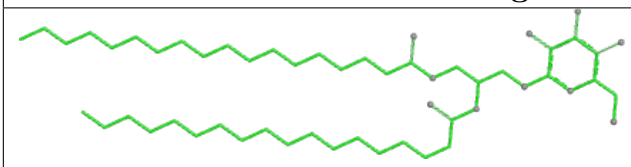
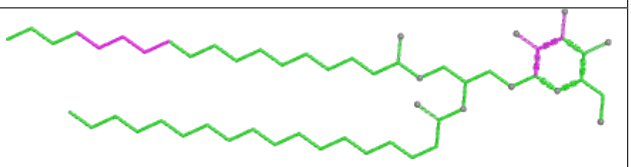
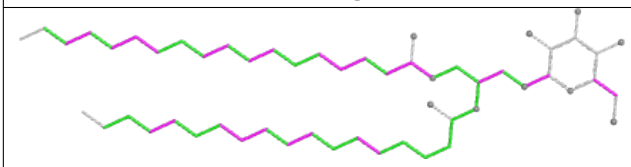
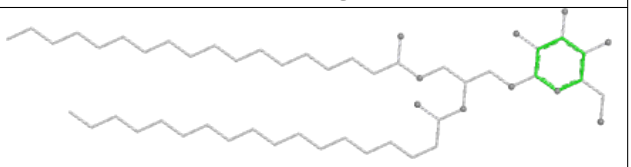
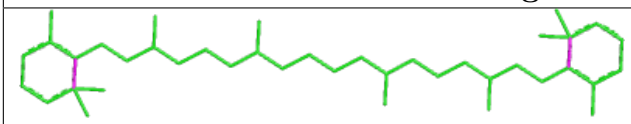
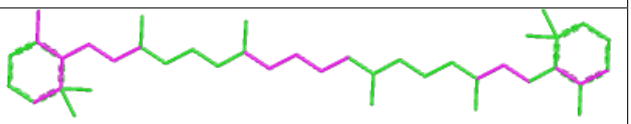
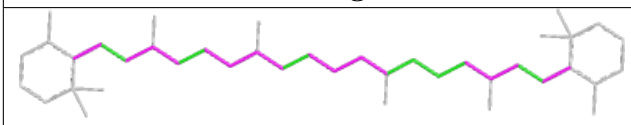
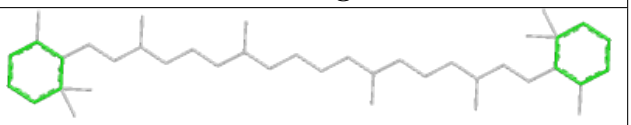
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG B2 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR II 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

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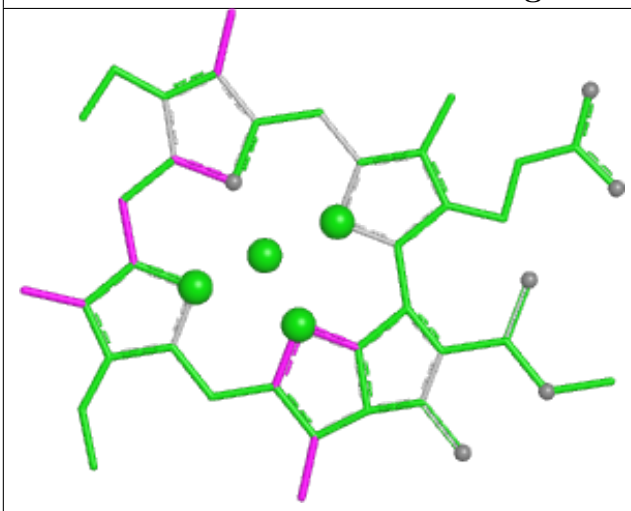
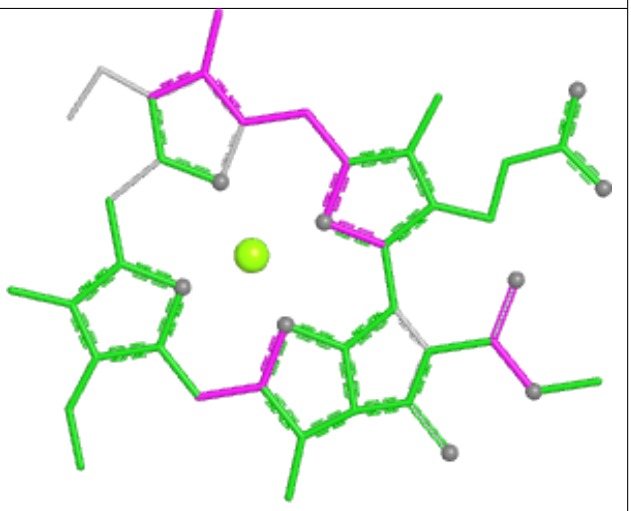
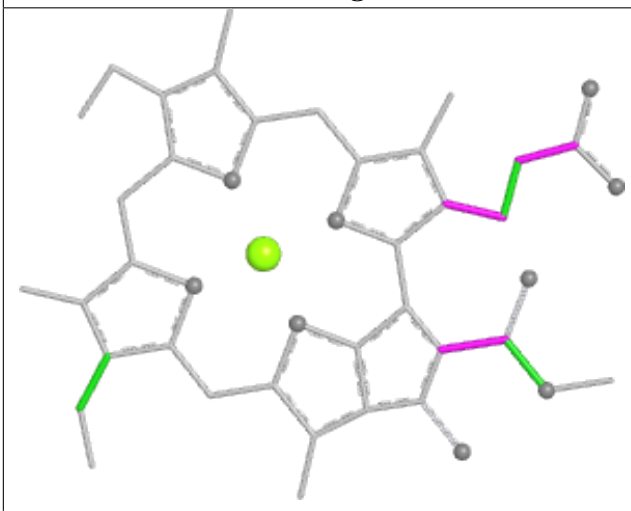
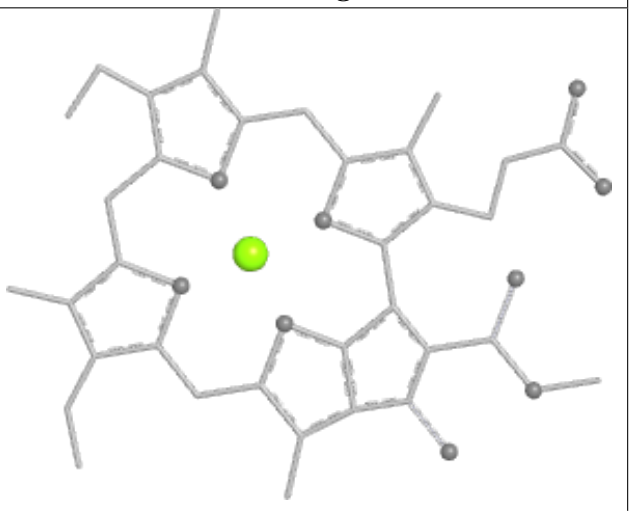
 Bond lengths	 Bond angles
 Torsions	 Rings

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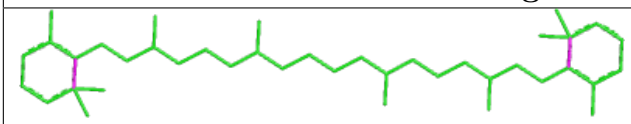
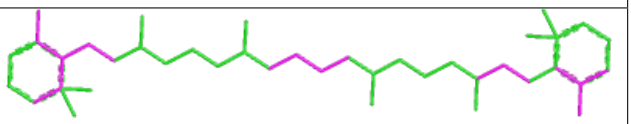
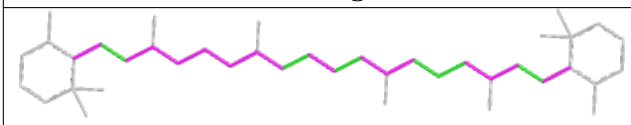
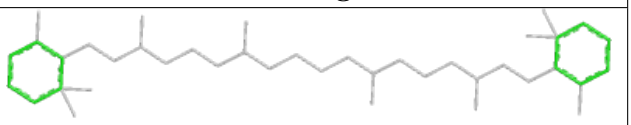
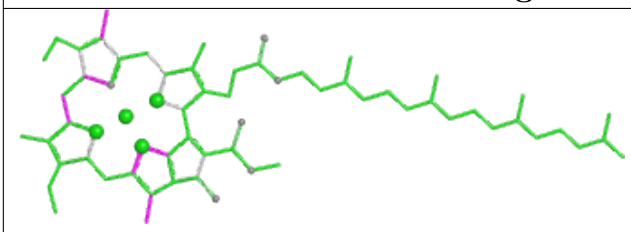
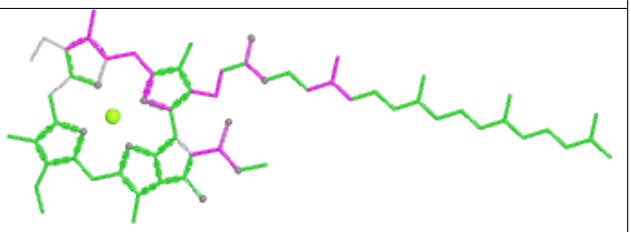
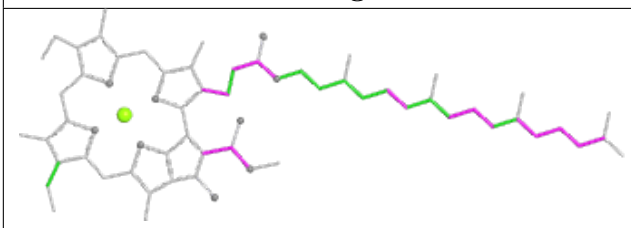
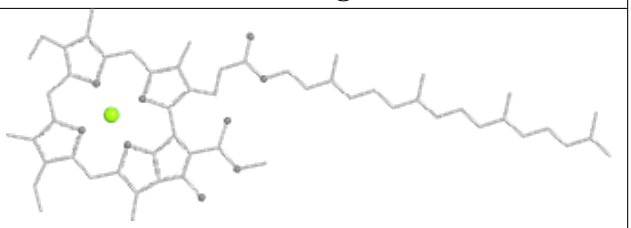
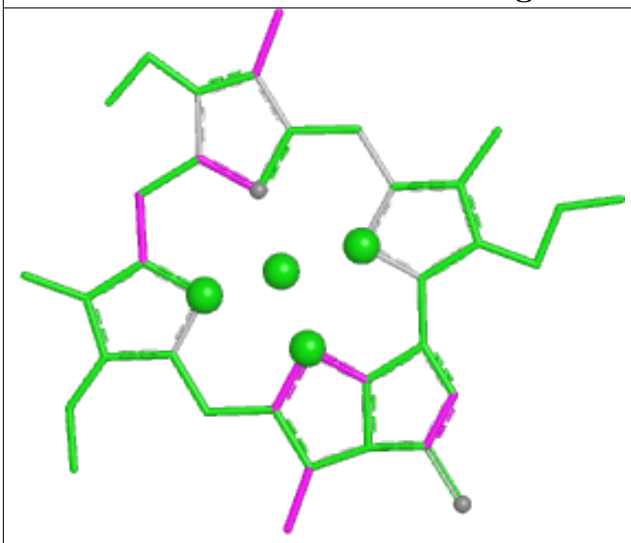
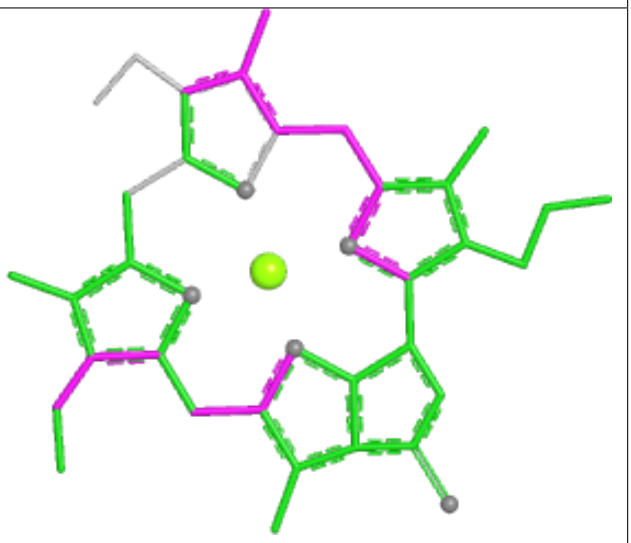
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 846	
	
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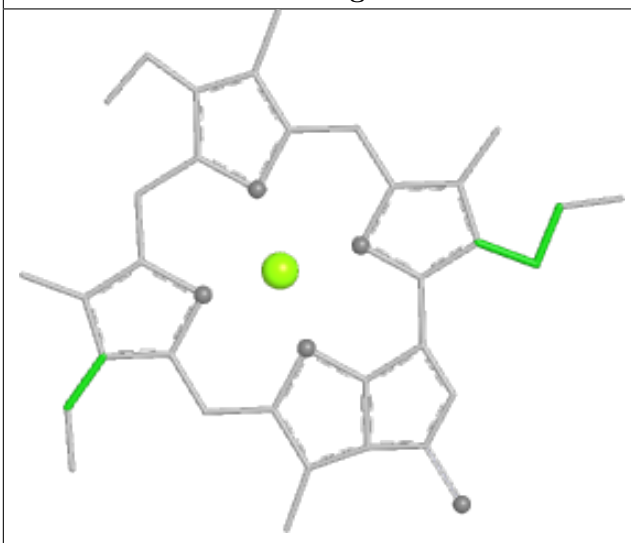
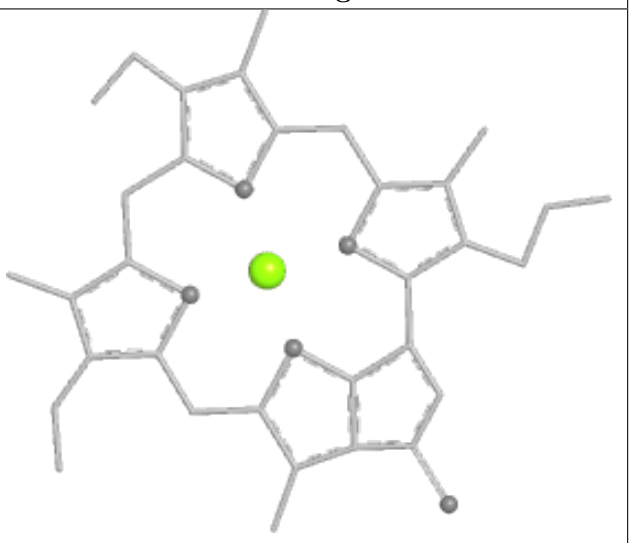
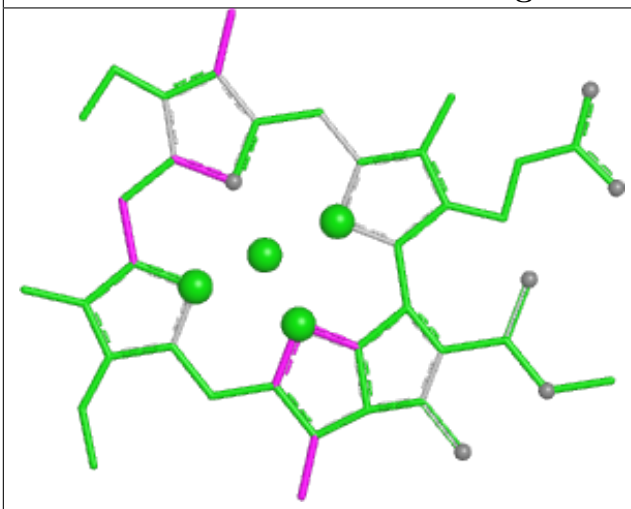
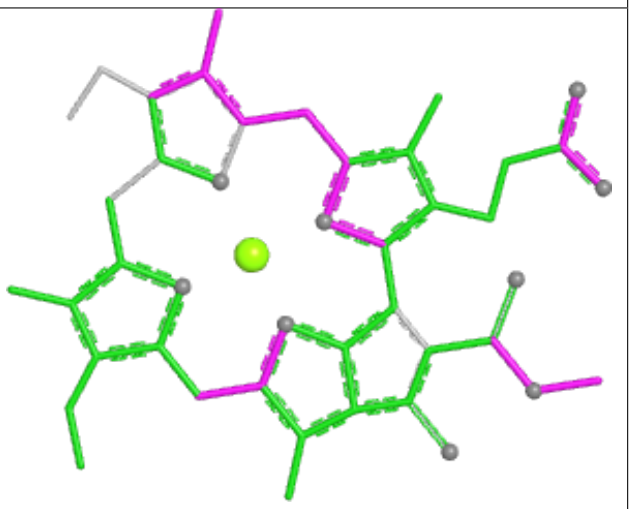
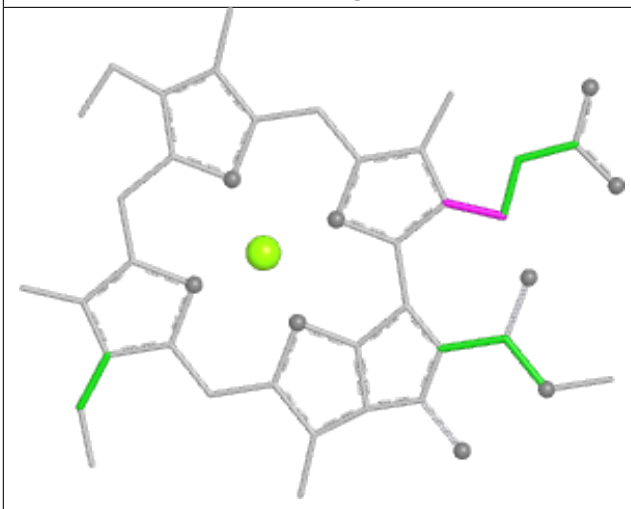
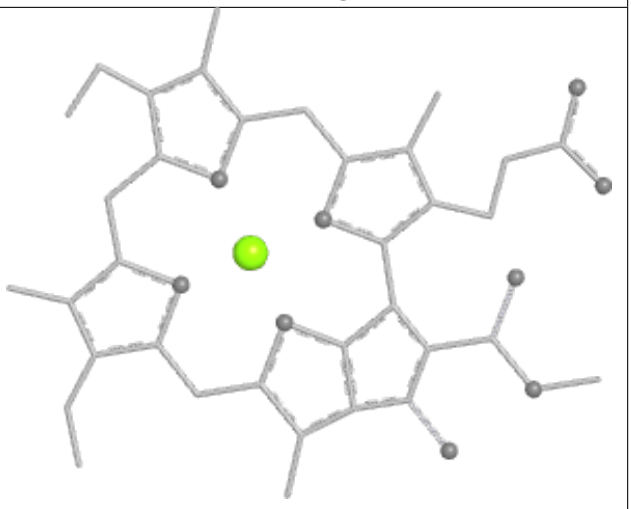
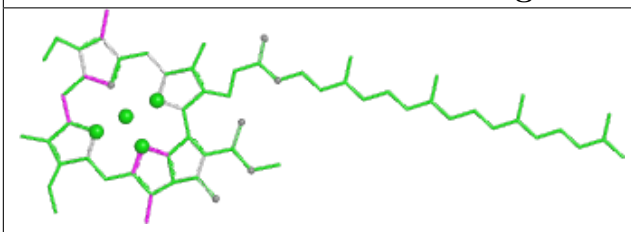
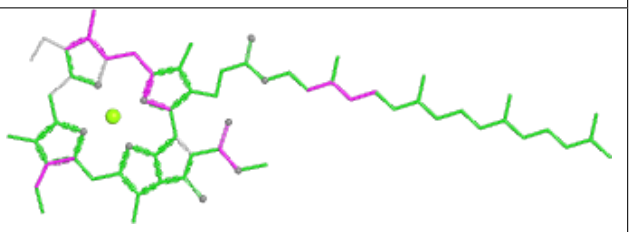
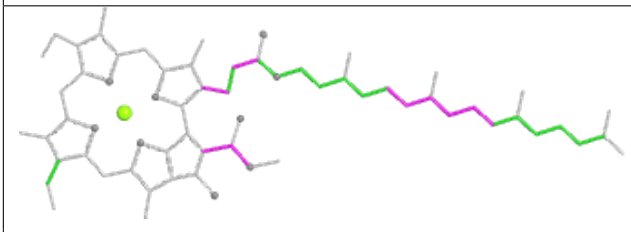
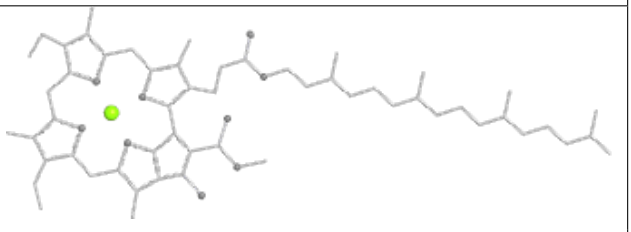
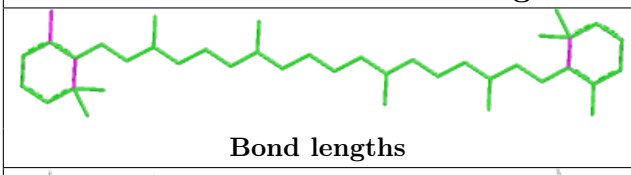
	
Torsions	**Rings**

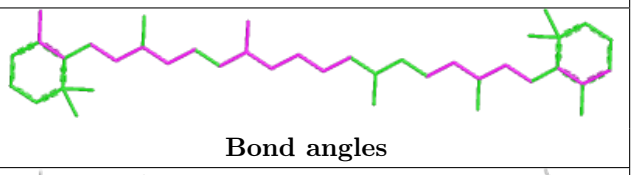
Ligand CLA B1 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

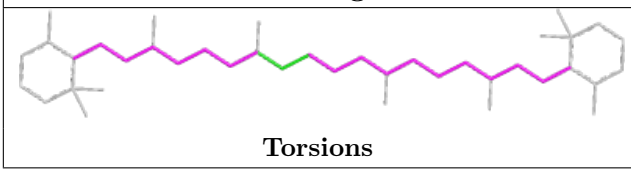
Ligand BCR FF 306



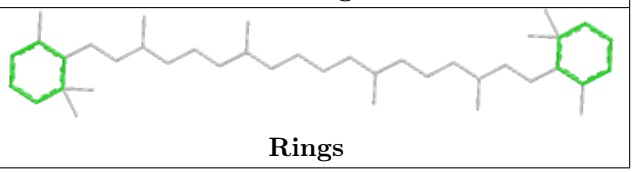
Bond lengths



Bond angles

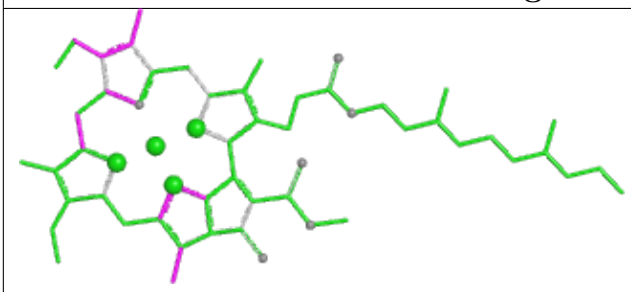


Torsions

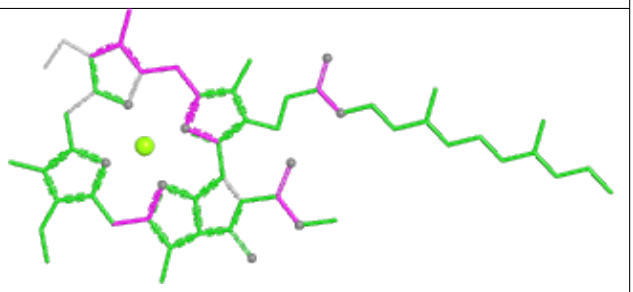


Rings

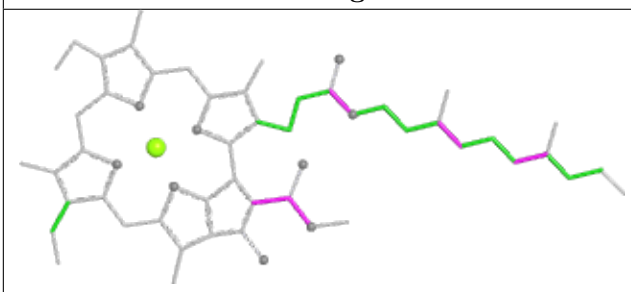
Ligand CLA B 816



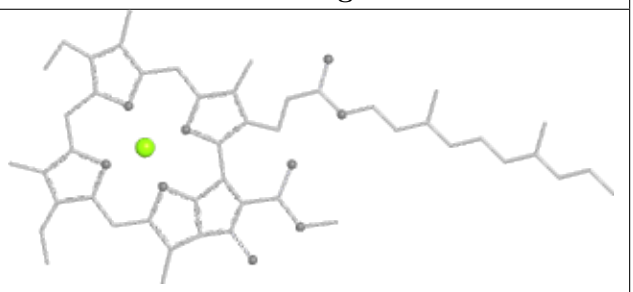
Bond lengths



Bond angles

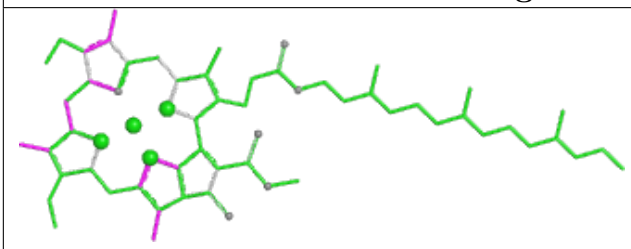


Torsions

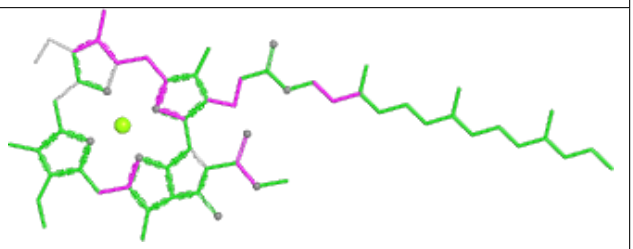


Rings

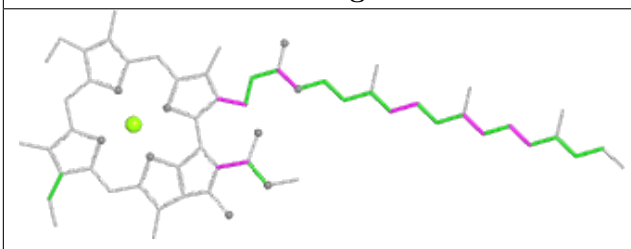
Ligand CLA B1 804



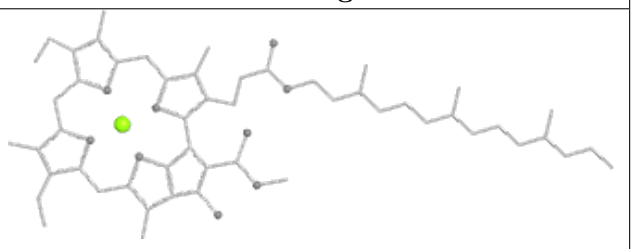
Bond lengths



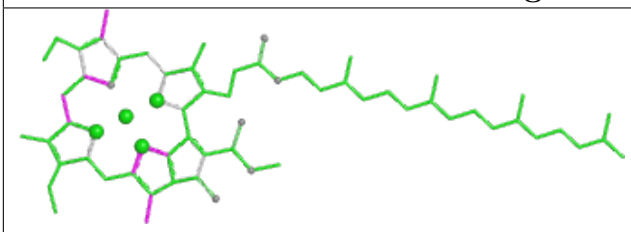
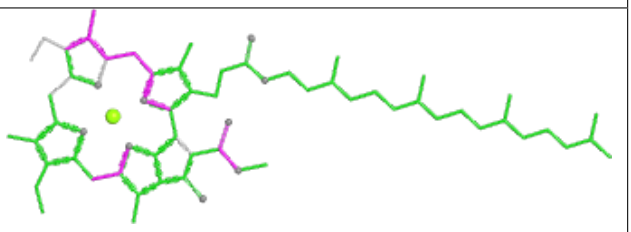
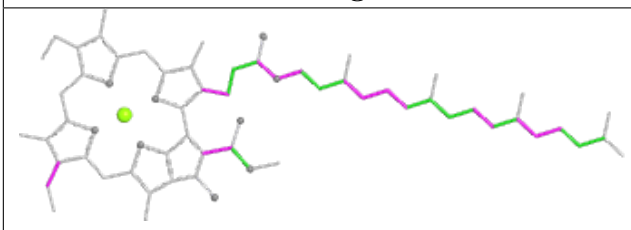
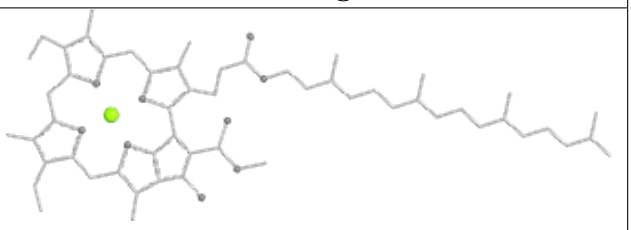
Bond angles

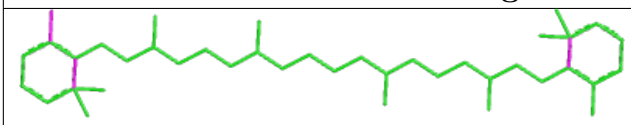
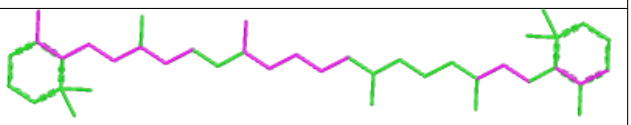
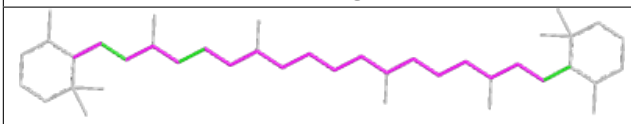
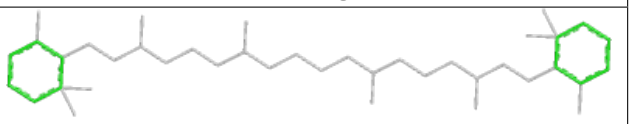


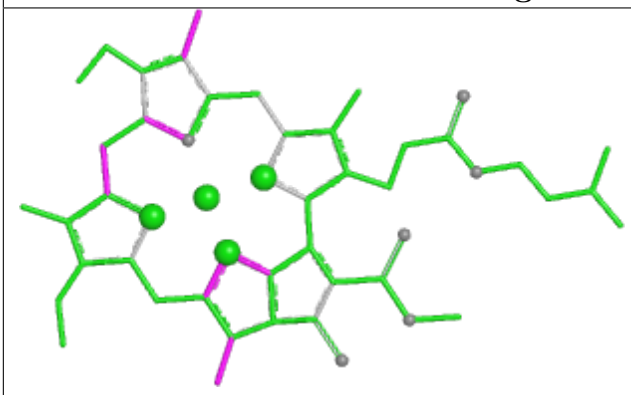
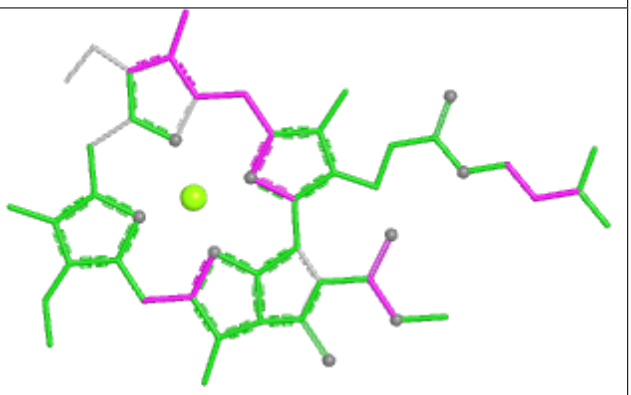
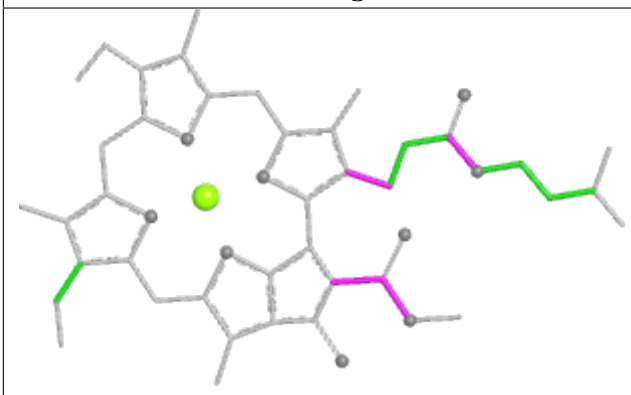
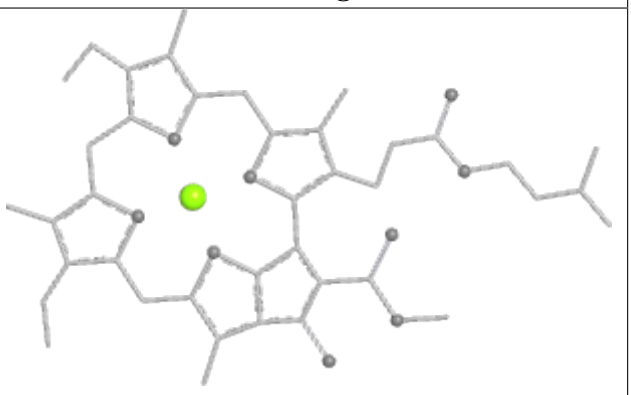
Torsions

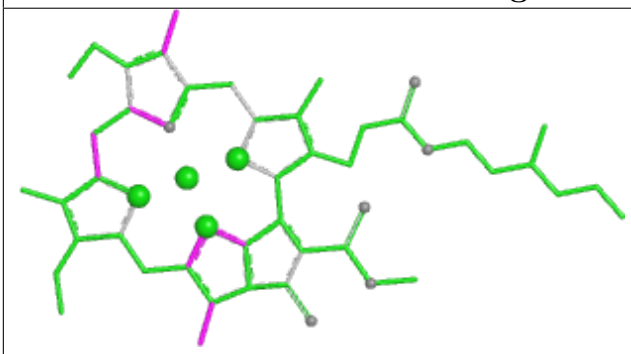
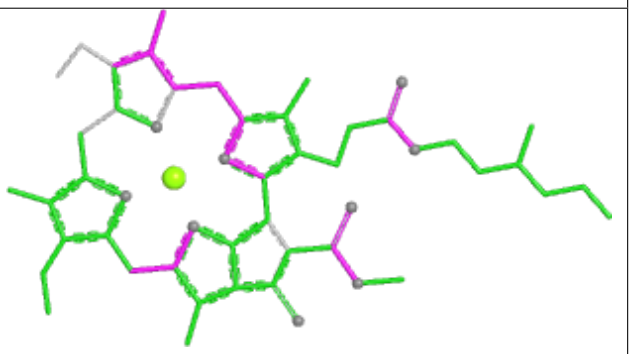
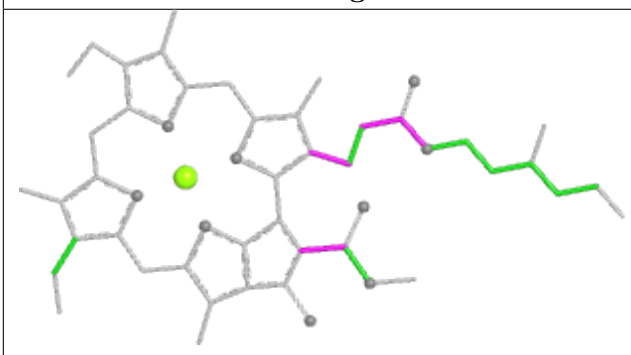
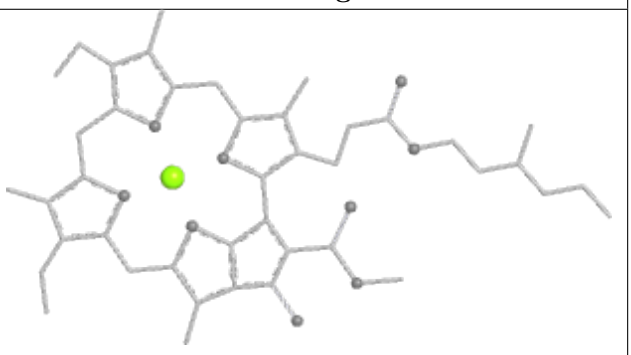


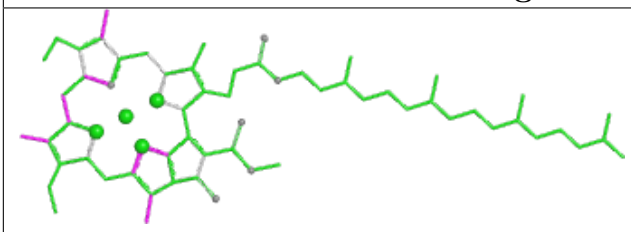
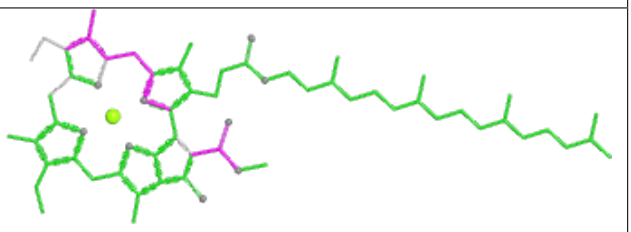
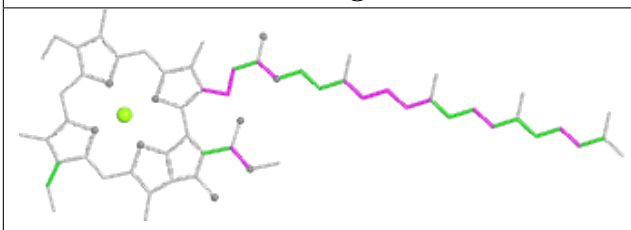
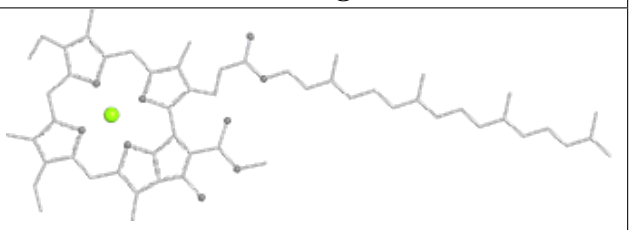
Rings

Ligand CLA B 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR MM 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

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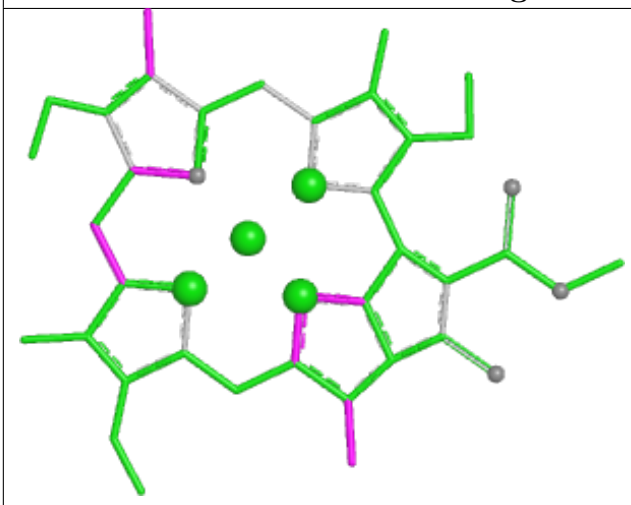
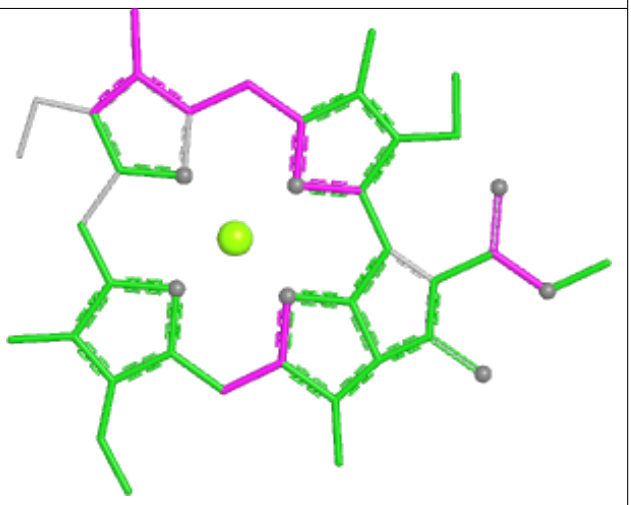
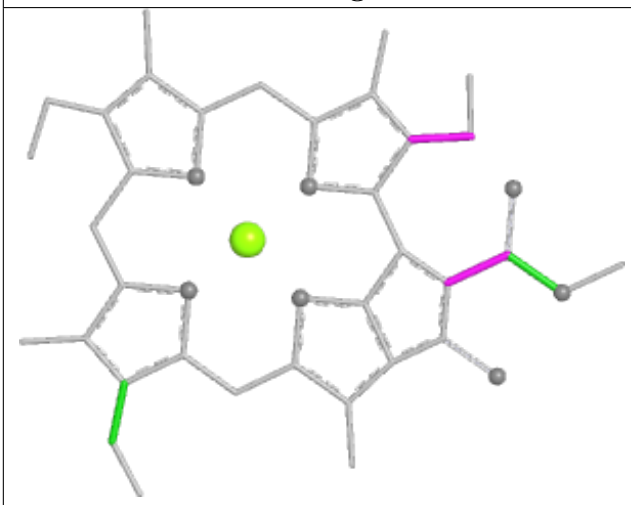
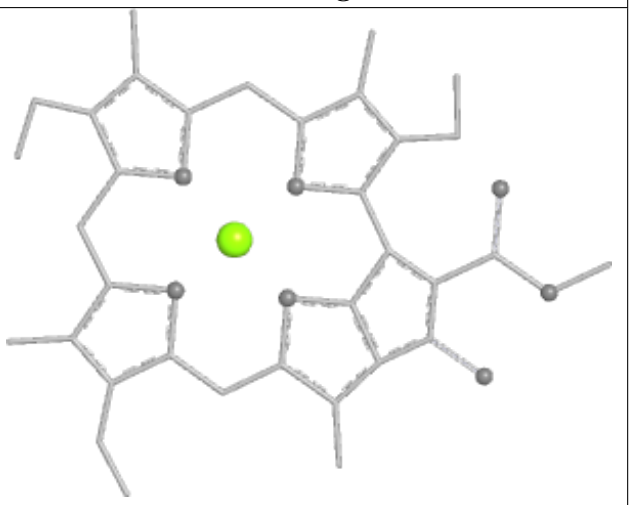
 Bond lengths	 Bond angles
 Torsions	 Rings

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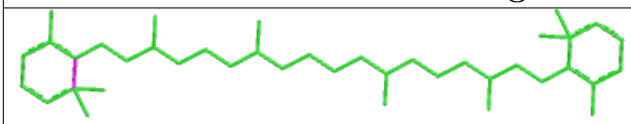
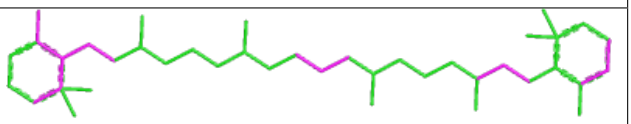
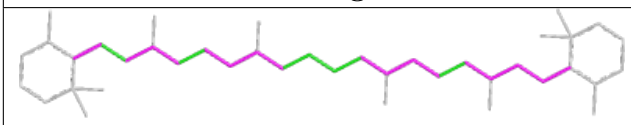
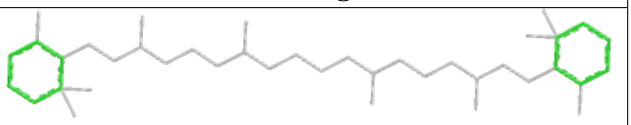
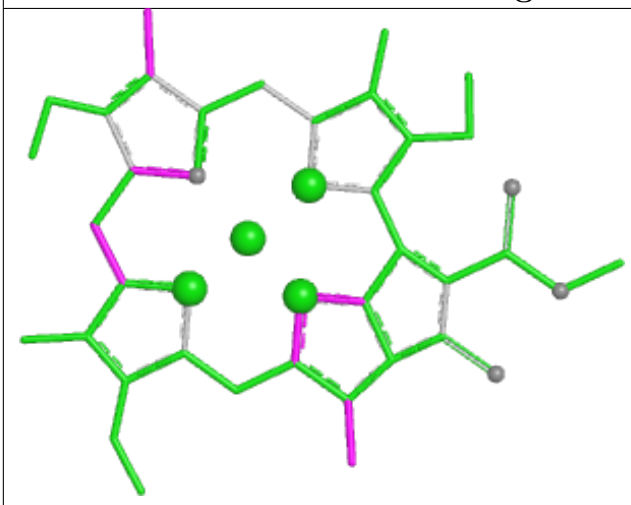
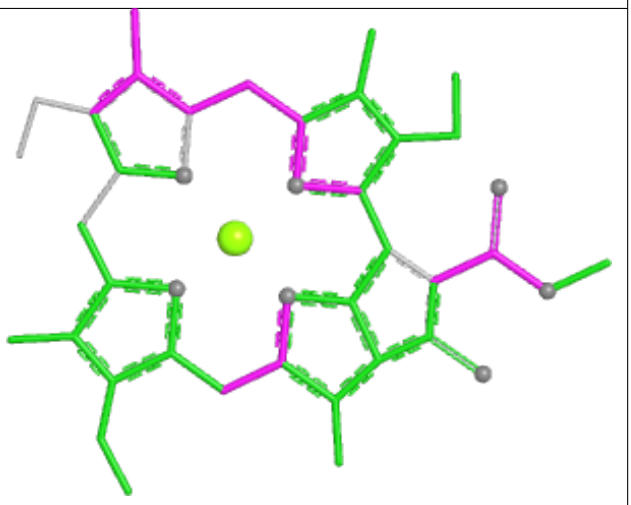
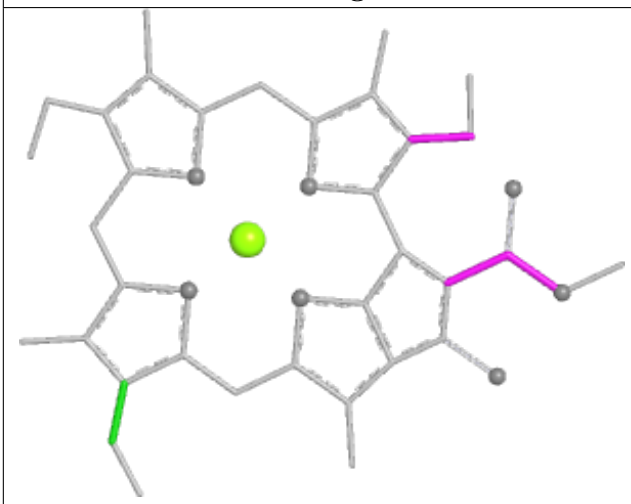
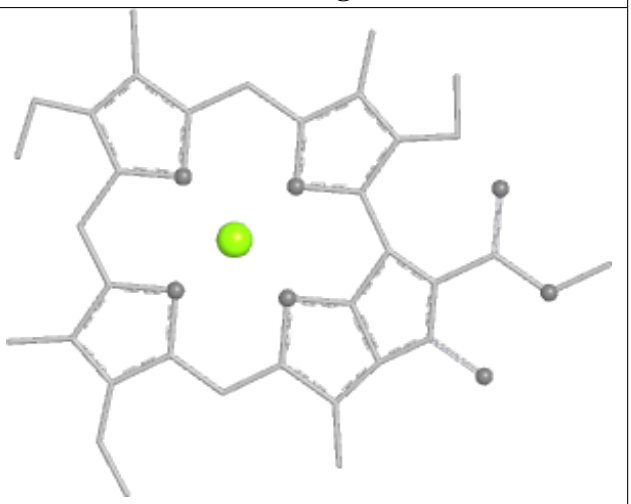
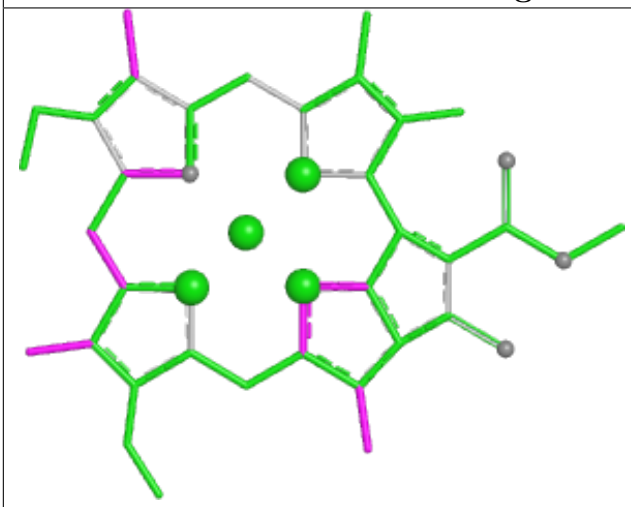
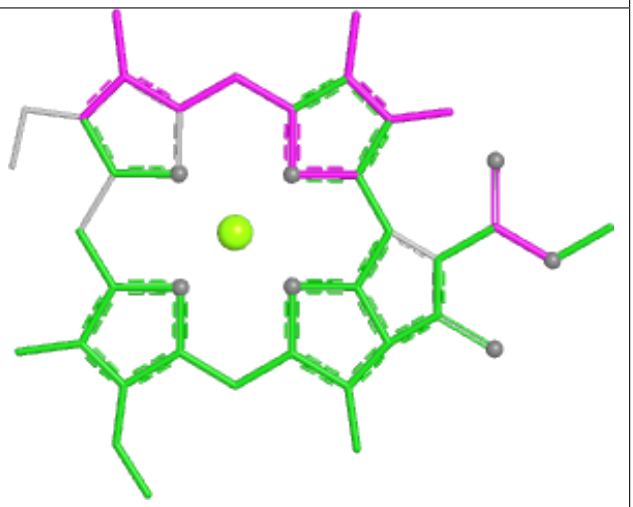
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

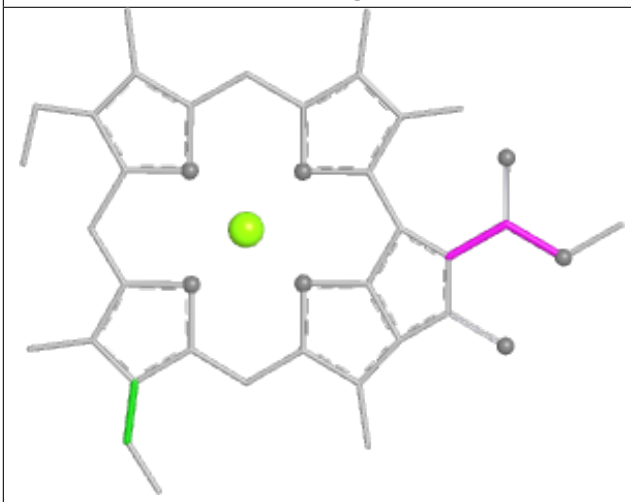
Ligand CLA A2 834



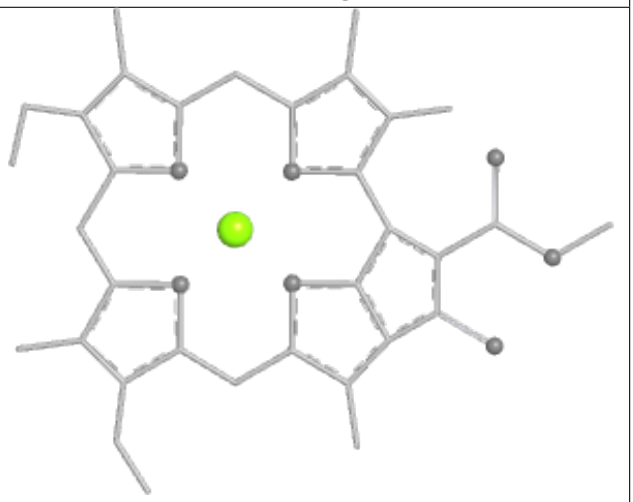
Bond lengths



Bond angles

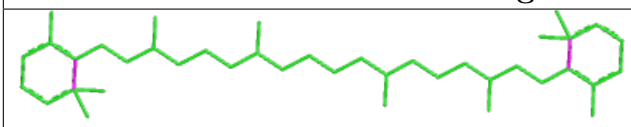


Torsions

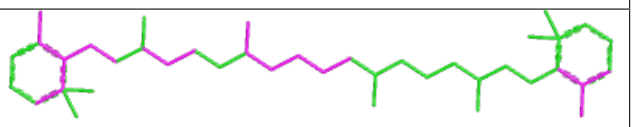


Rings

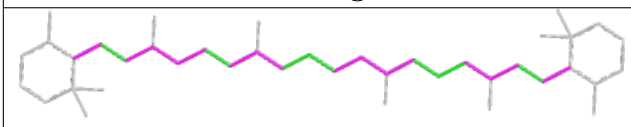
Ligand BCR JJ 102



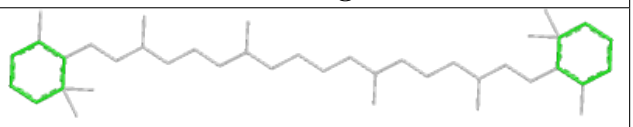
Bond lengths



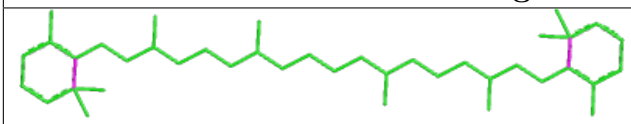
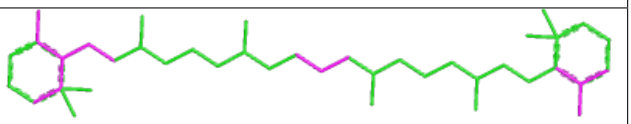
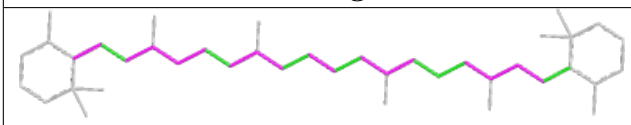
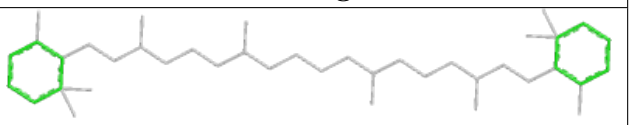
Bond angles

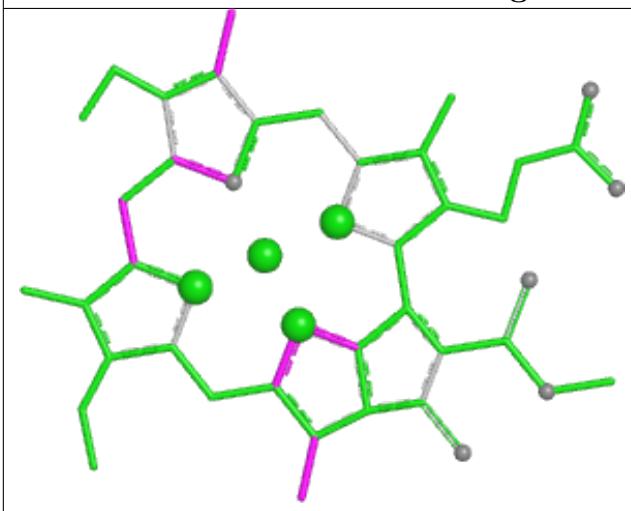
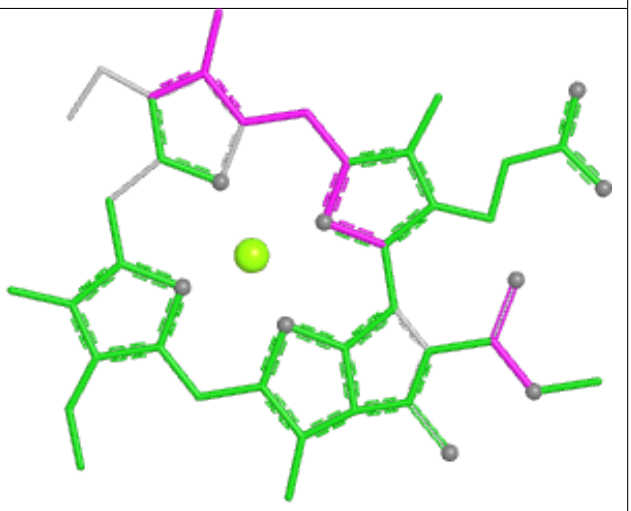
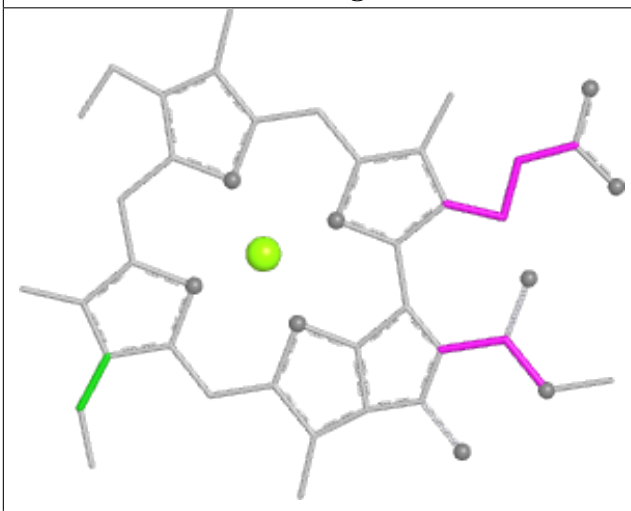
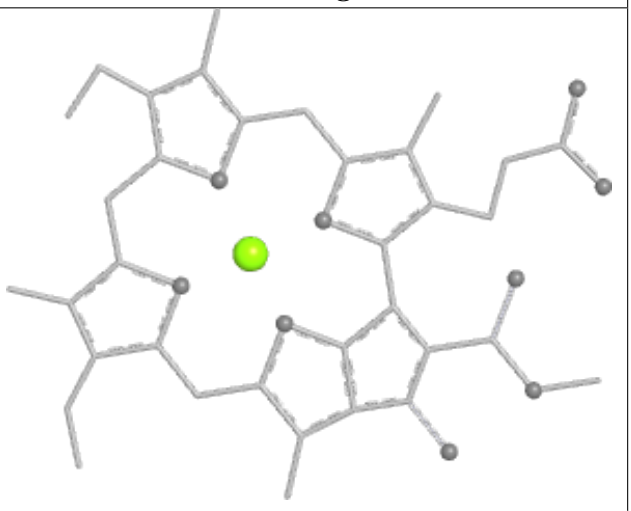


Torsions

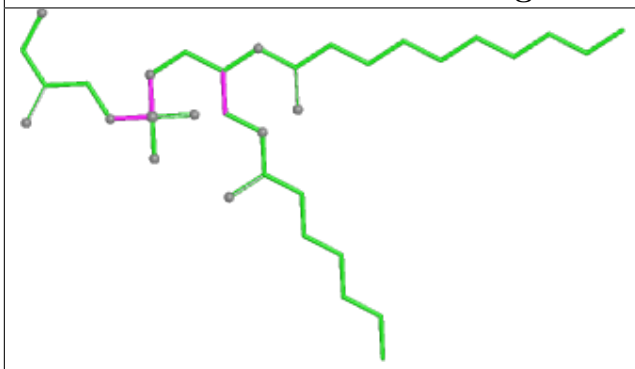


Rings

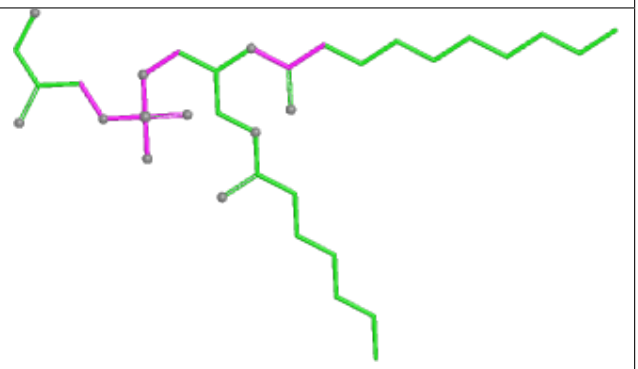
Ligand BCR A2 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA XX 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

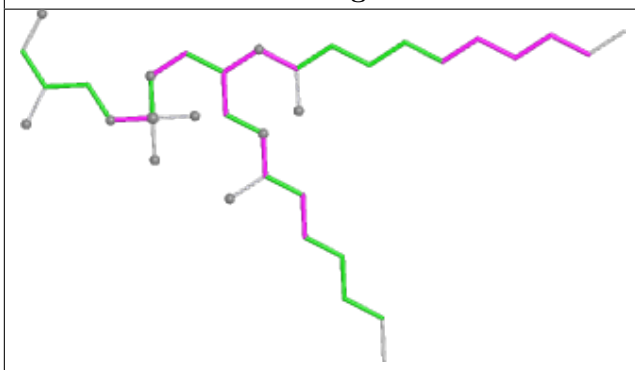
Ligand LHG LL 205



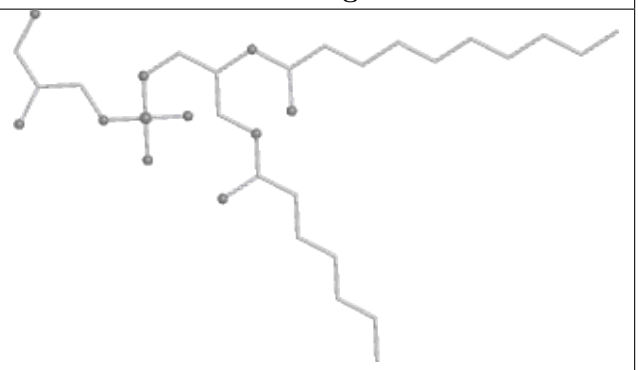
Bond lengths



Bond angles

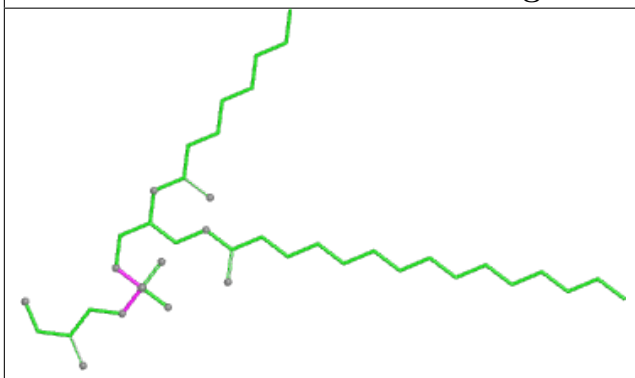


Torsions

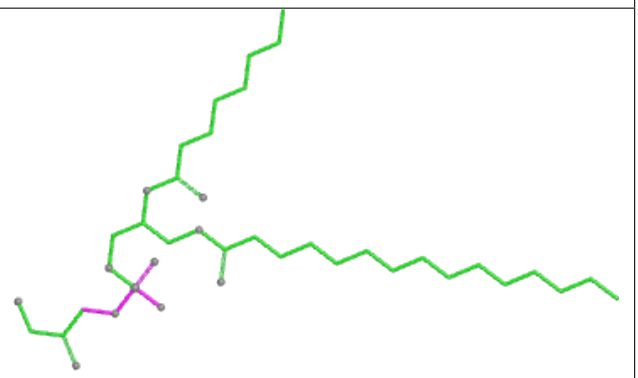


Rings

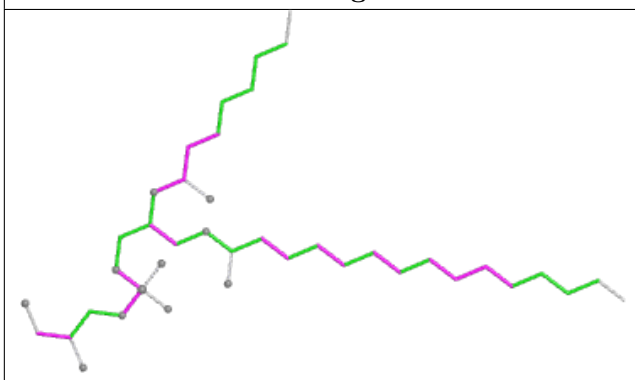
Ligand LHG X 102



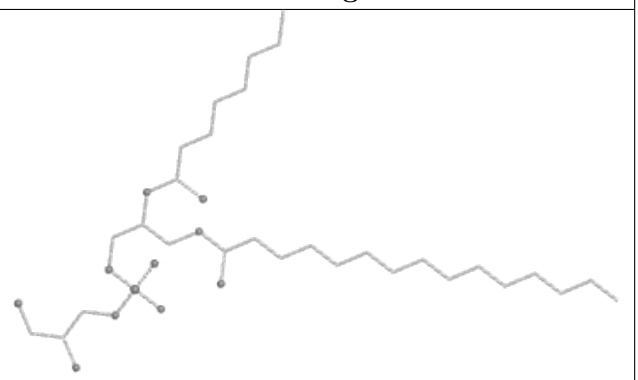
Bond lengths



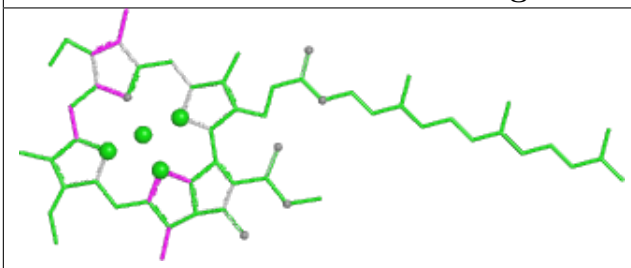
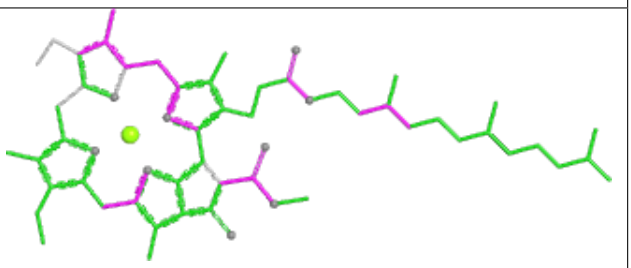
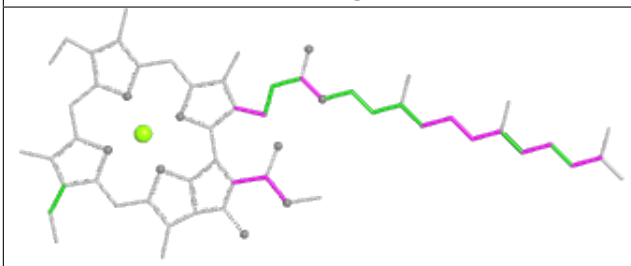
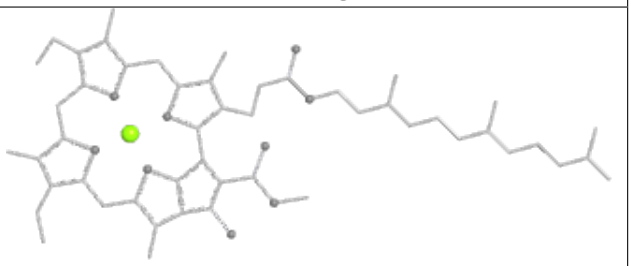
Bond angles

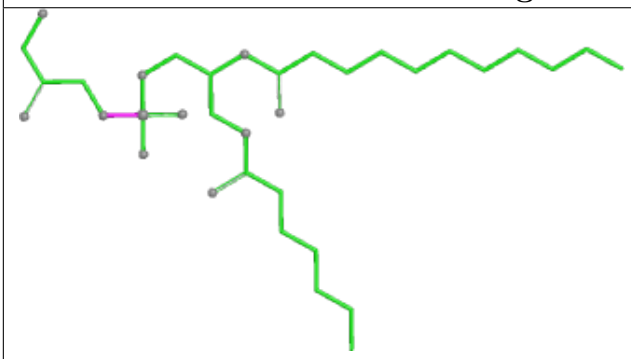
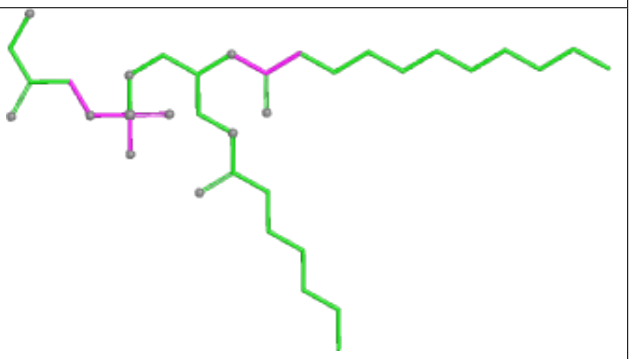
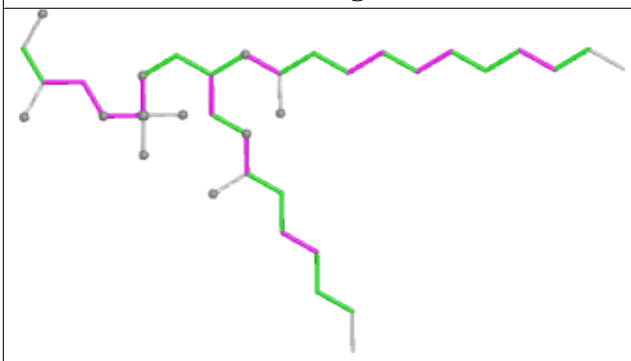
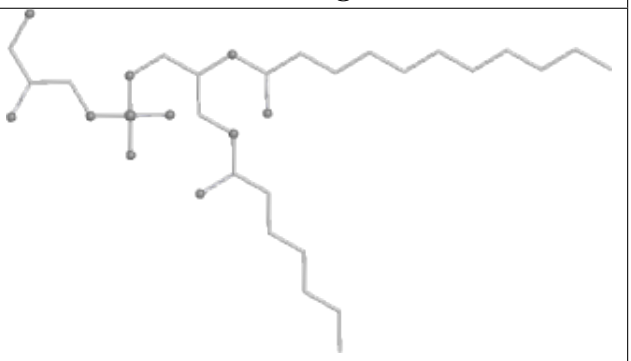


Torsions



Rings

Ligand CLA AA 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG L2 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

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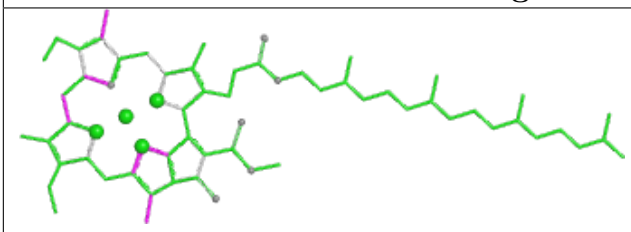
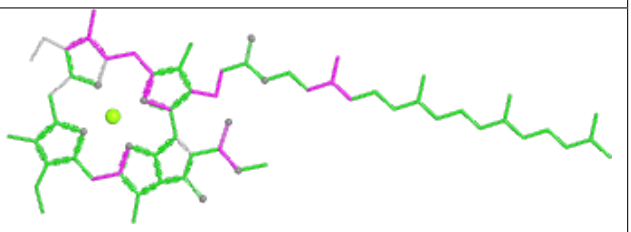
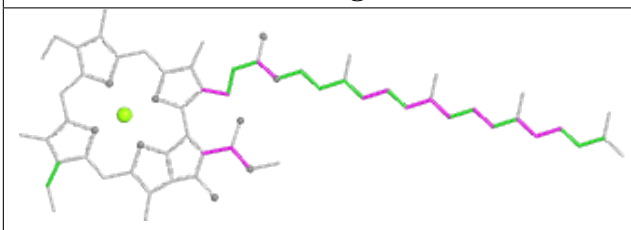
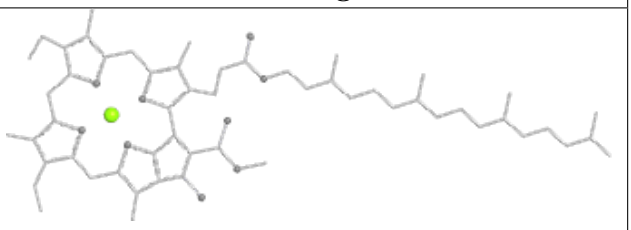
 Bond lengths	 Bond angles
 Torsions	 Rings

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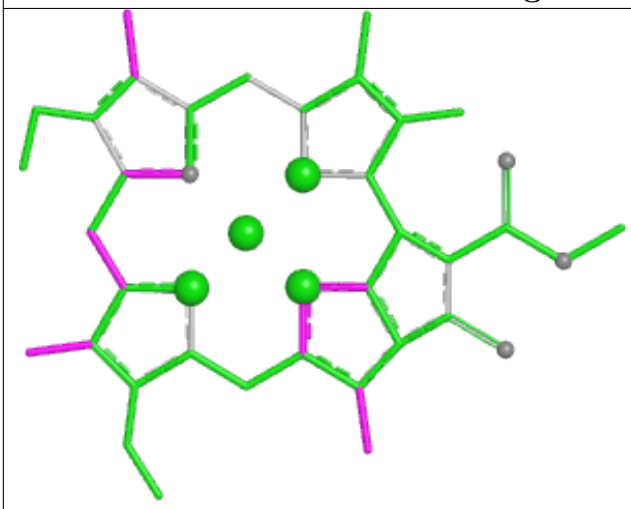
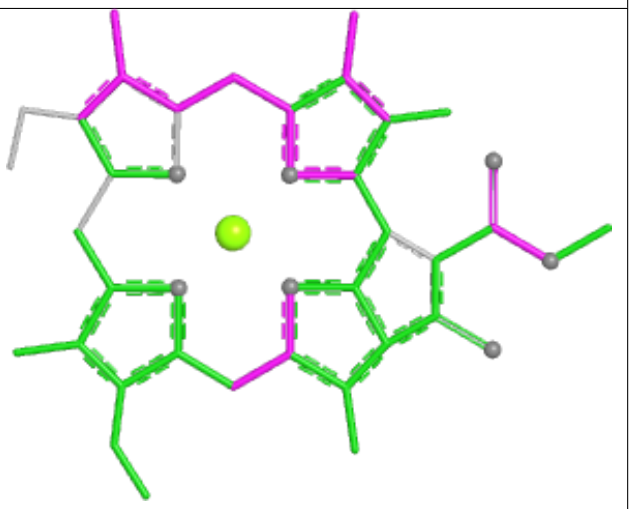
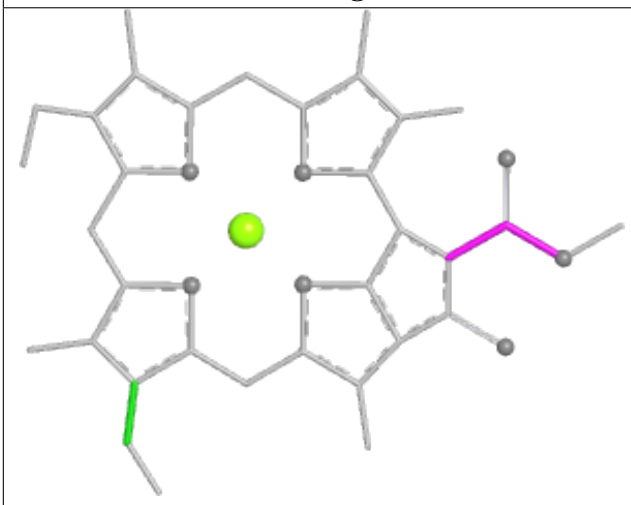
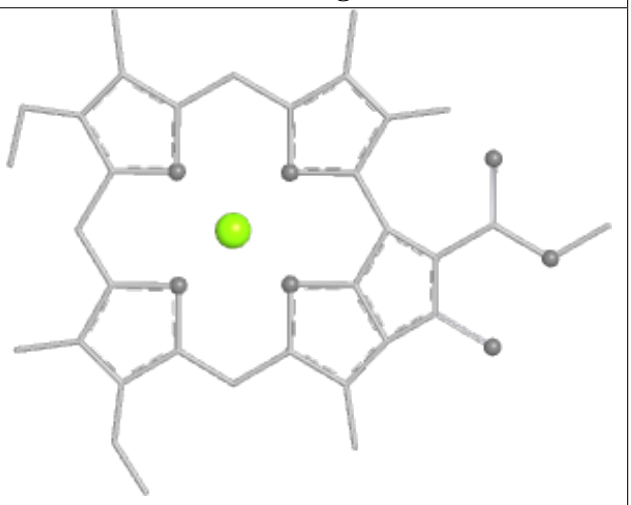
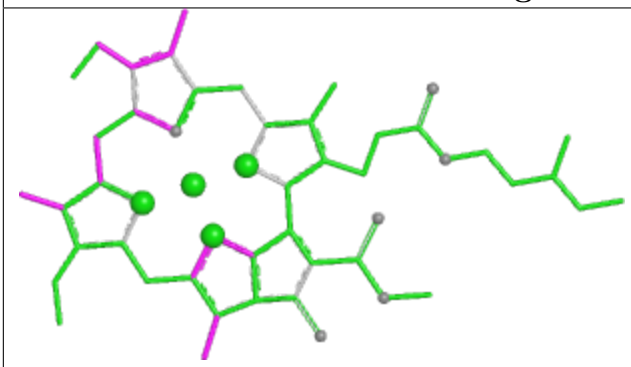
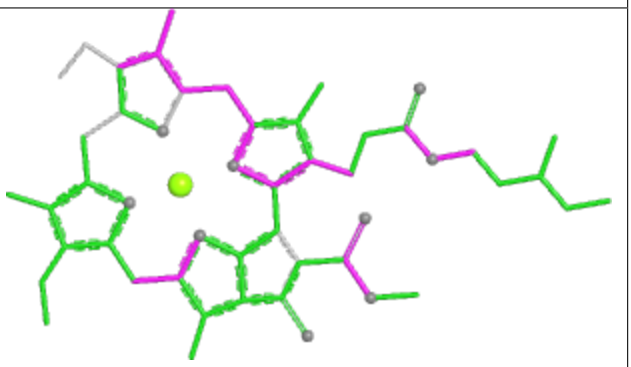
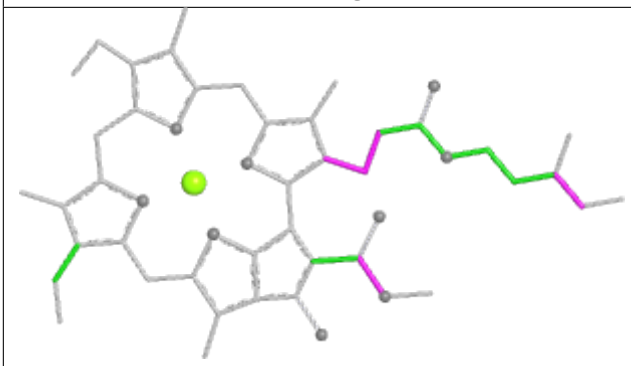
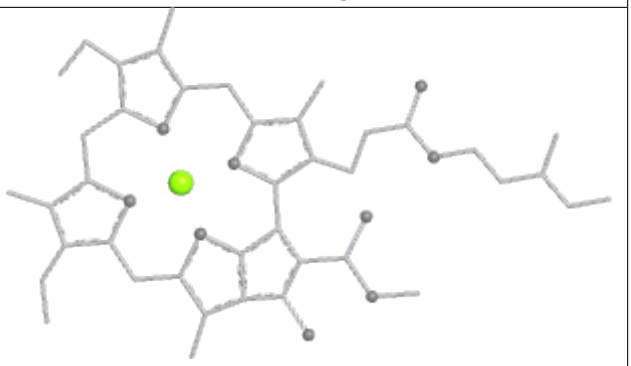
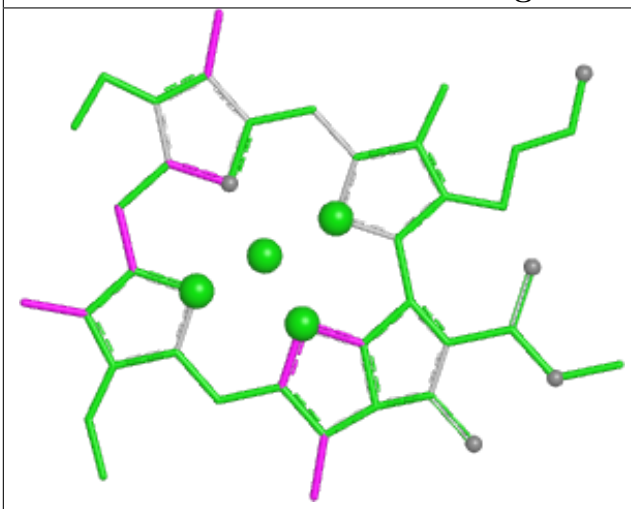
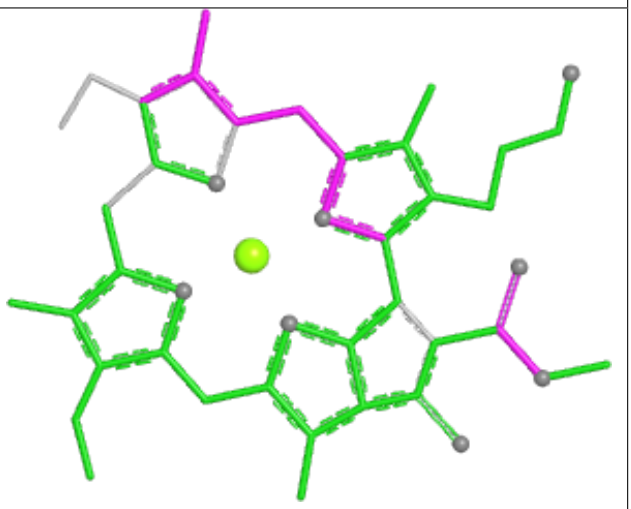
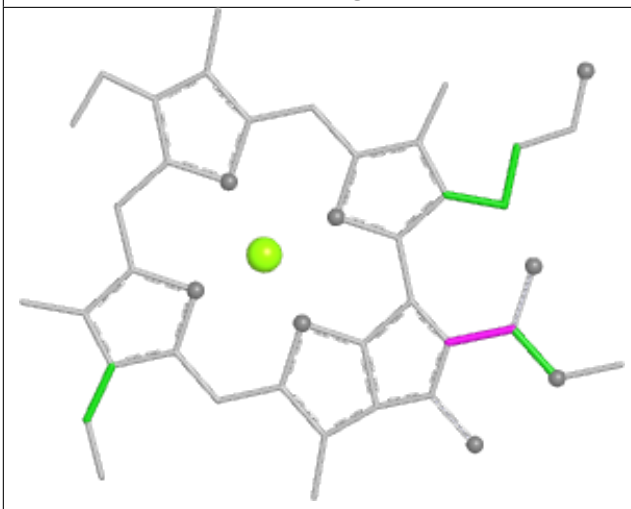
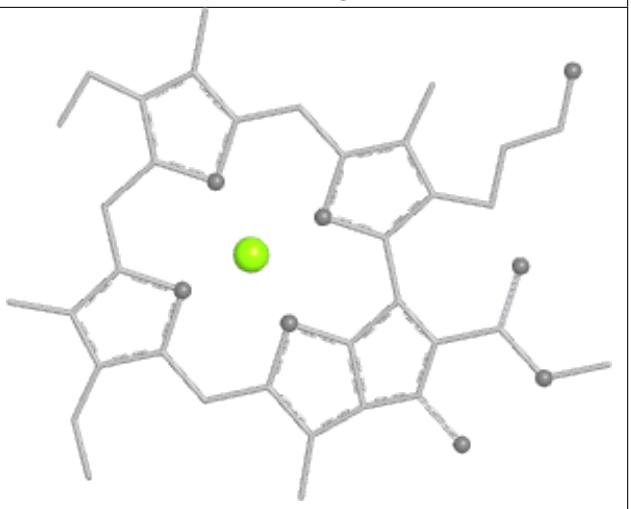
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 810	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A2 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

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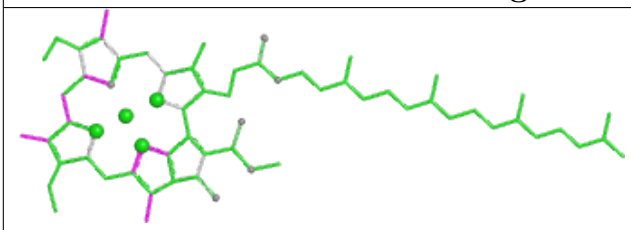
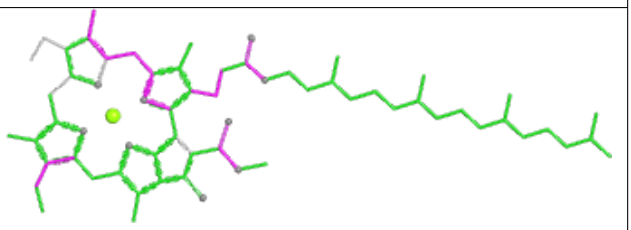
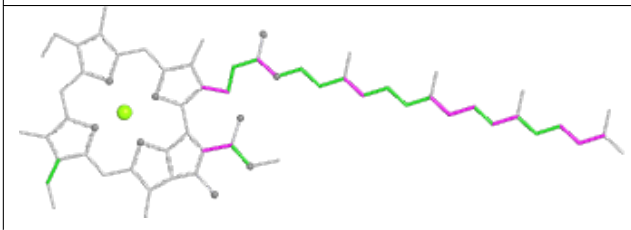
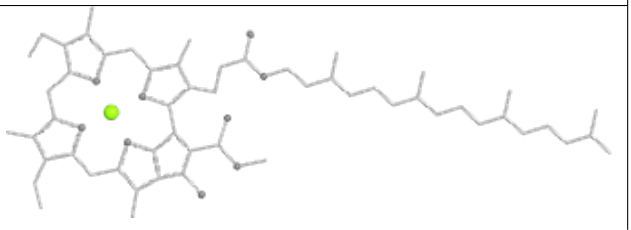
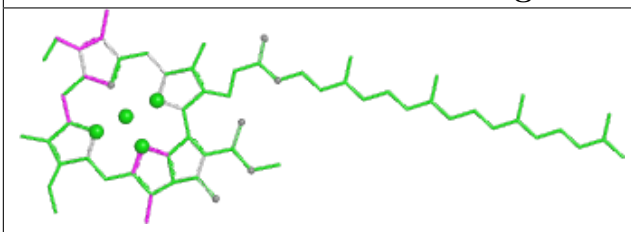
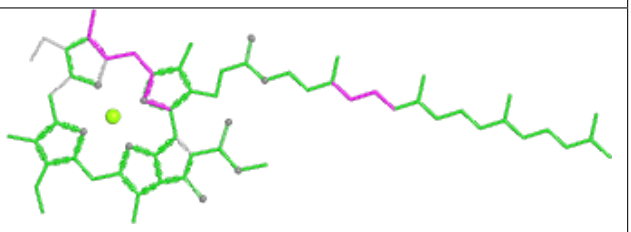
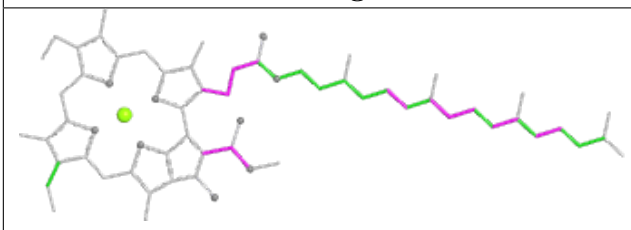
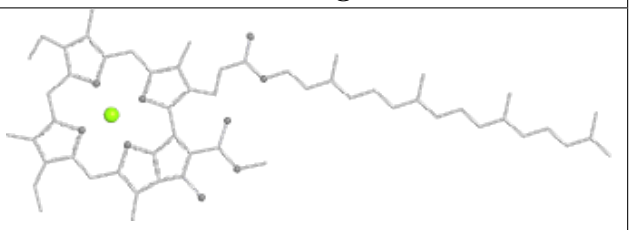
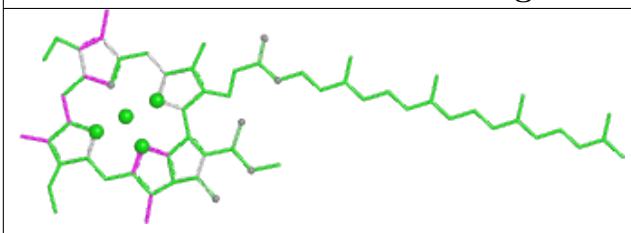
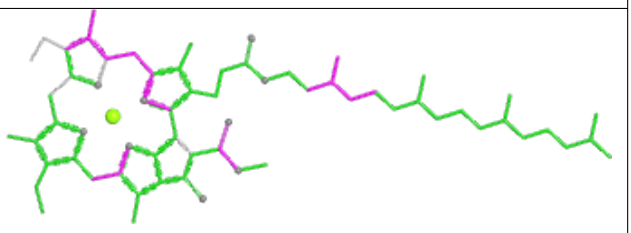
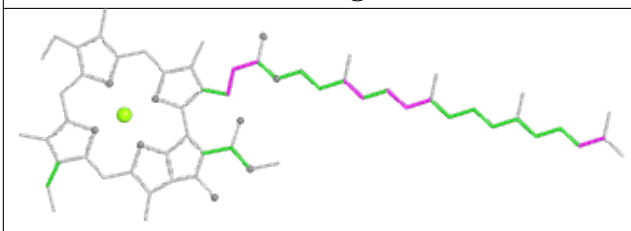
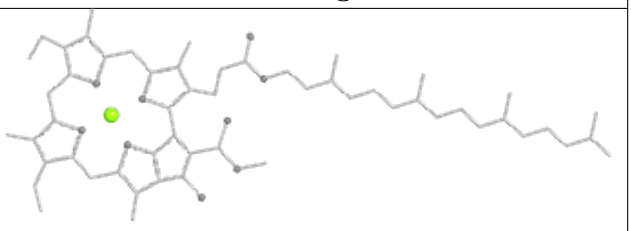
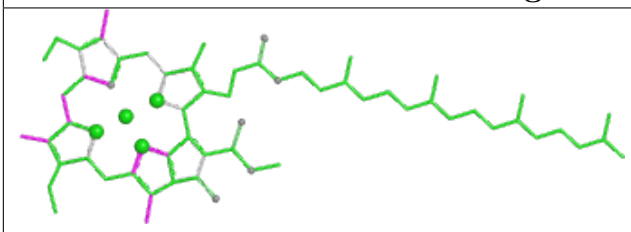
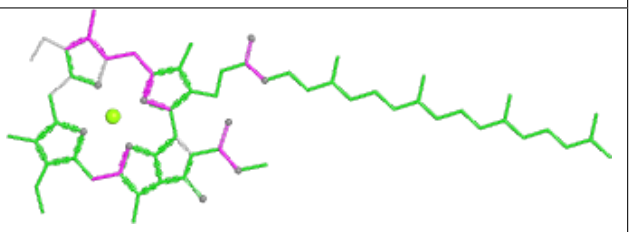
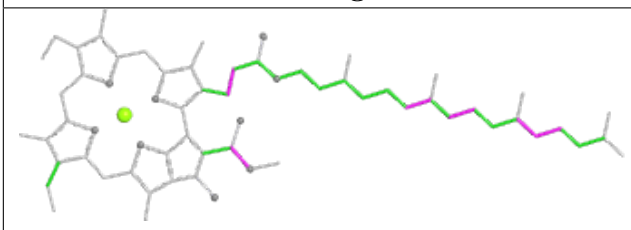
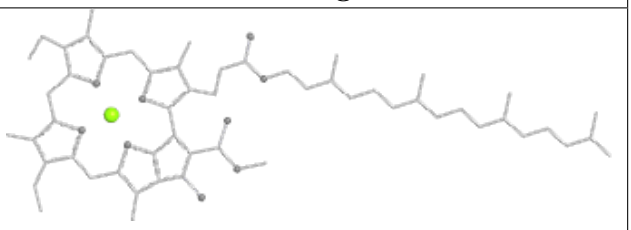
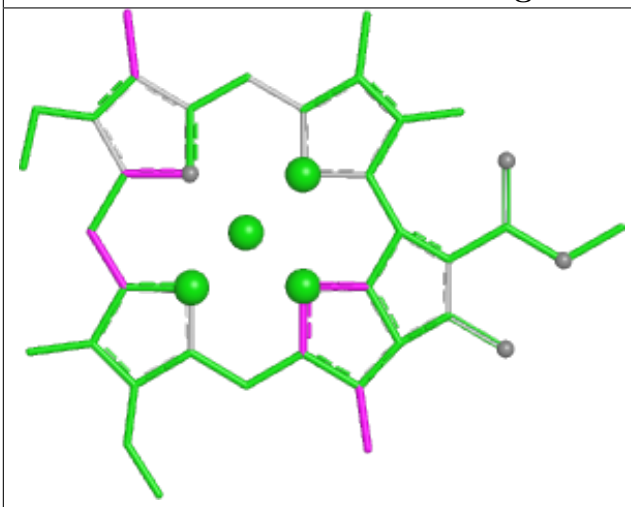
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

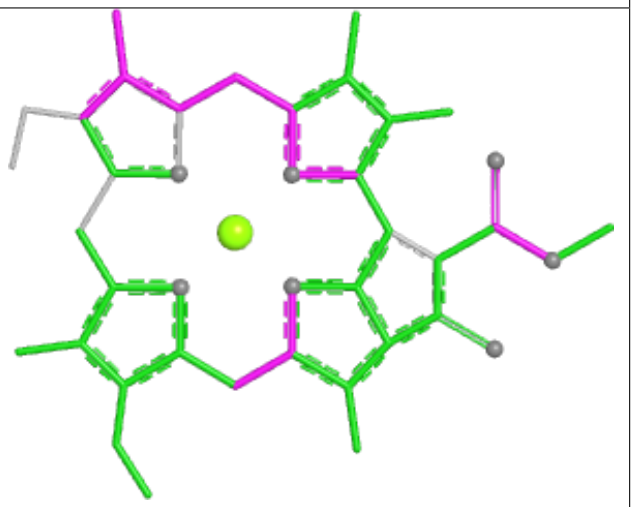
Ligand CLA A1 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

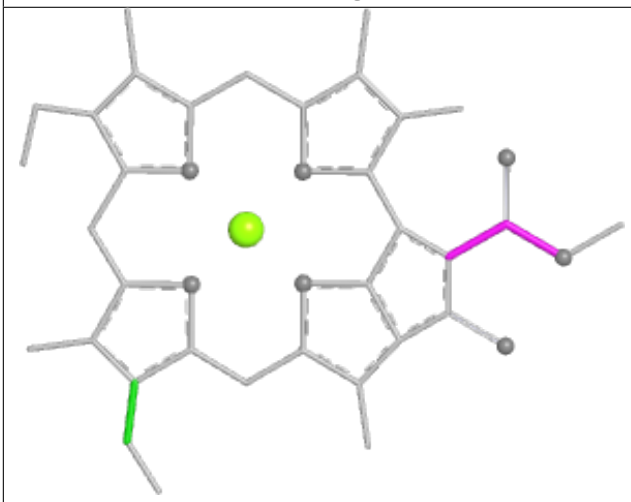
Ligand CLA A1 844



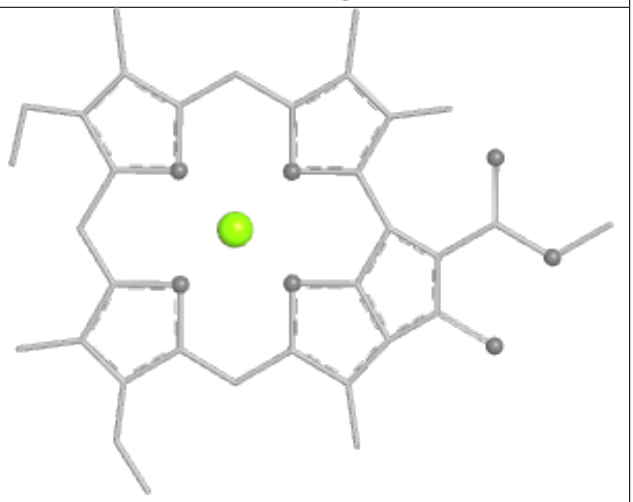
Bond lengths



Bond angles

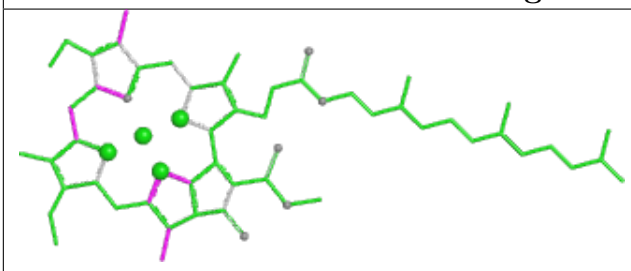


Torsions

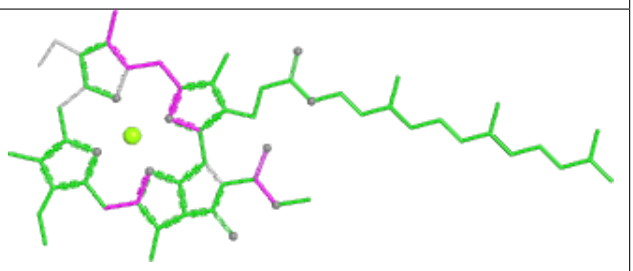


Rings

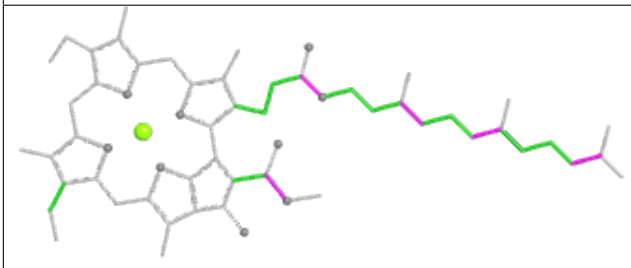
Ligand CLA B 808



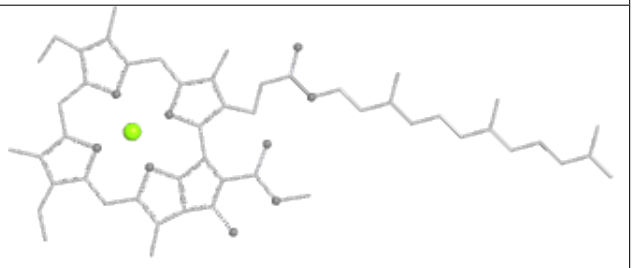
Bond lengths



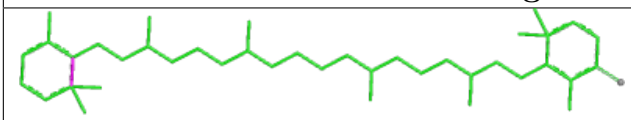
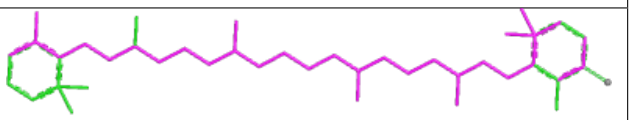
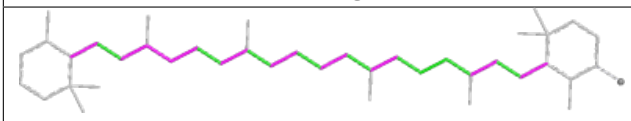
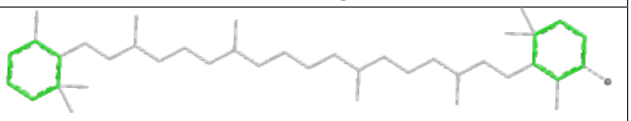
Bond angles

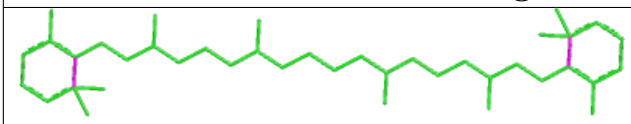
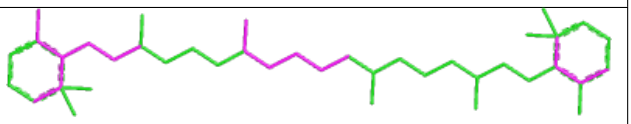
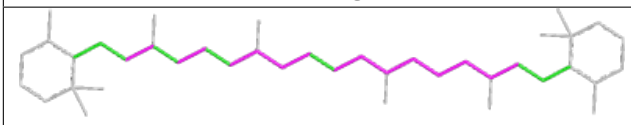
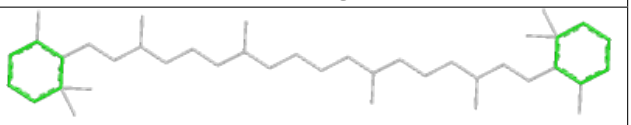


Torsions

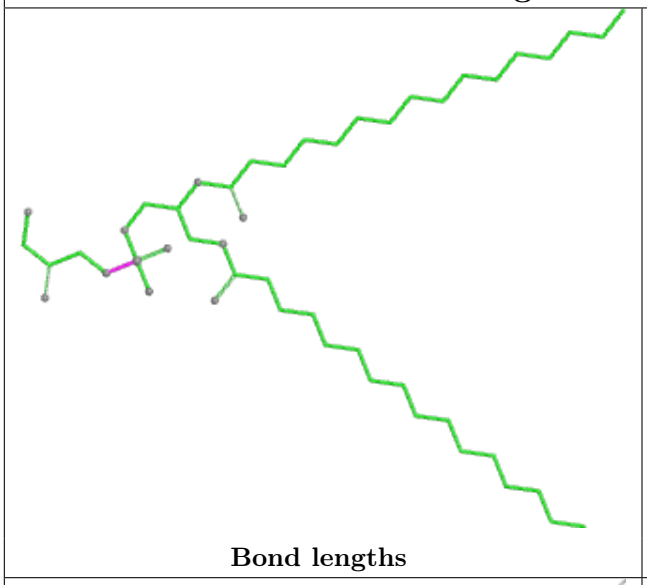


Rings

Ligand ECH B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A1 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG X2 103



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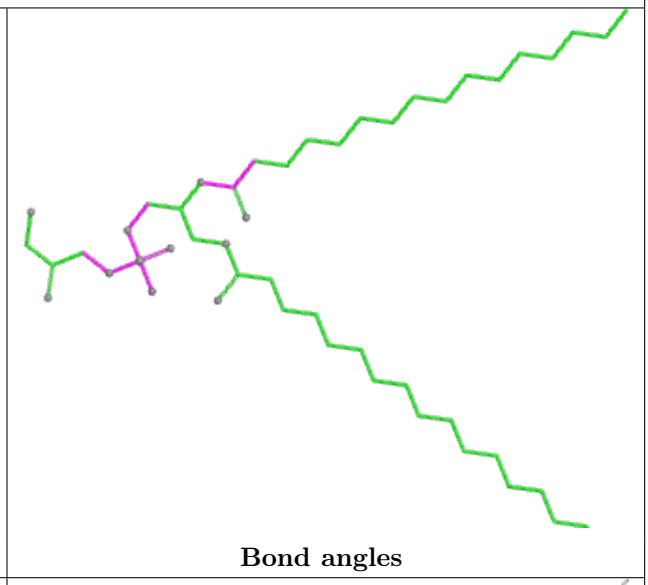

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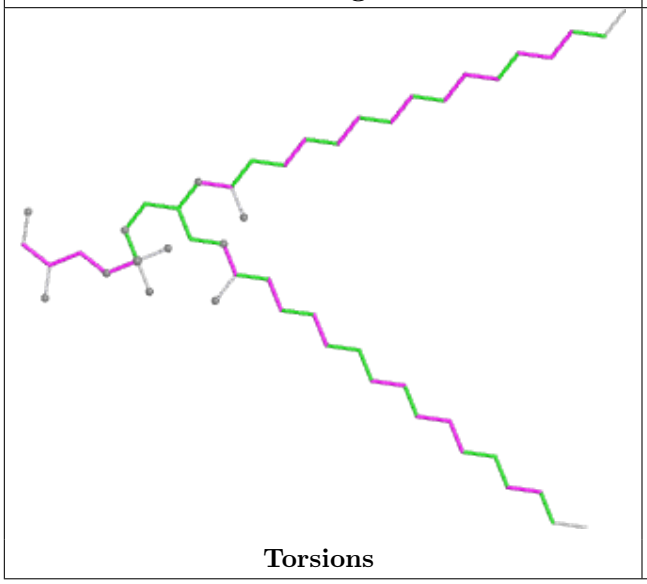
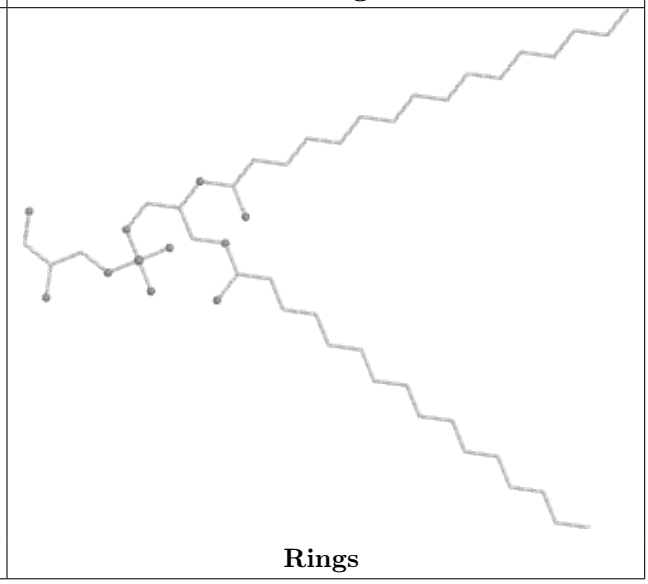
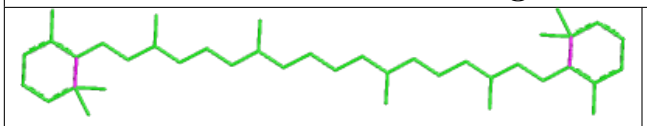


Torsions



Rings

Ligand BCR AA 851



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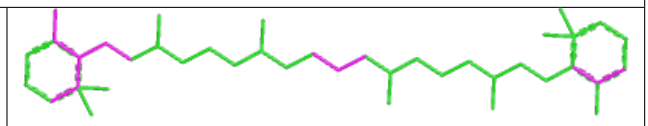

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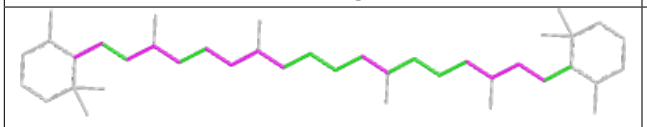
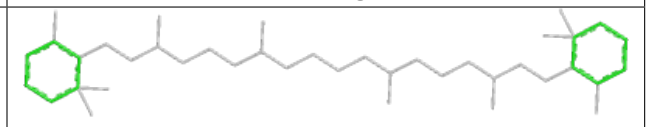
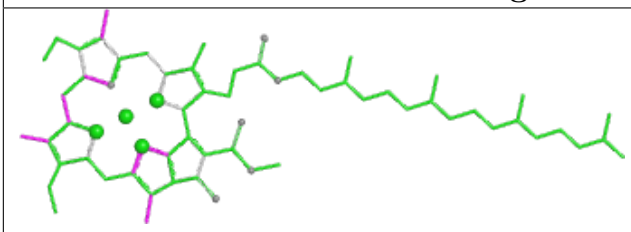
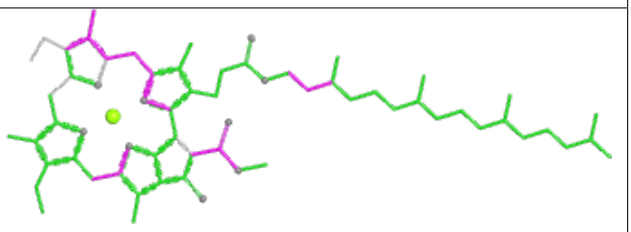
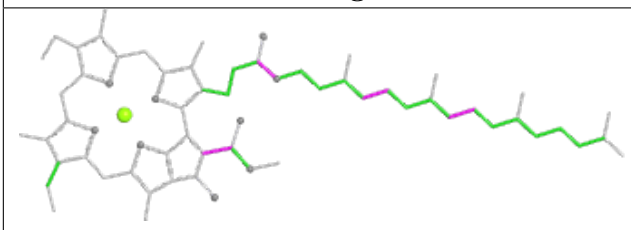
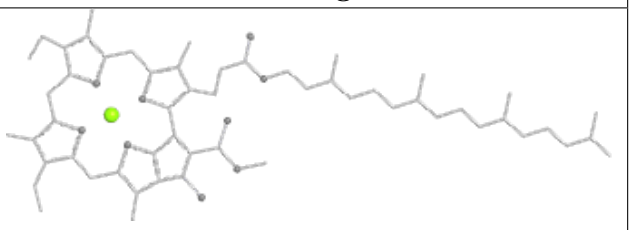
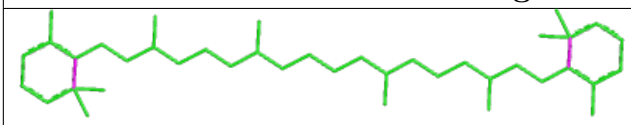
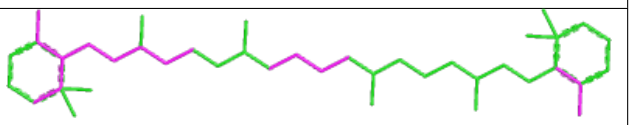
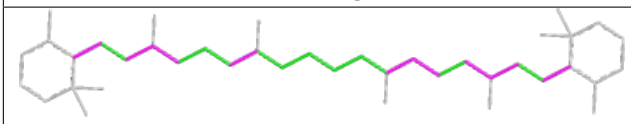
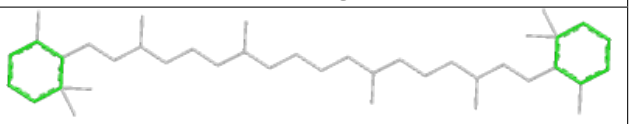


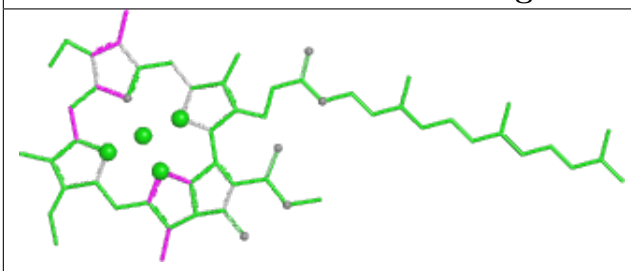
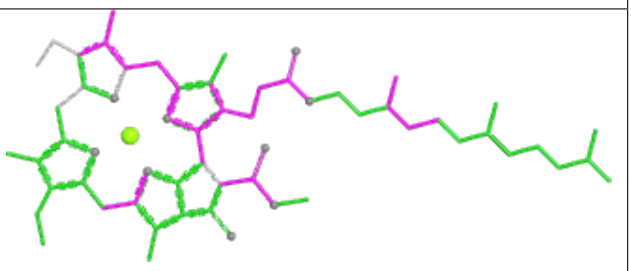
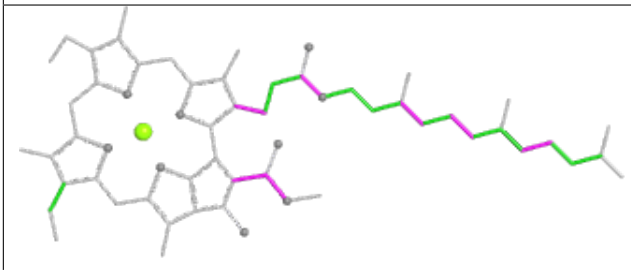
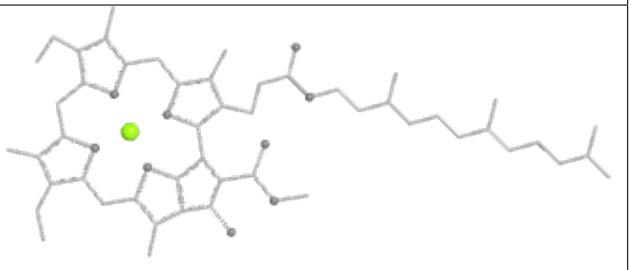
Torsions

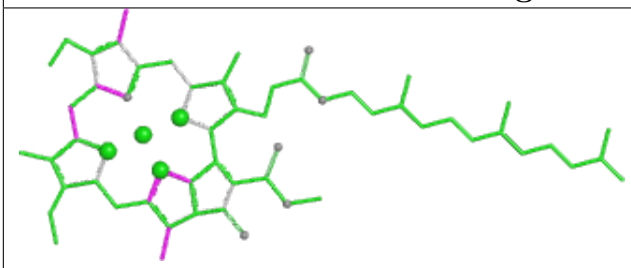
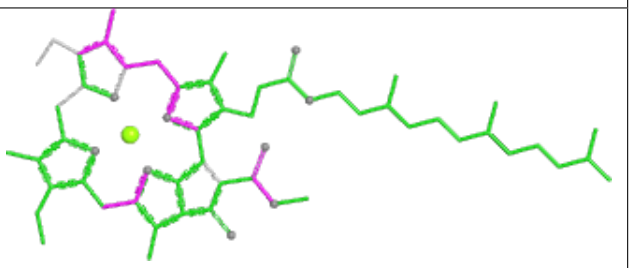
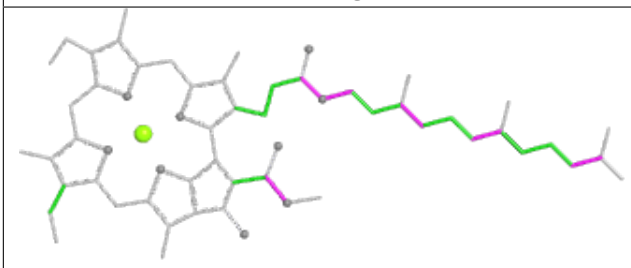
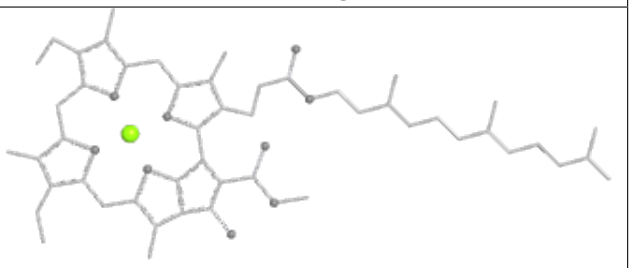


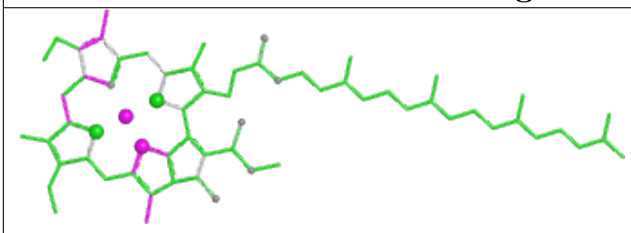
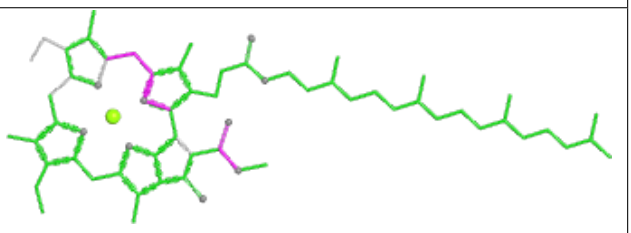
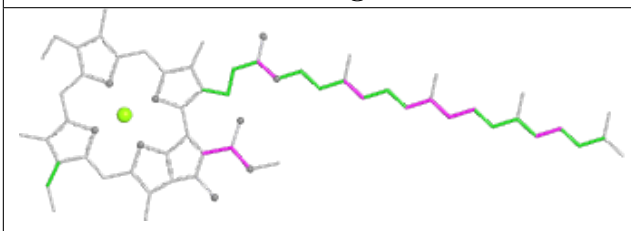
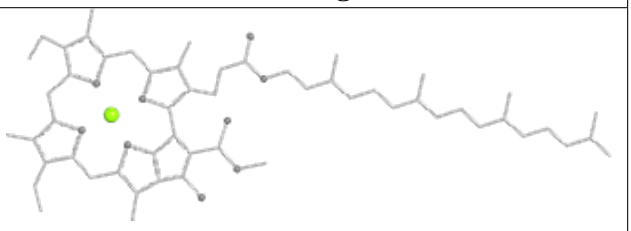
Rings

Ligand CLA AA 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A1 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

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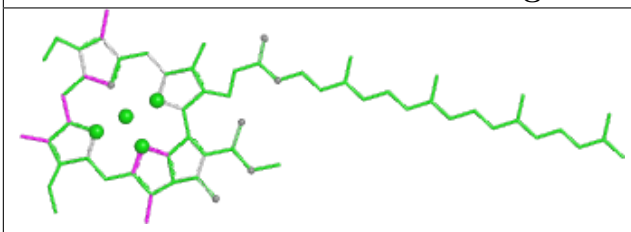
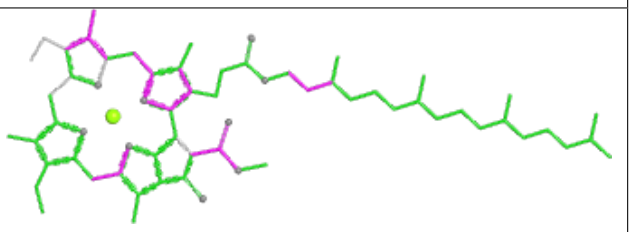
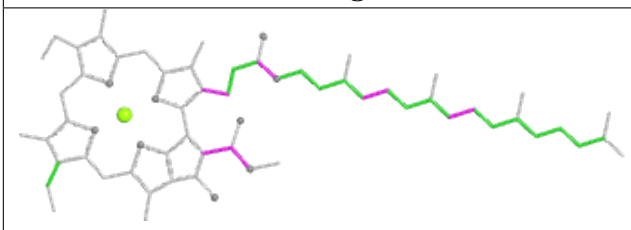
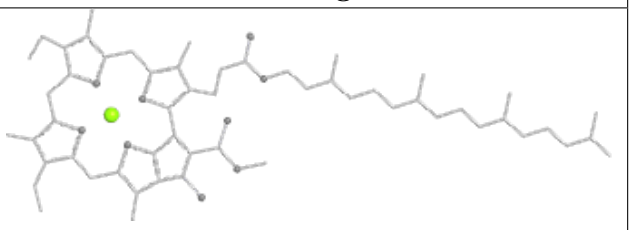
 Bond lengths	 Bond angles
 Torsions	 Rings

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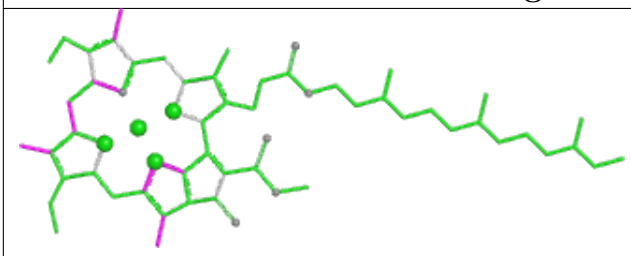
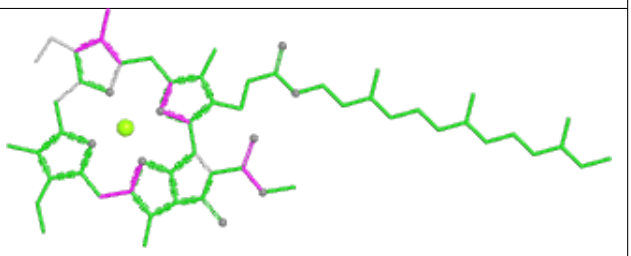
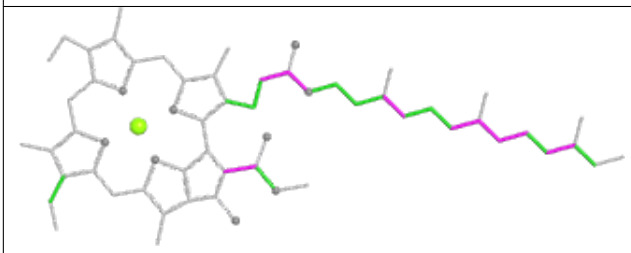
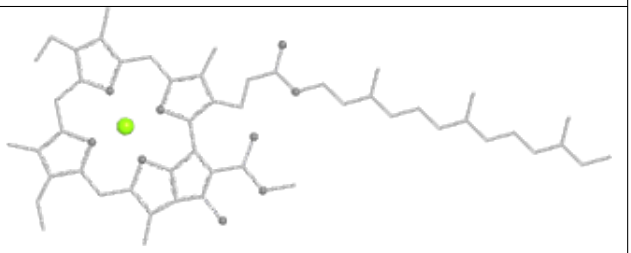
 Bond lengths	 Bond angles
 Torsions	 Rings

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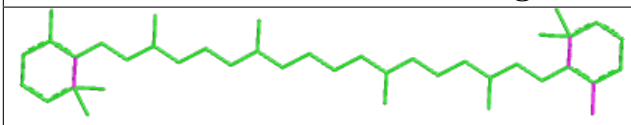
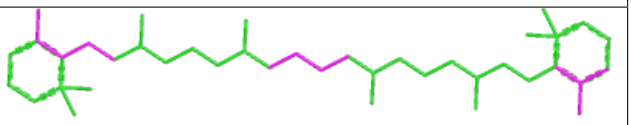
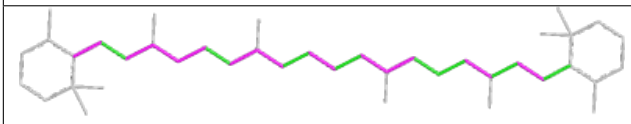
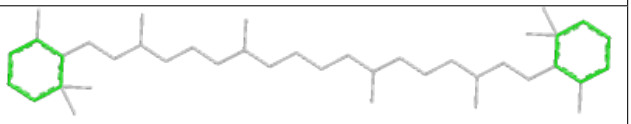
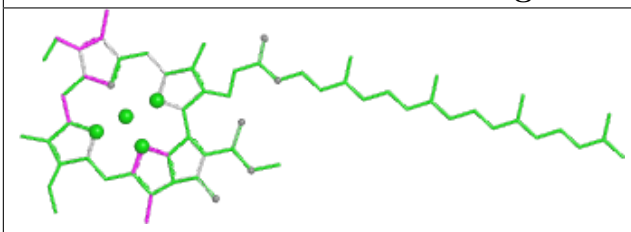
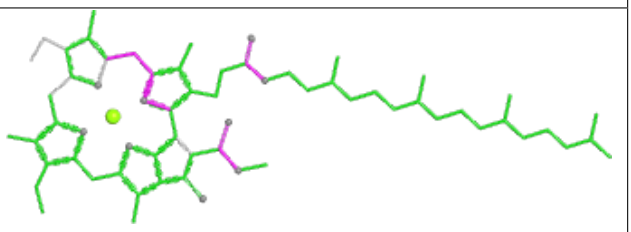
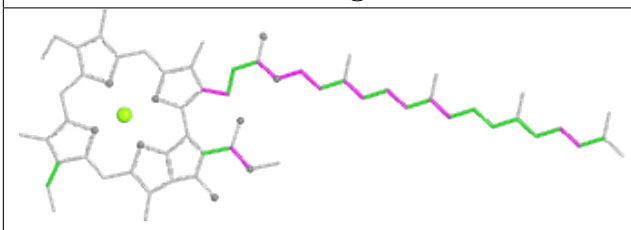
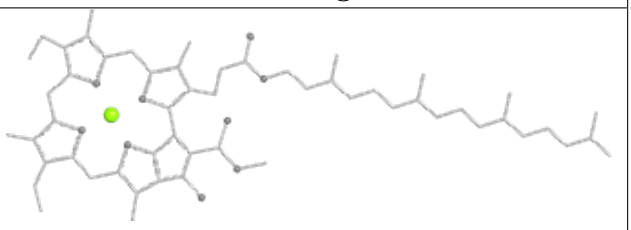
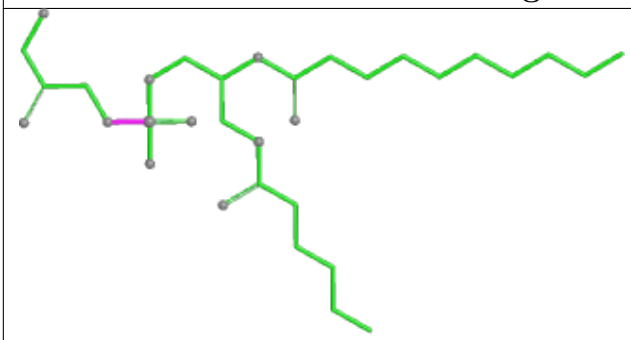
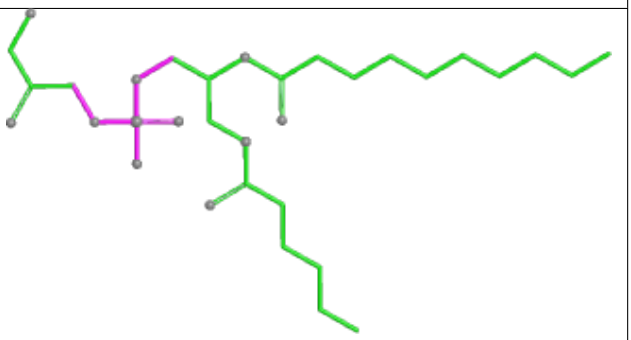
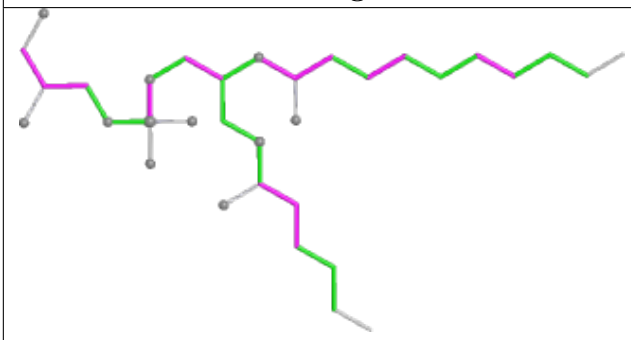
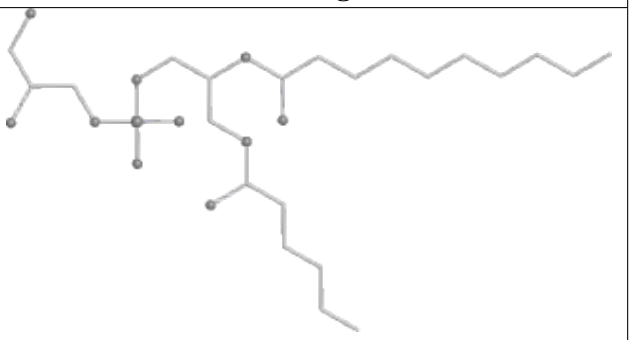
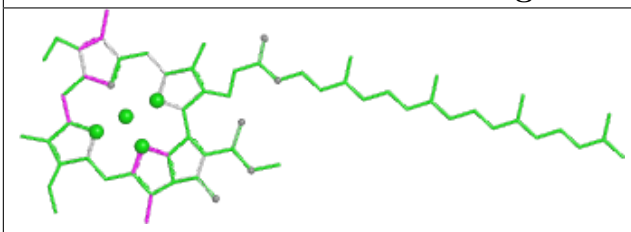
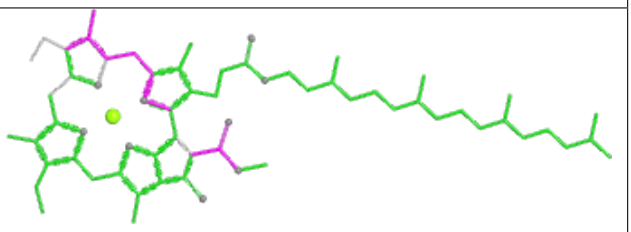
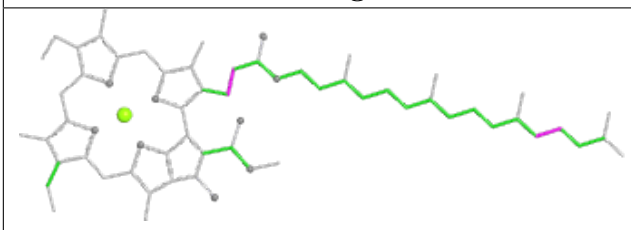
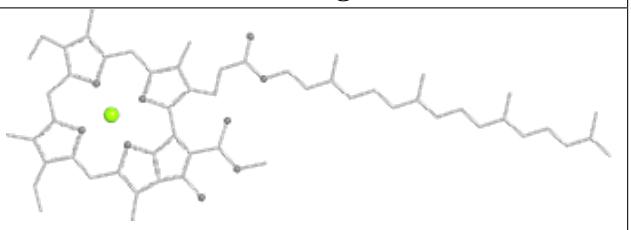
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG B 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

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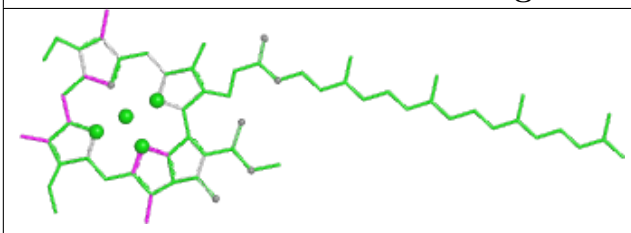
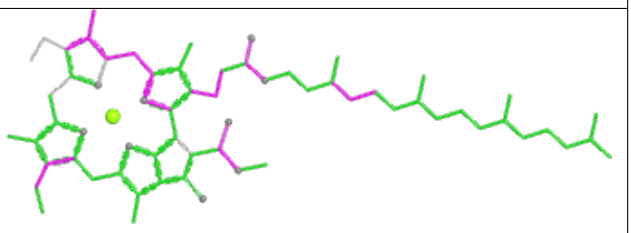
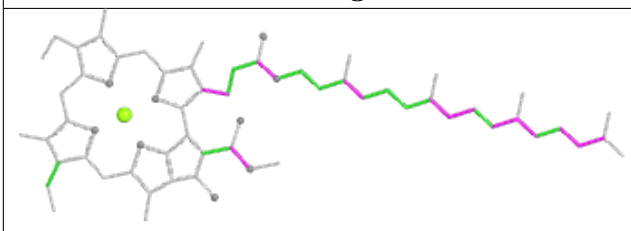
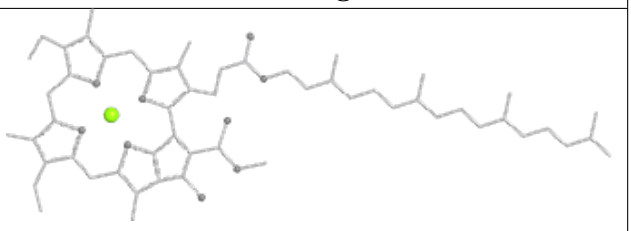
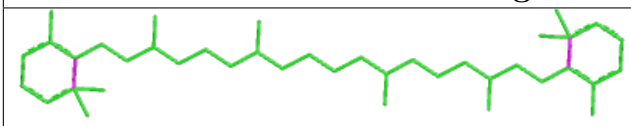
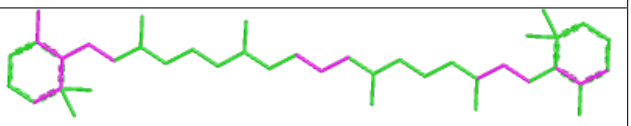
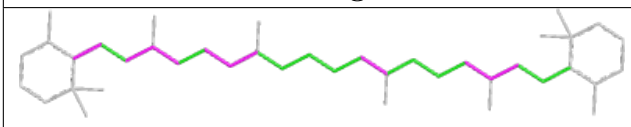
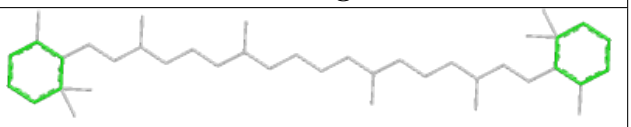
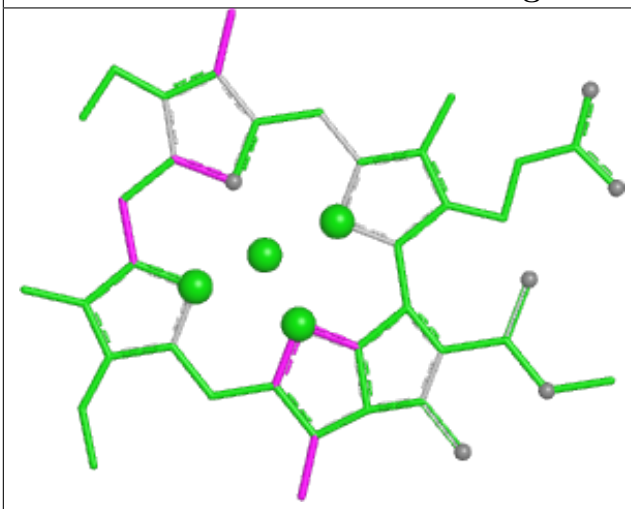
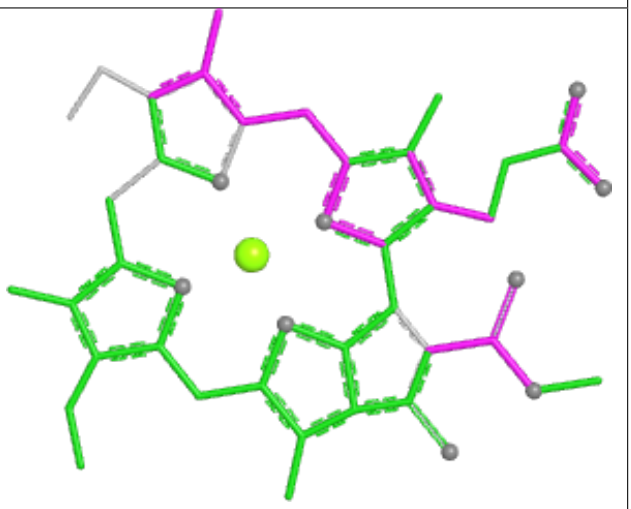
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A2 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

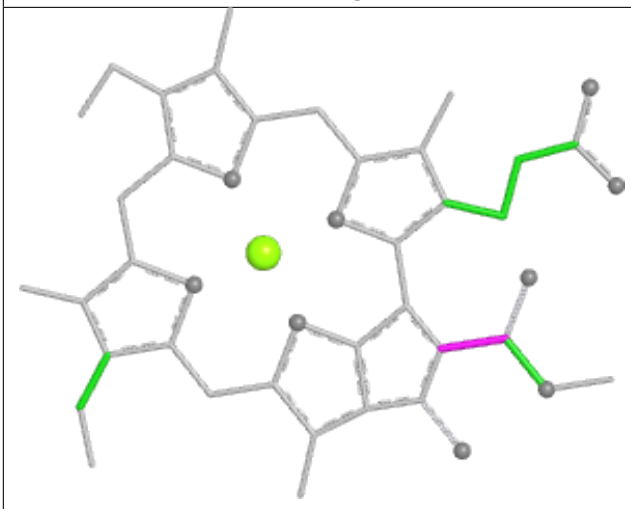
Ligand CLA K 101



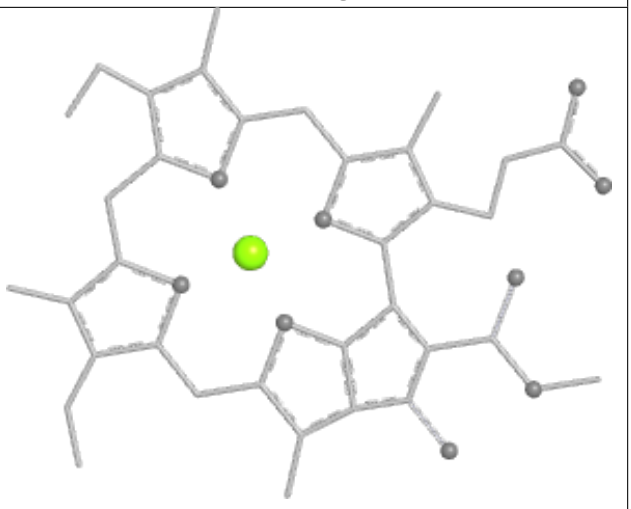
Bond lengths



Bond angles

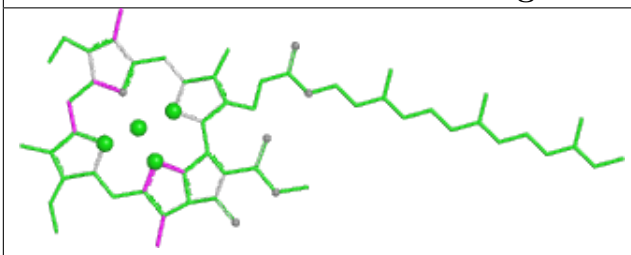


Torsions



Rings

Ligand CLA L2 204



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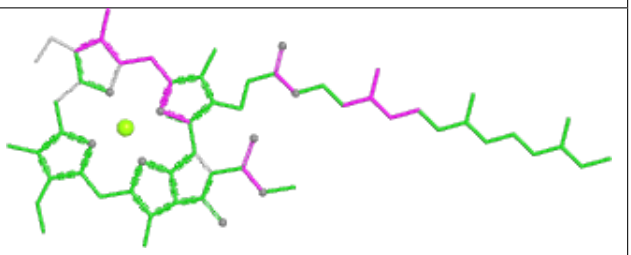

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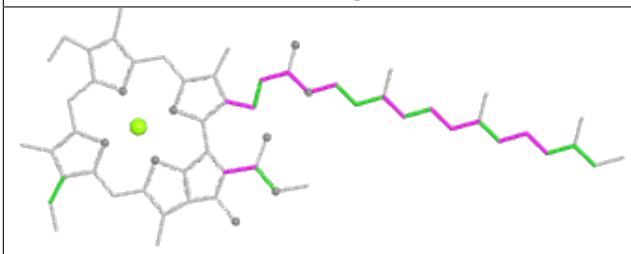

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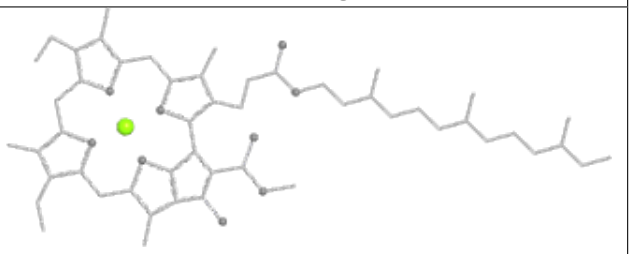
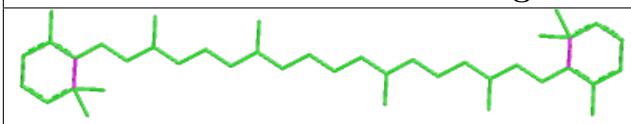
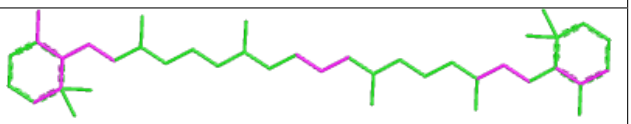
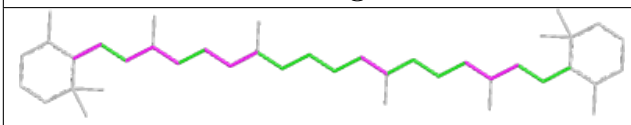
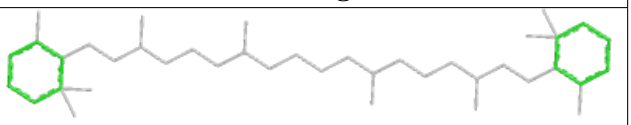


Rings

Ligand BCR A1 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

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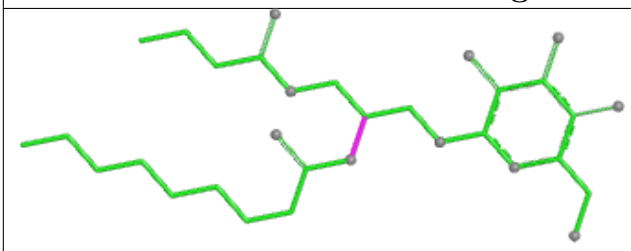
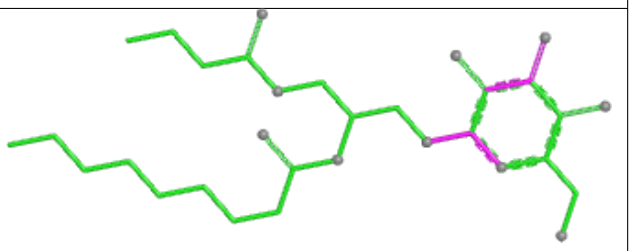
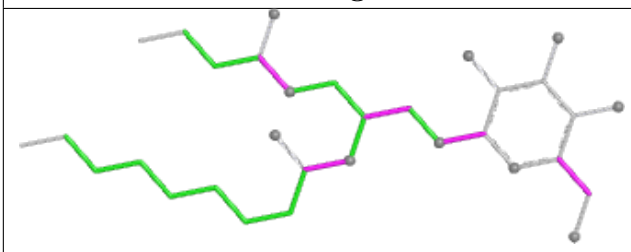
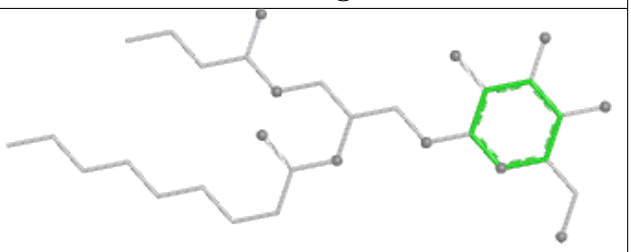
 Bond lengths	 Bond angles
 Torsions	 Rings

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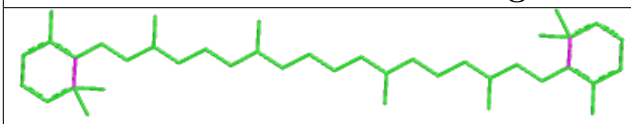
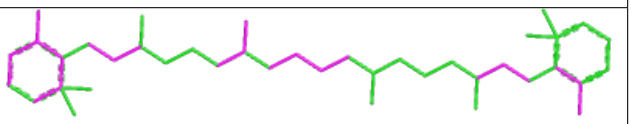
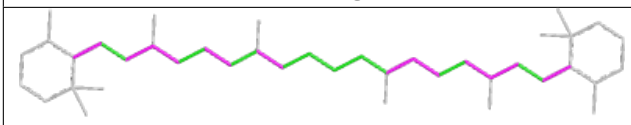
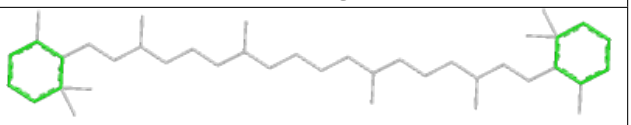
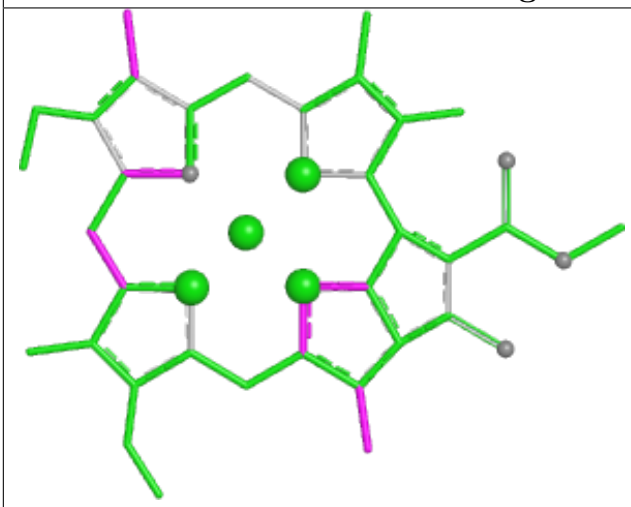
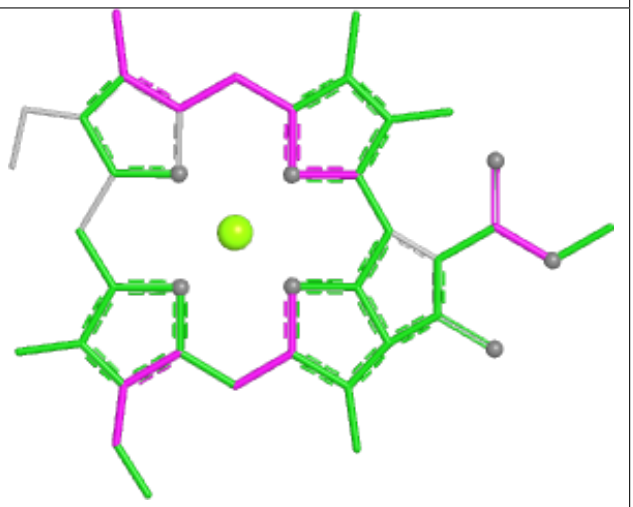
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J2 103



Bond lengths



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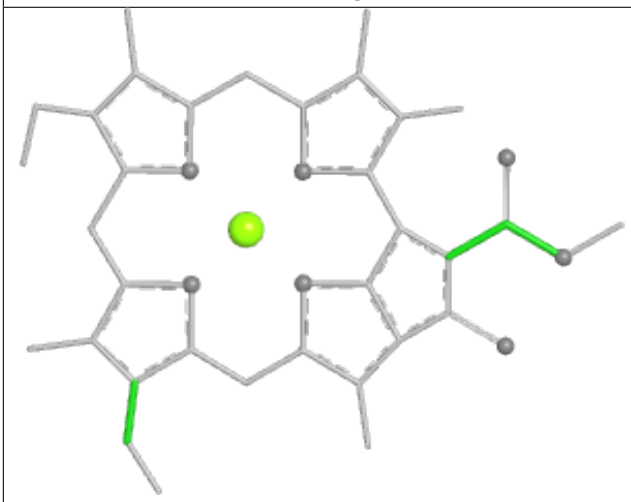

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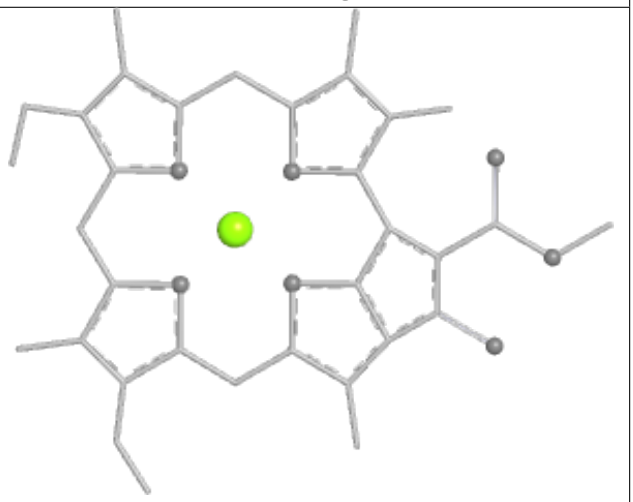
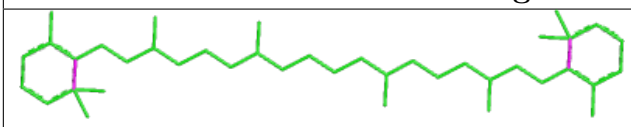


Rings

Ligand BCR FF 303



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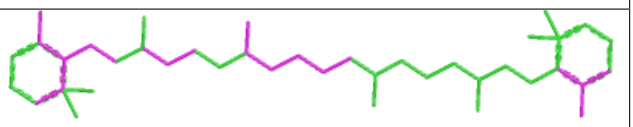

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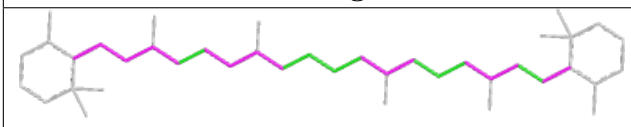

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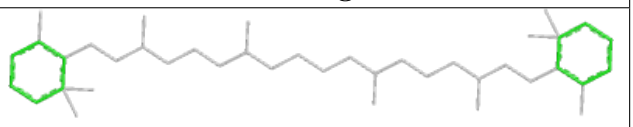
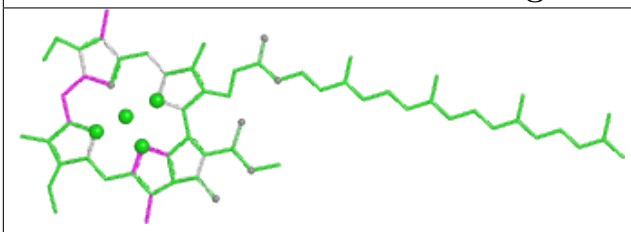
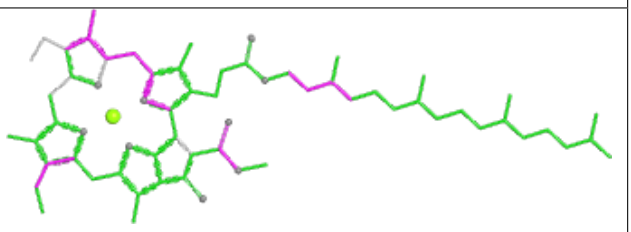
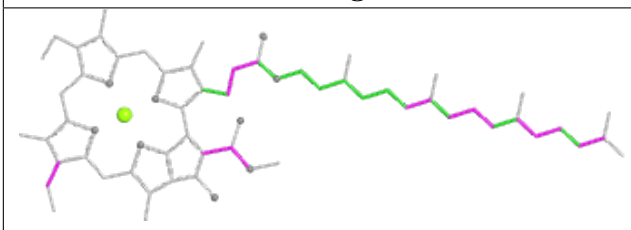
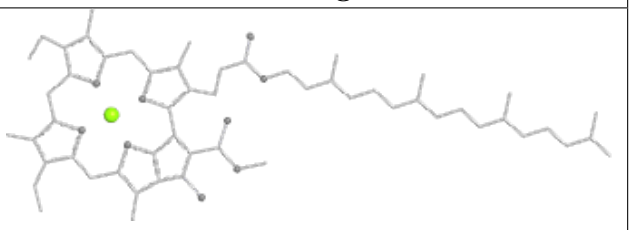


Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

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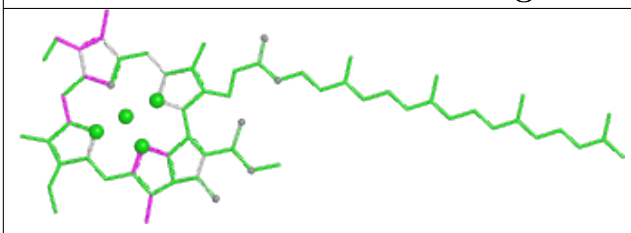
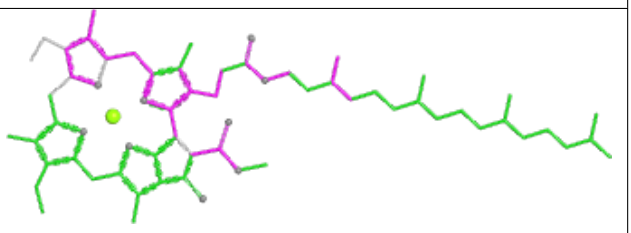
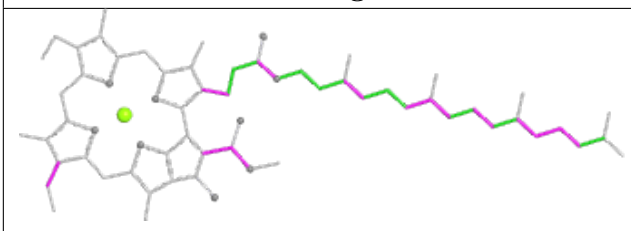
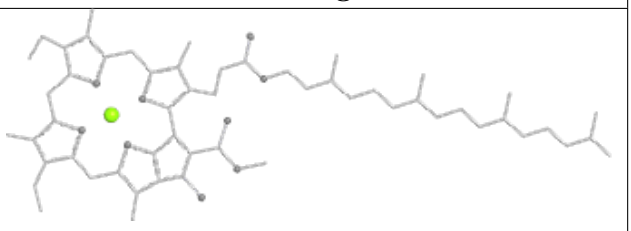
 Bond lengths	 Bond angles
 Torsions	 Rings

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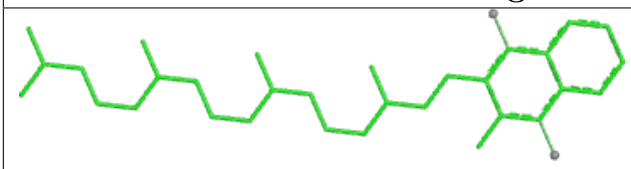
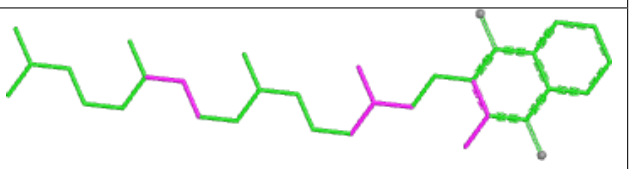
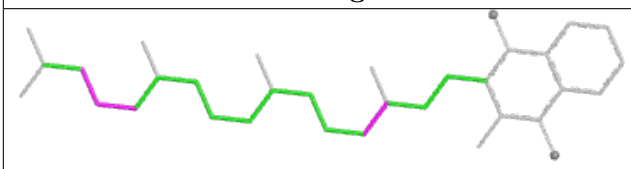
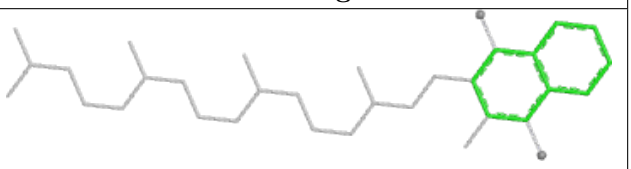
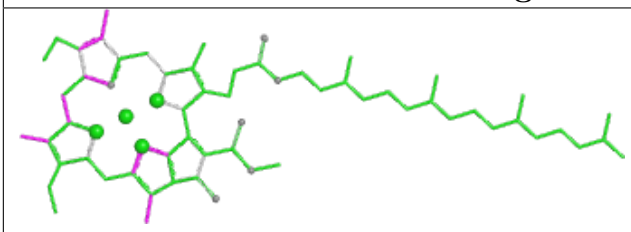
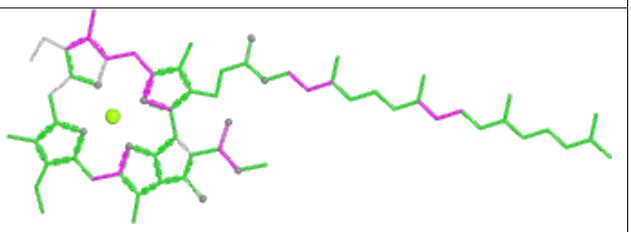
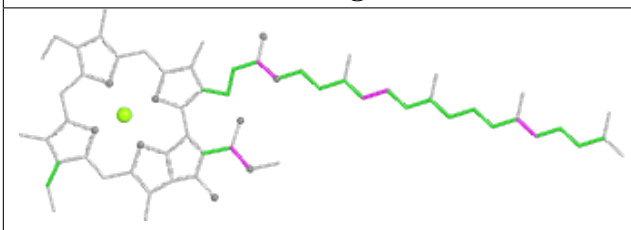
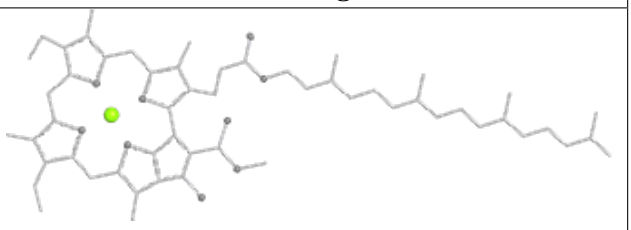
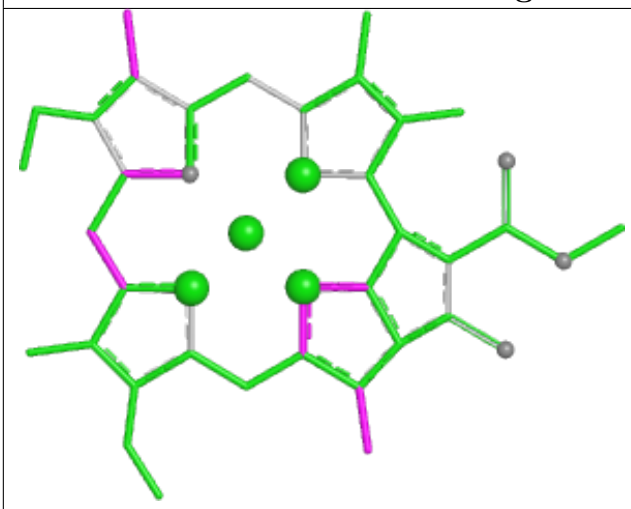
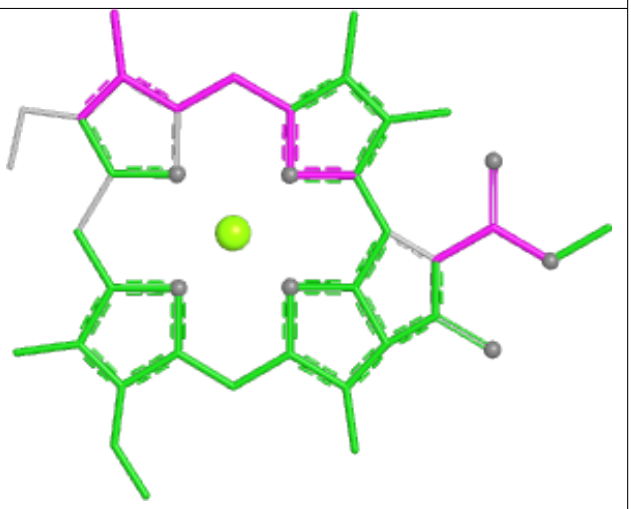
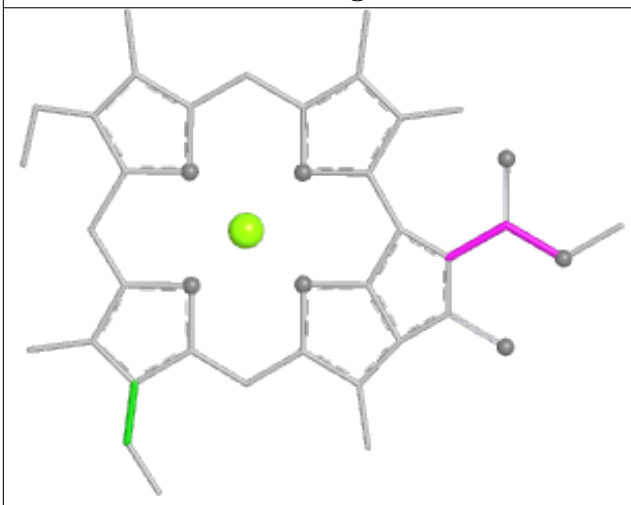
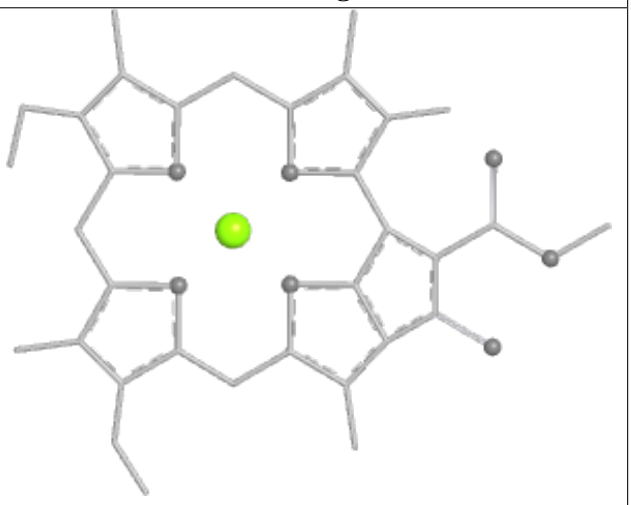
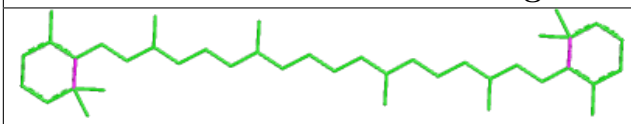
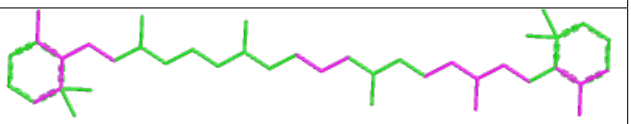
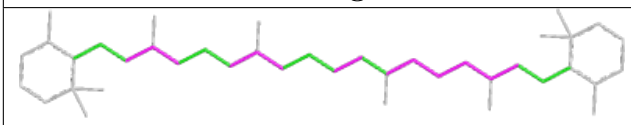
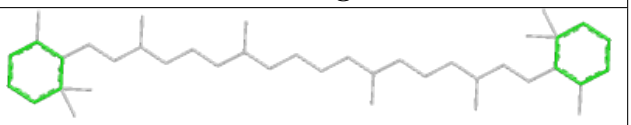
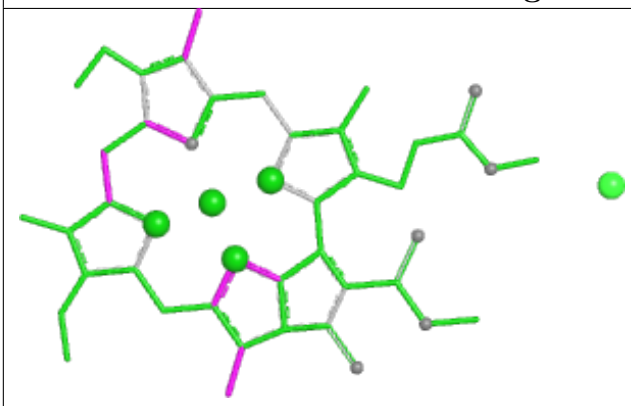
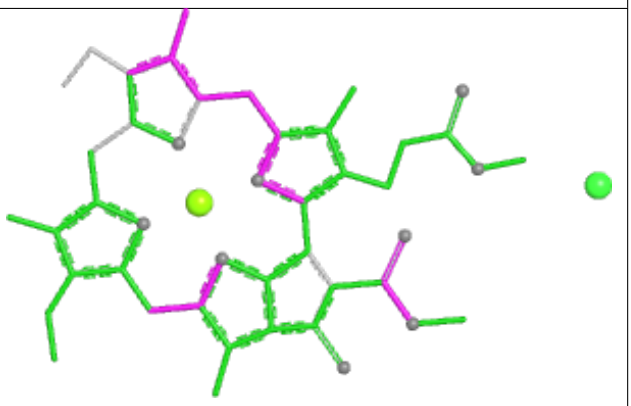
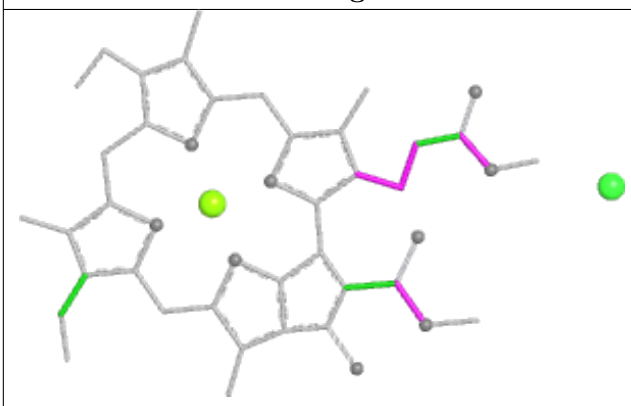
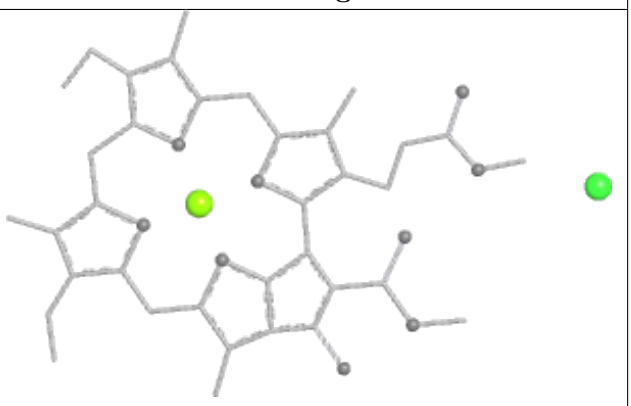
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR F 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

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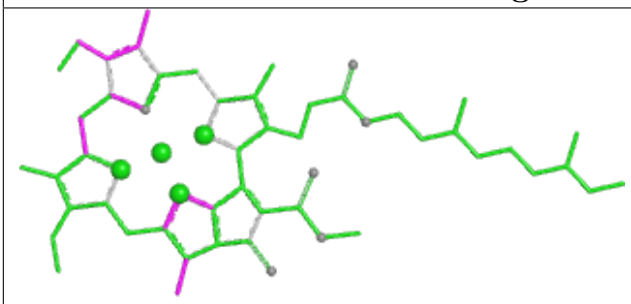
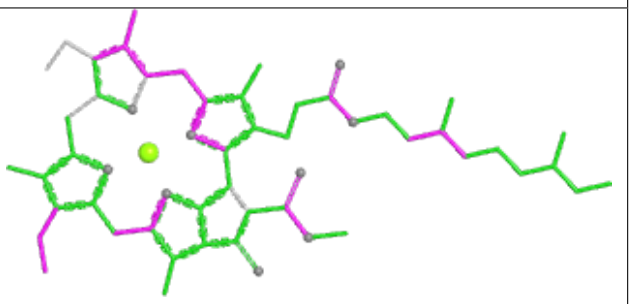
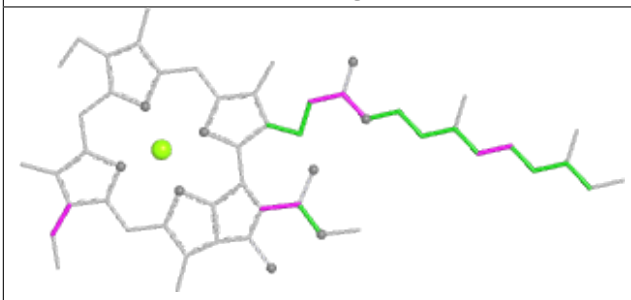
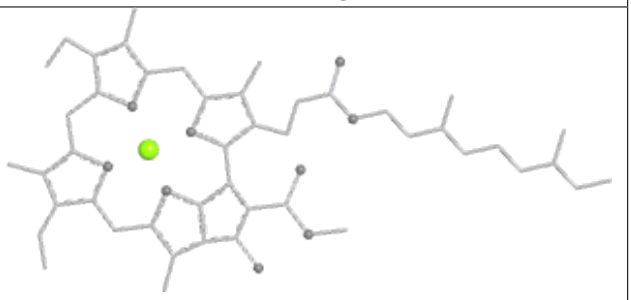
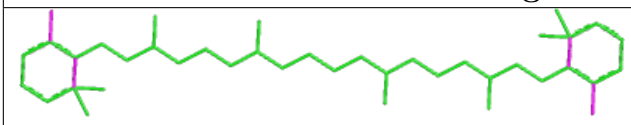
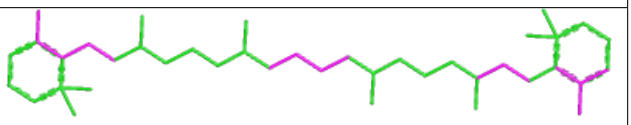
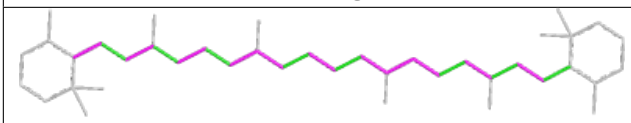
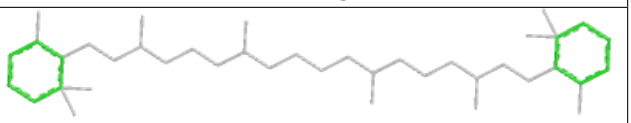
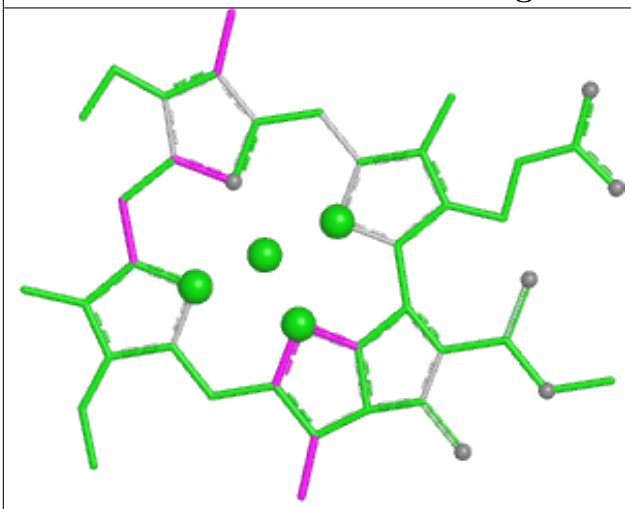
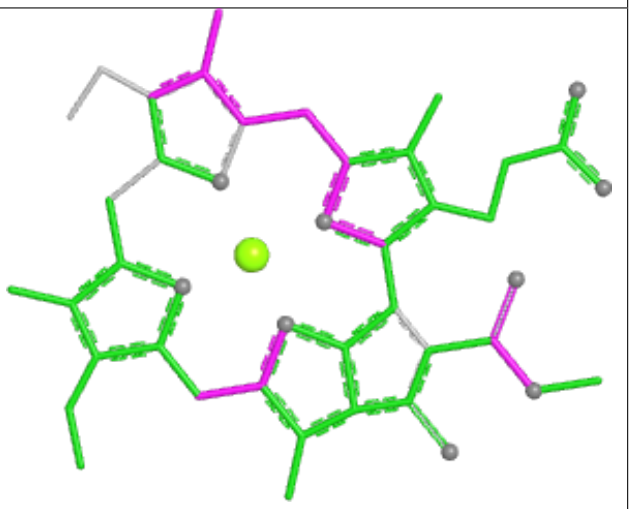
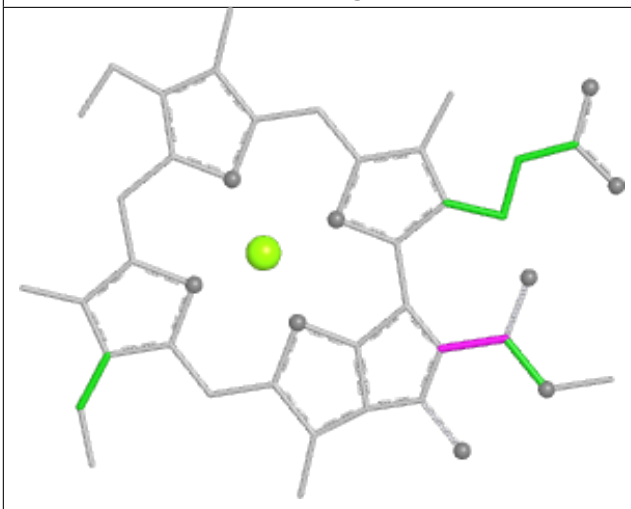
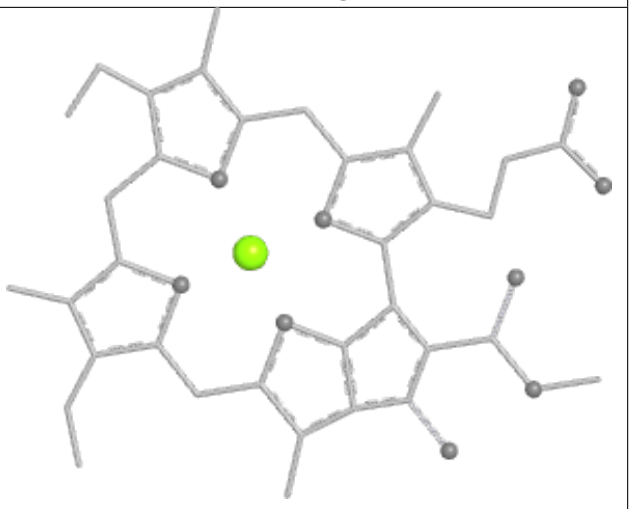
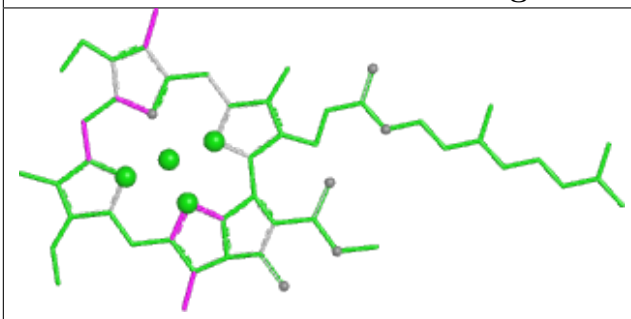
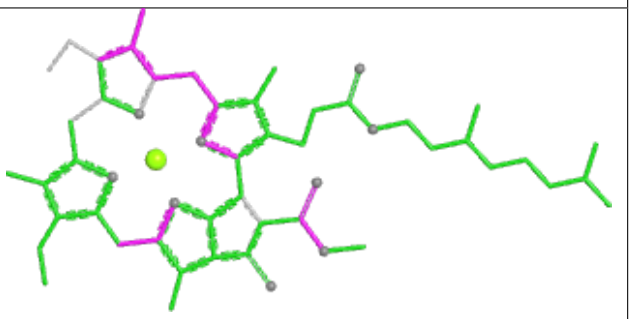
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 828	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA AA 815	
	
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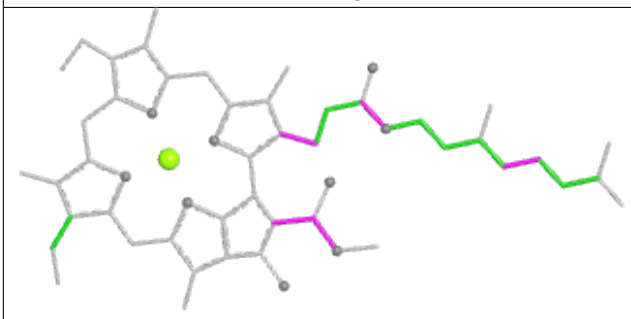
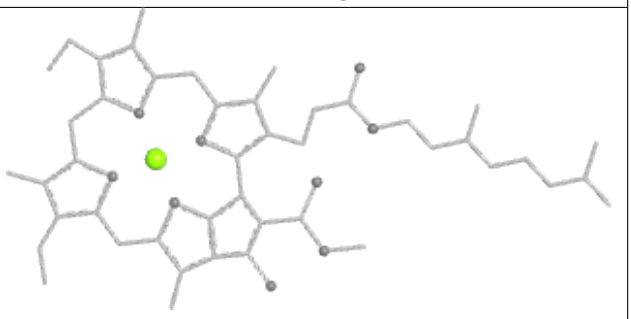
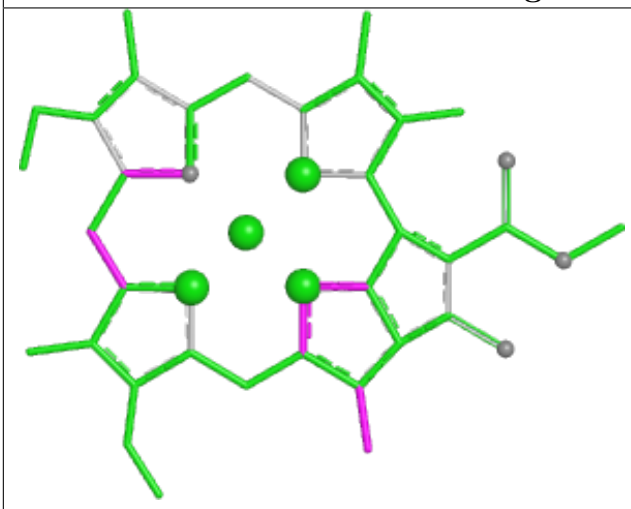
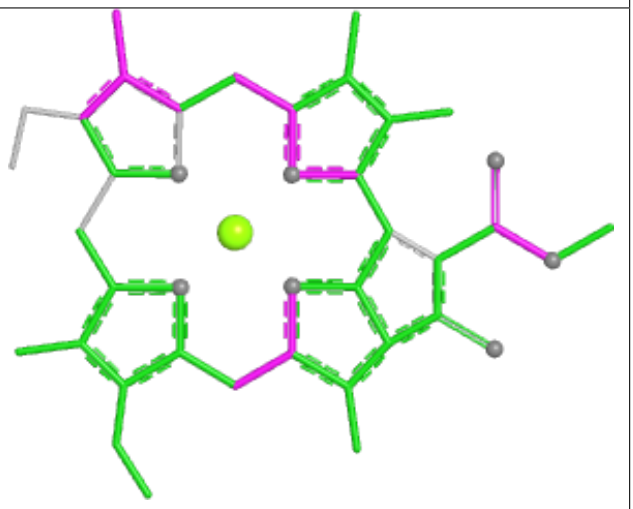
	
Torsions	**Rings**

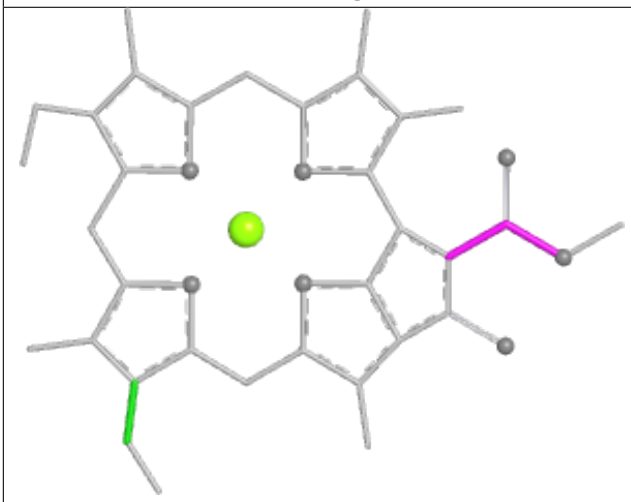
Ligand CLA B 818



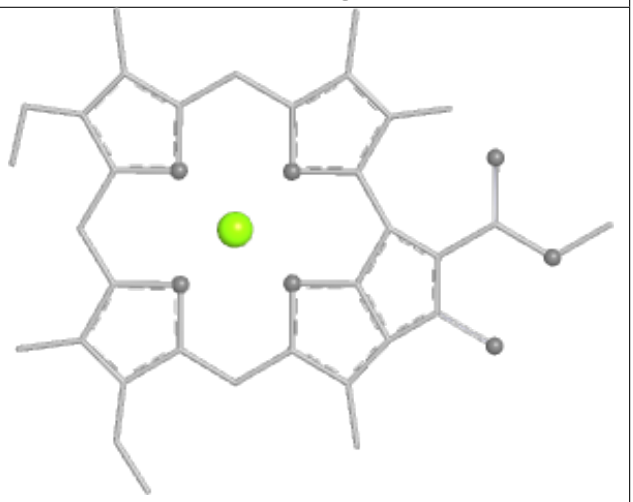
Bond lengths



Bond angles

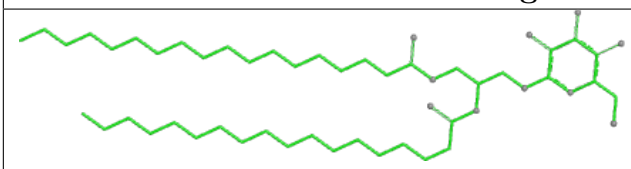


Torsions

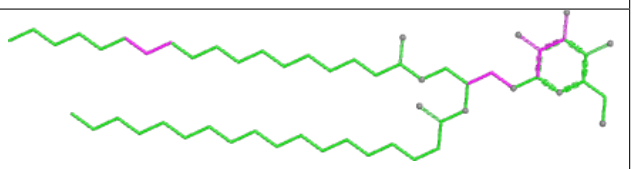


Rings

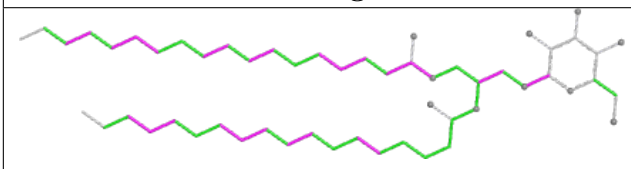
Ligand LMG B 845



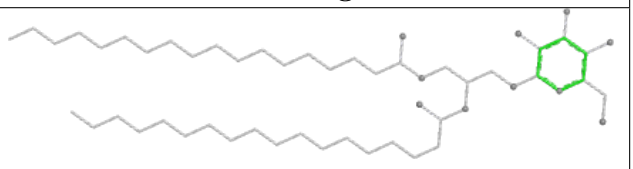
Bond lengths



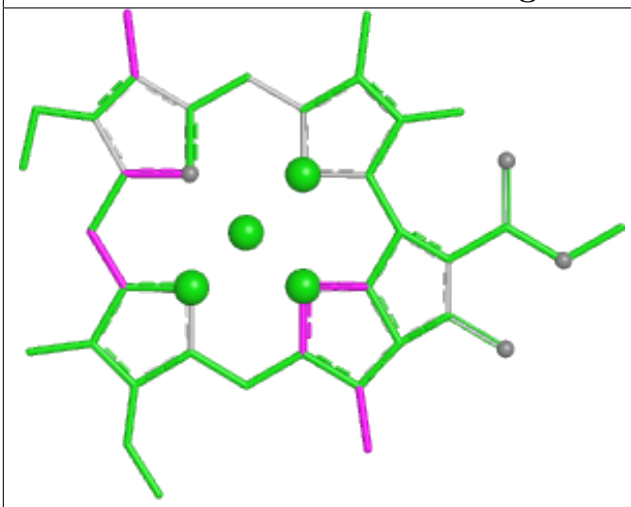
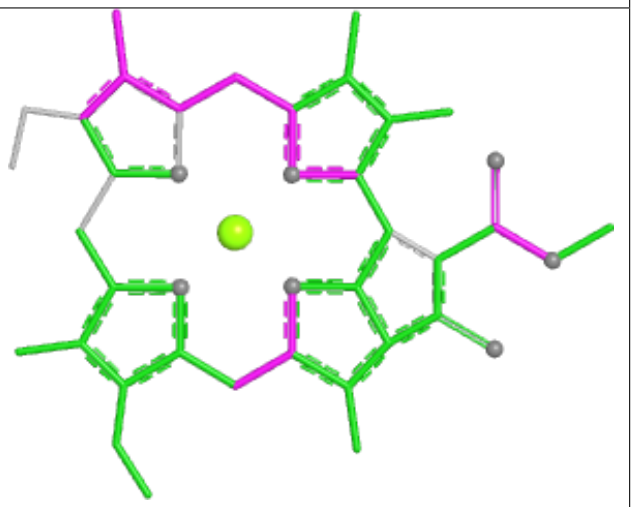
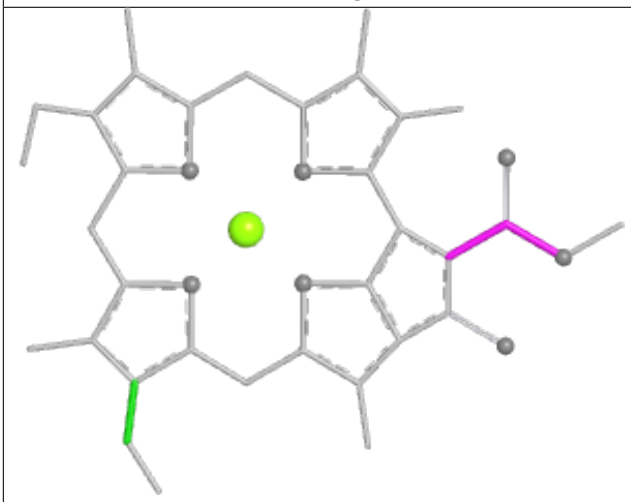
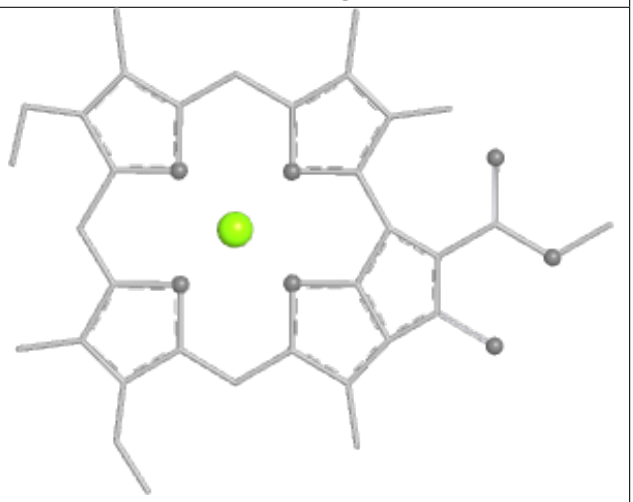
Bond angles



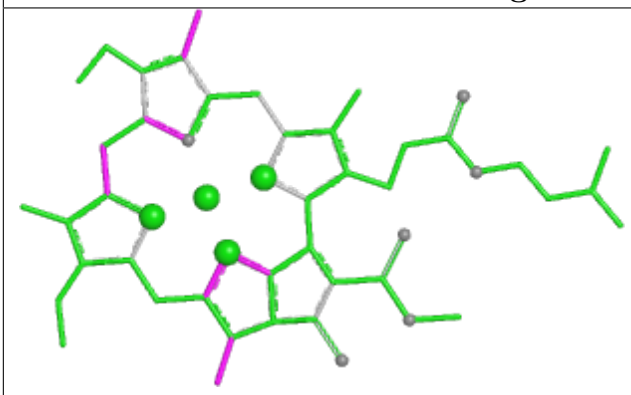
Torsions



Rings

Ligand CLA J2 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA AA 809



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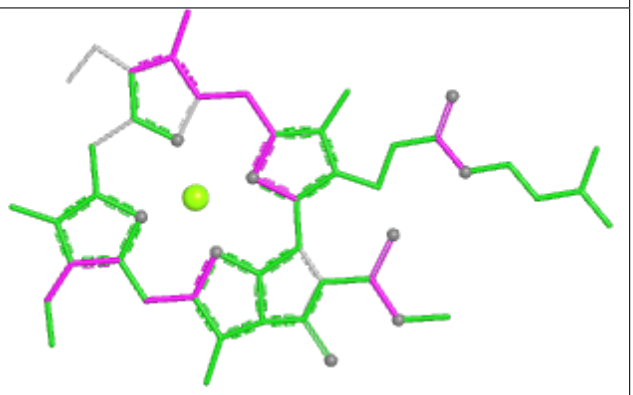
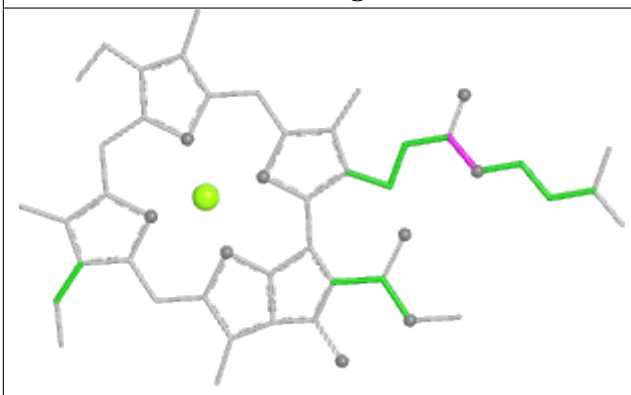
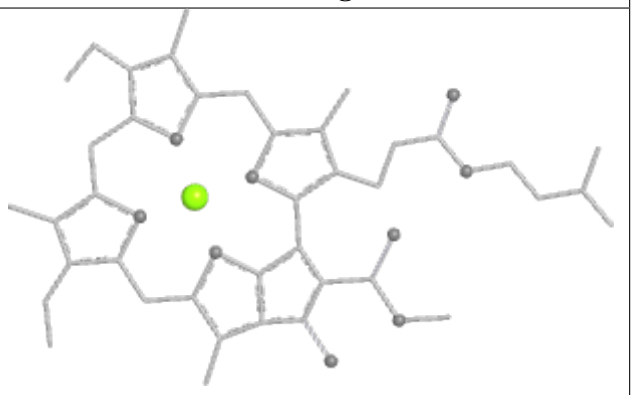


Bond angles

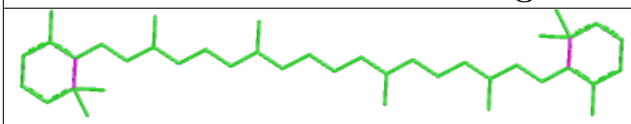


Torsions



Rings

Ligand BCR L1 209



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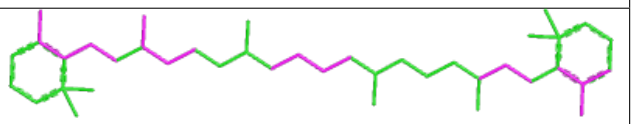
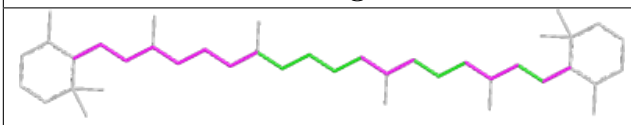
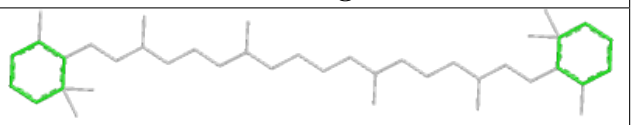


Bond angles

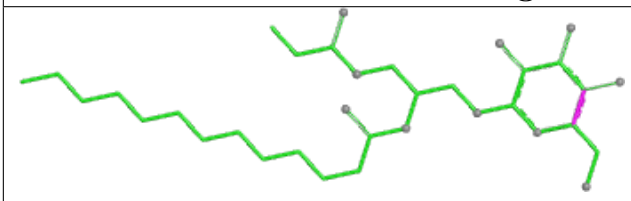


Torsions

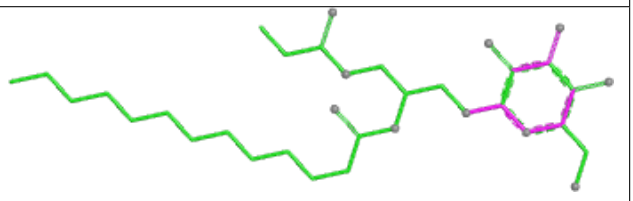


Rings

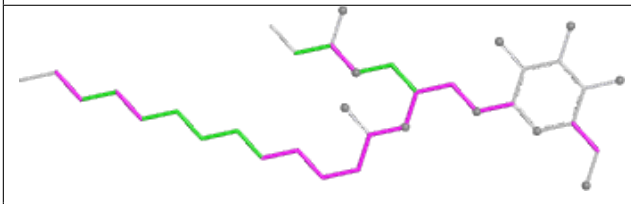
Ligand LMG I1 102



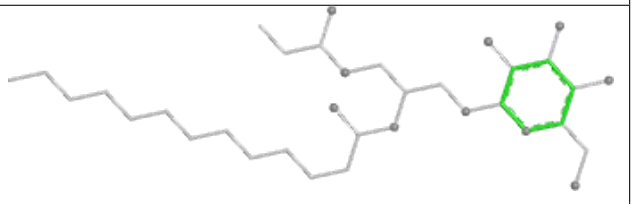
Bond lengths



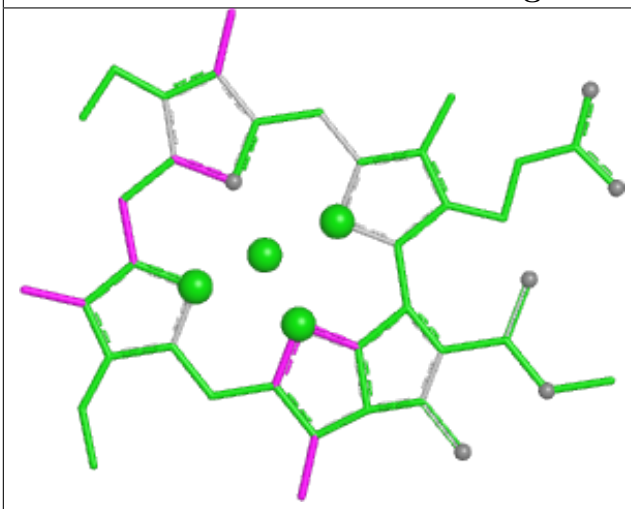
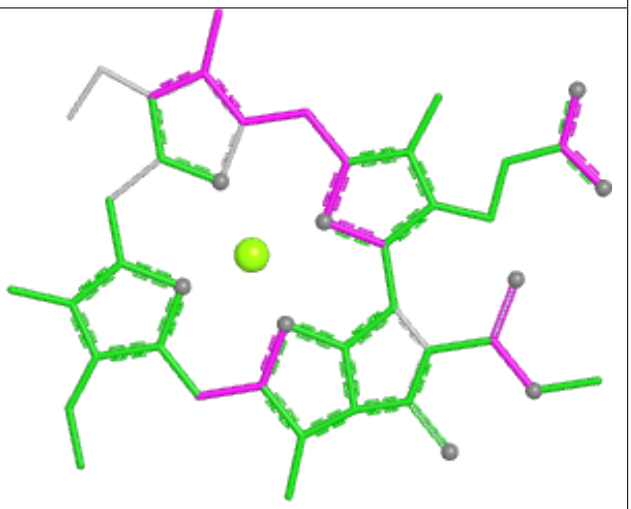
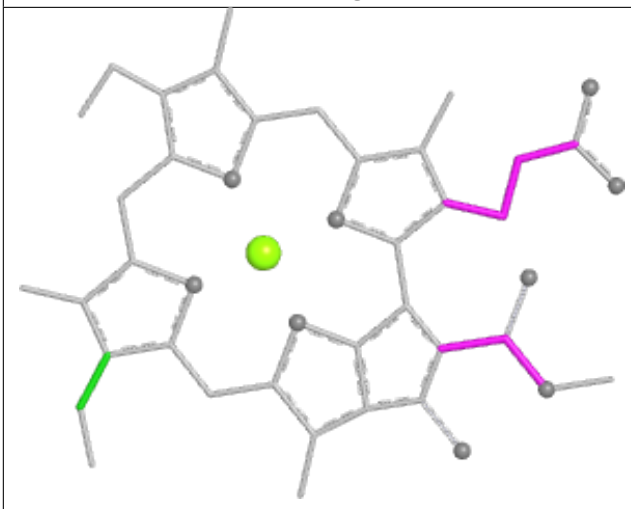
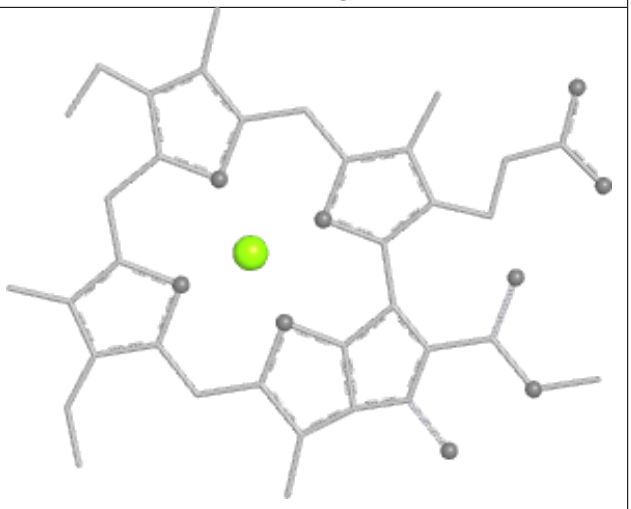
Bond angles



Torsions



Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

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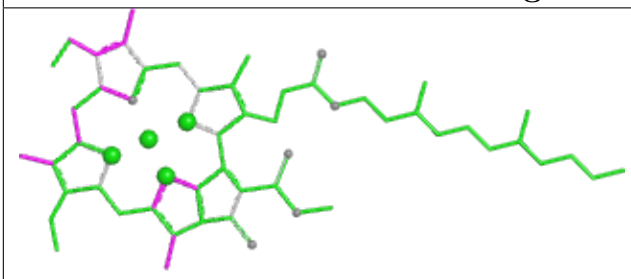
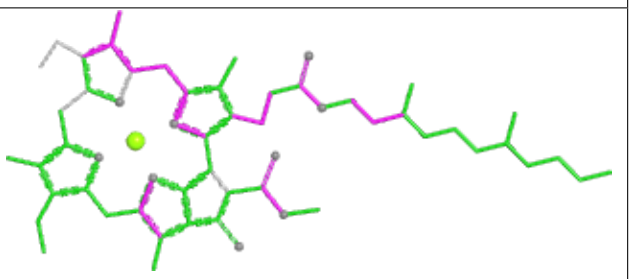
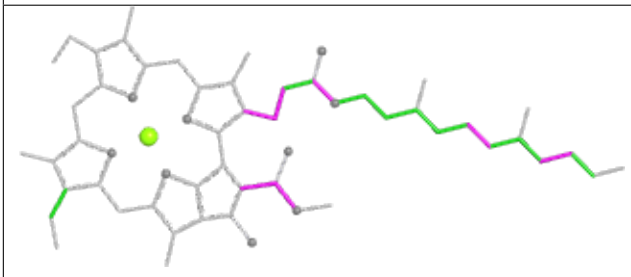
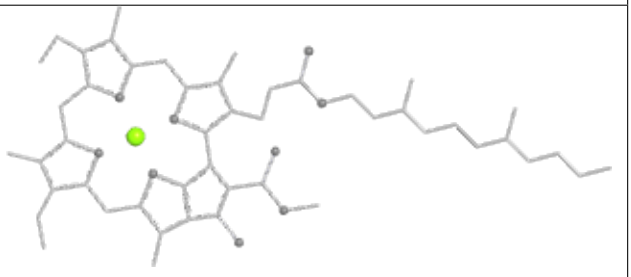
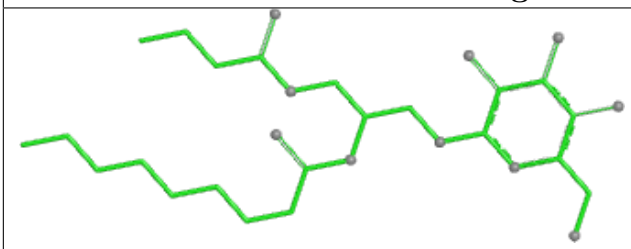
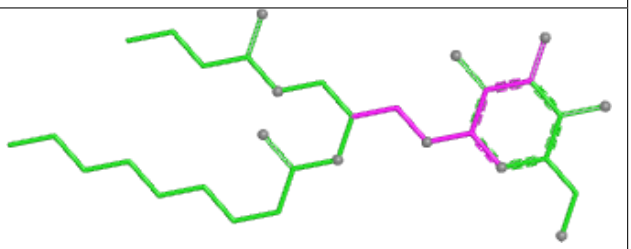
	
Bond lengths	Bond angles
	
Torsions	Rings

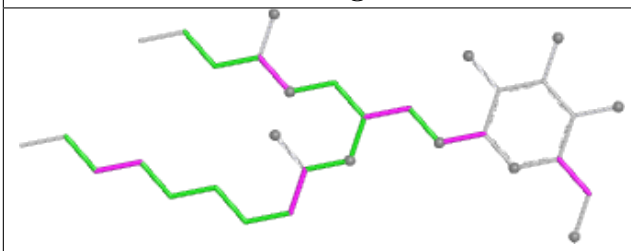
Ligand LMG B1 846



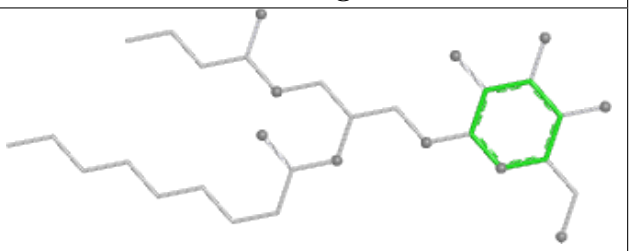
Bond lengths



Bond angles

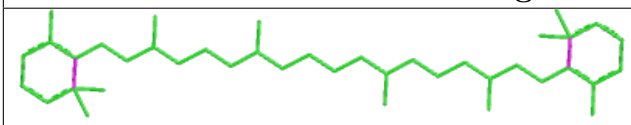


Torsions



Rings

Ligand BCR F2 305



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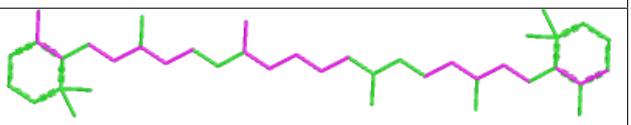
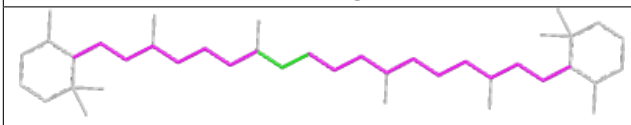


Bond angles



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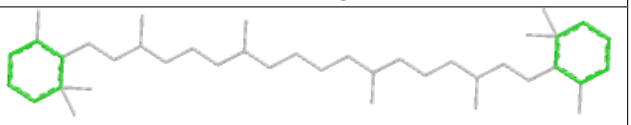
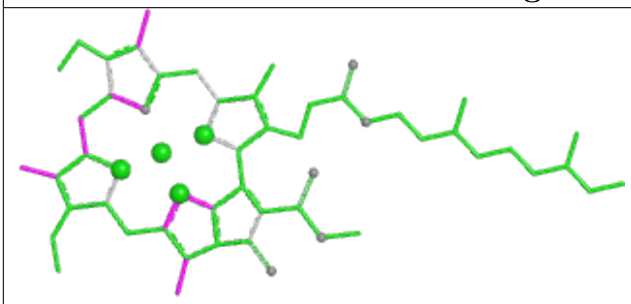


Rings

Ligand CLA A 840



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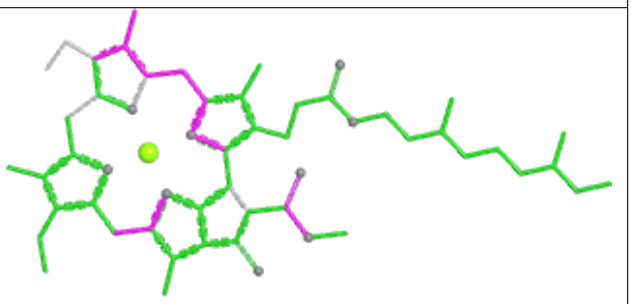
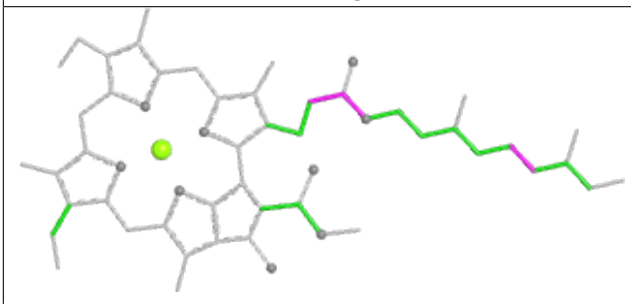
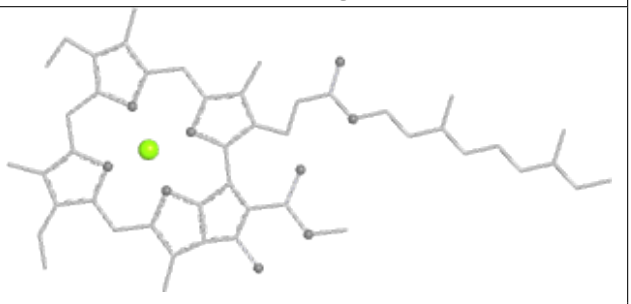


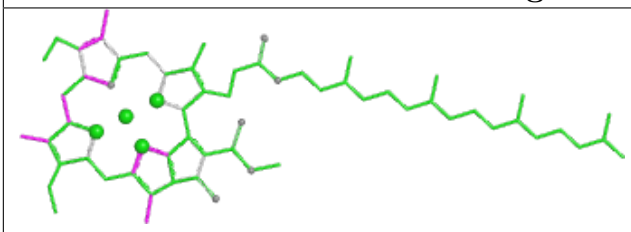
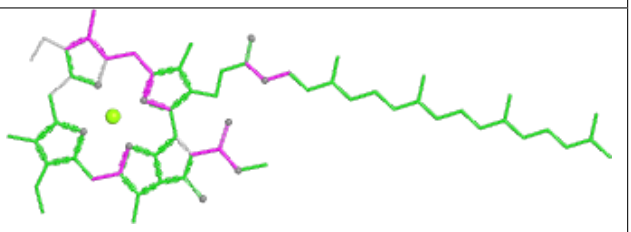
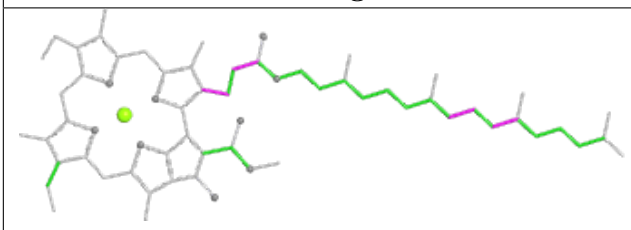
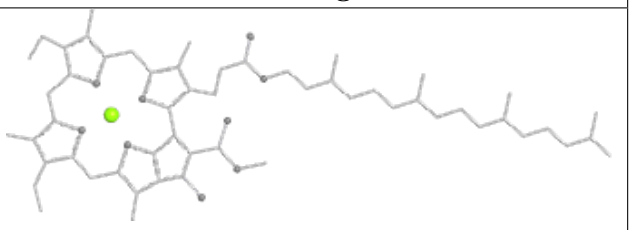
Bond angles

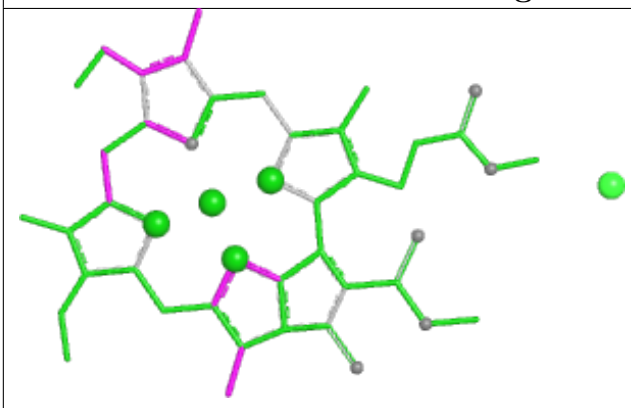
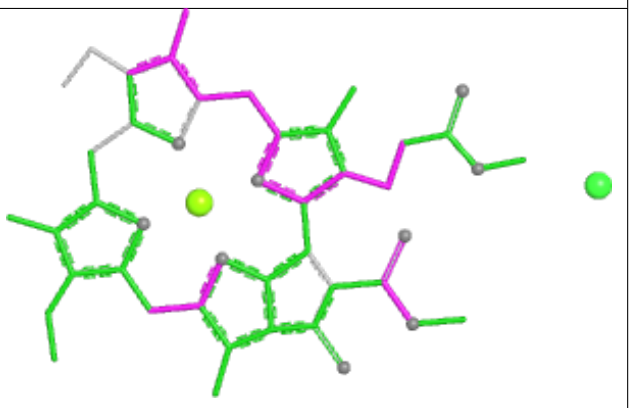
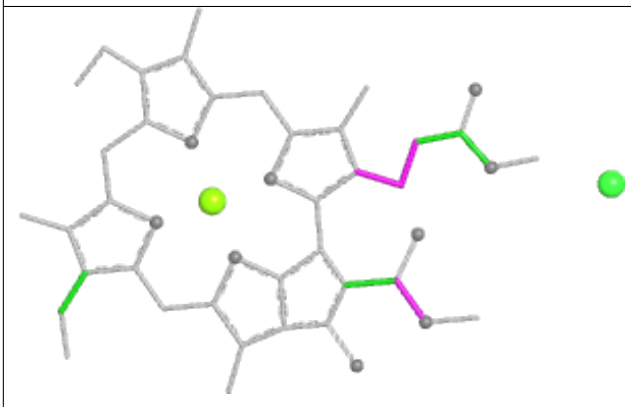
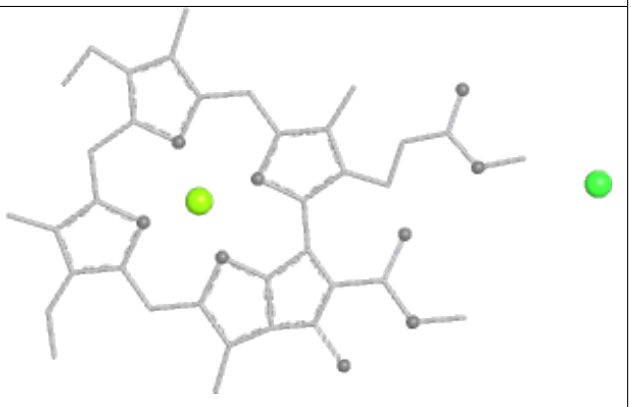


Torsions

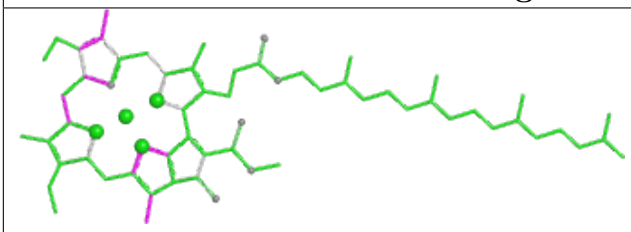


Rings

Ligand CLA L 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 826



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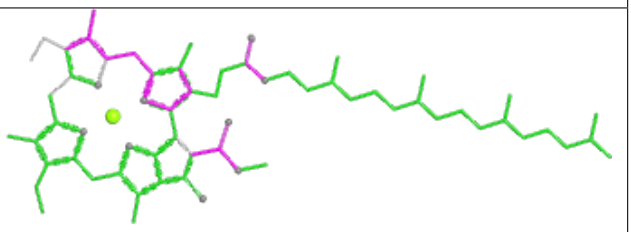
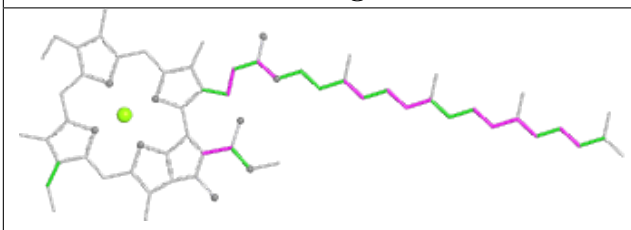


Bond angles



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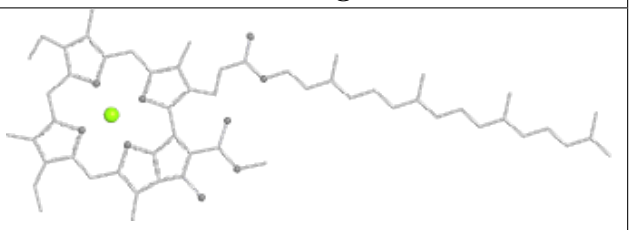
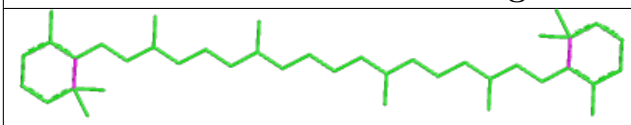


Rings

Ligand BCR AA 855



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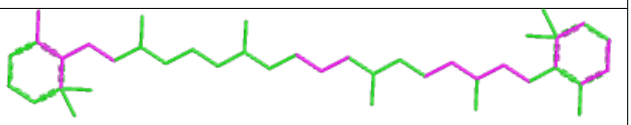
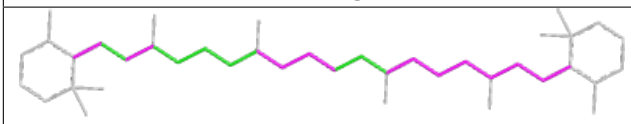
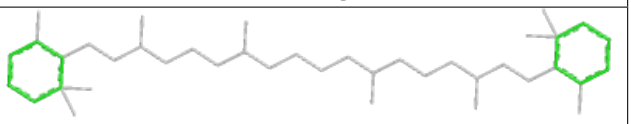


Bond angles

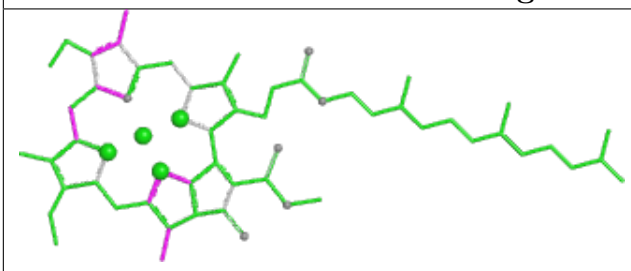


Torsions



Rings

Ligand CLA F2 301



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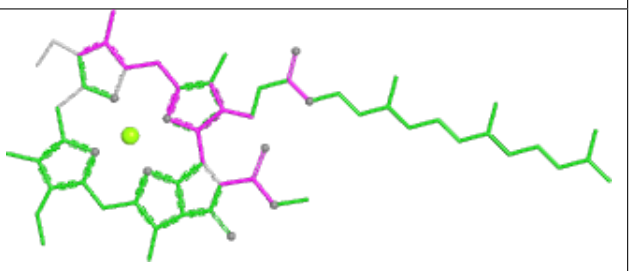
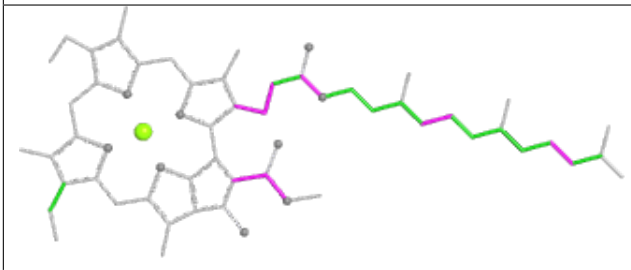
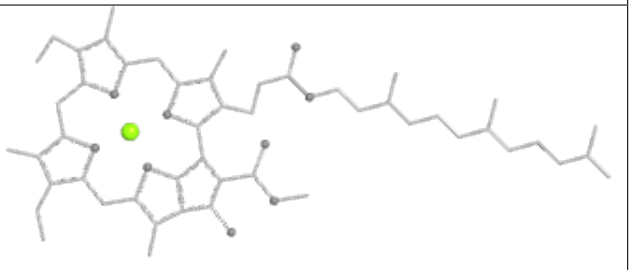


Bond angles

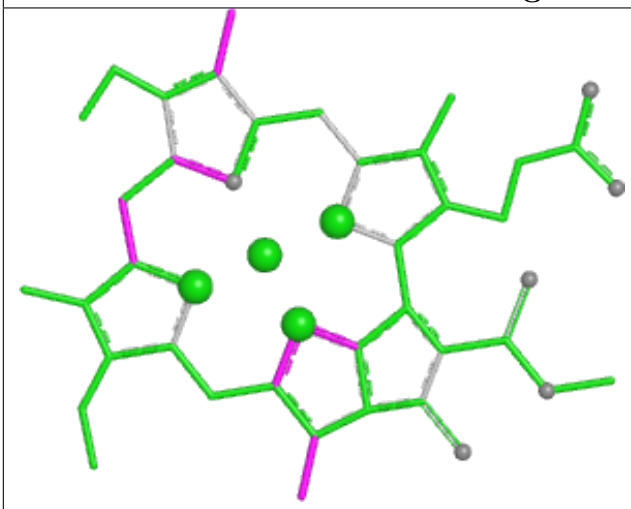


Torsions



Rings

Ligand CLA A 818



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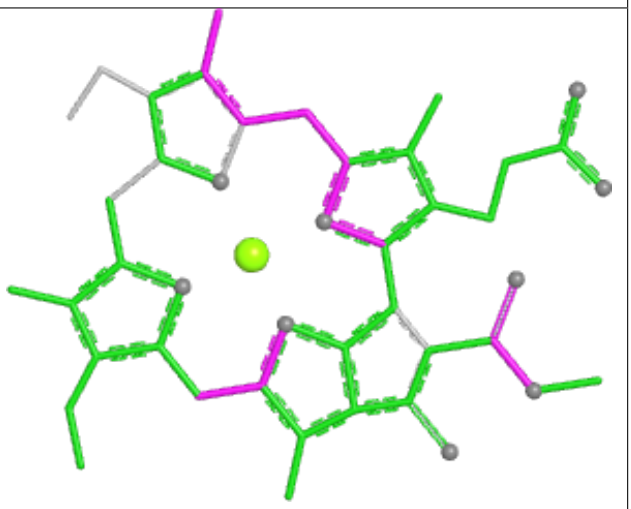
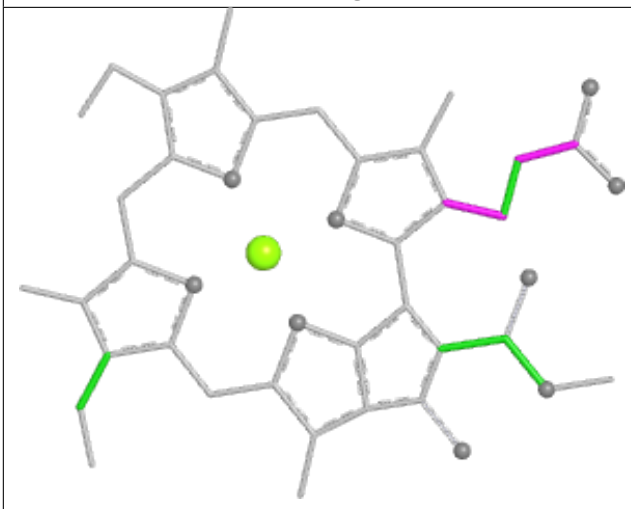
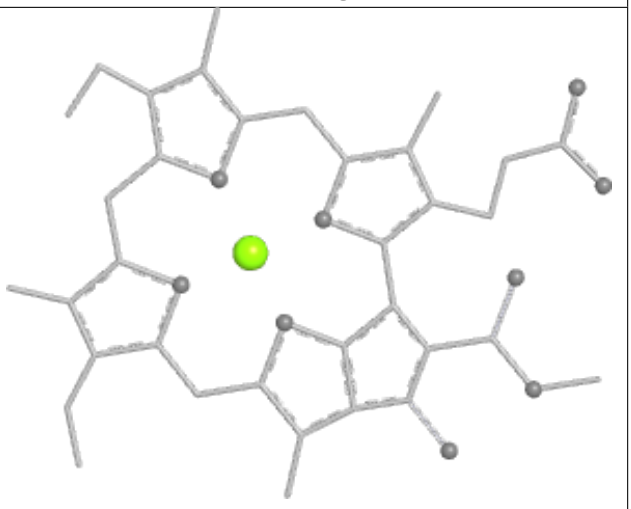


Bond angles

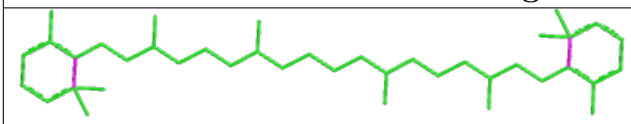


Torsions



Rings

Ligand BCR A 854



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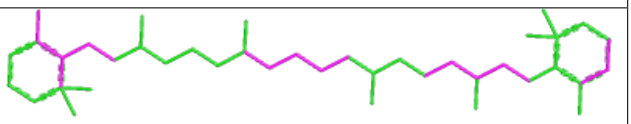
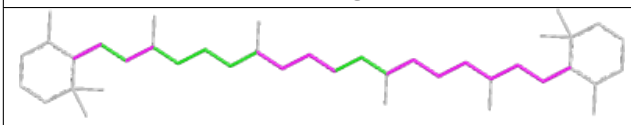
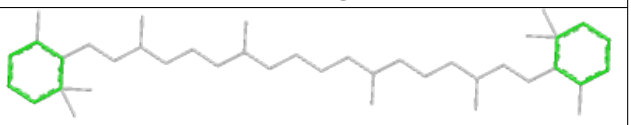


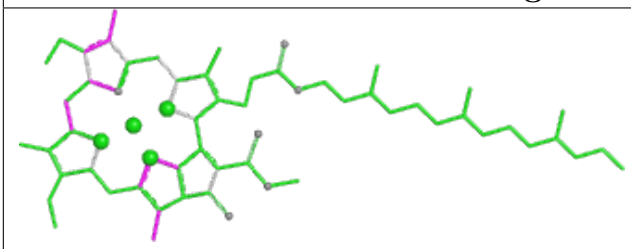
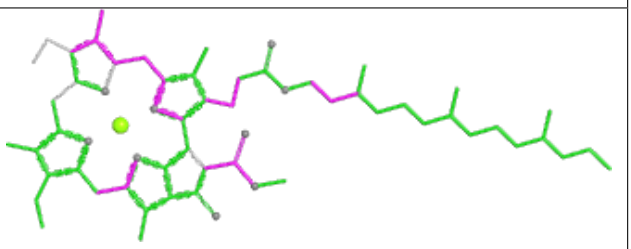
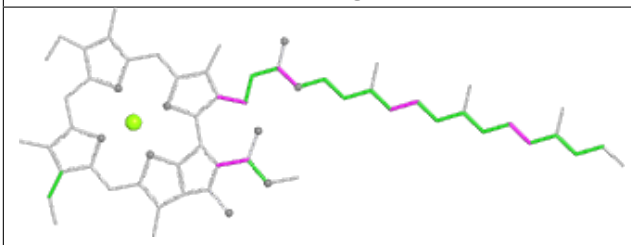
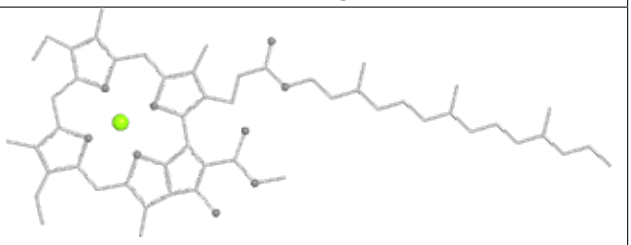
Bond angles

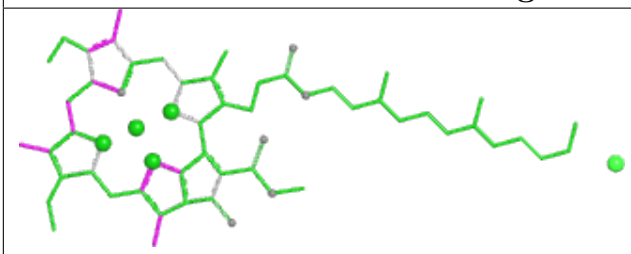
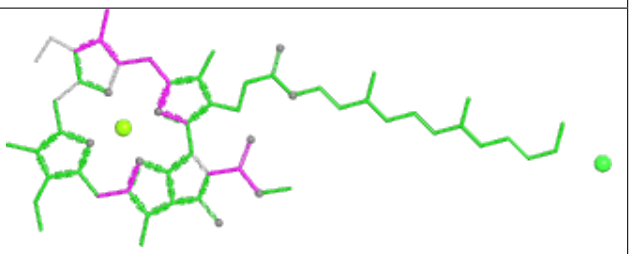
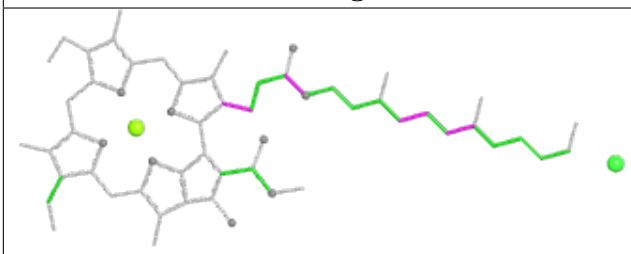
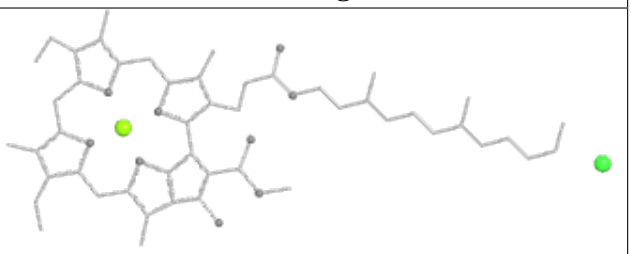


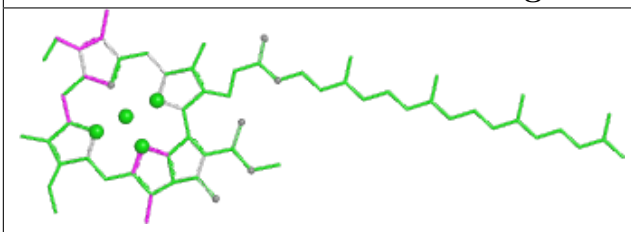
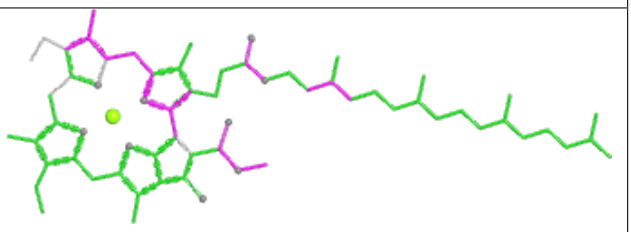
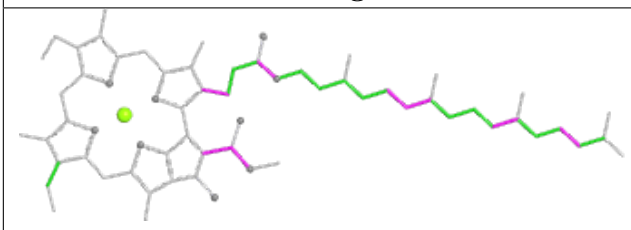
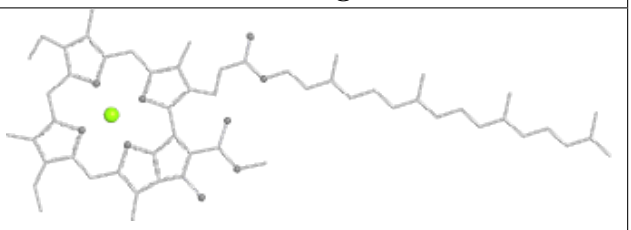
Torsions

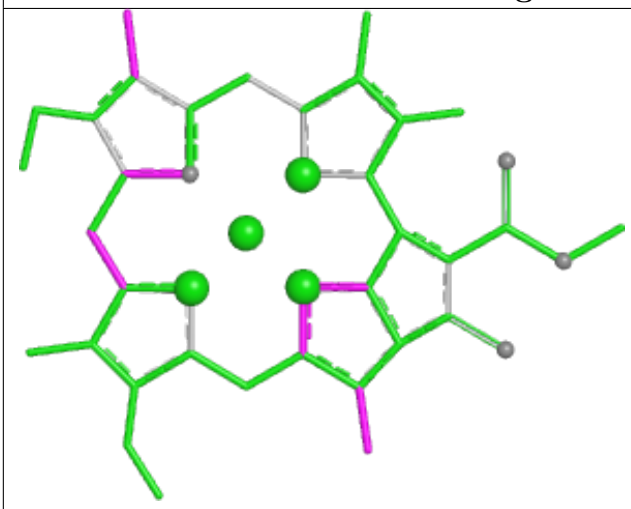
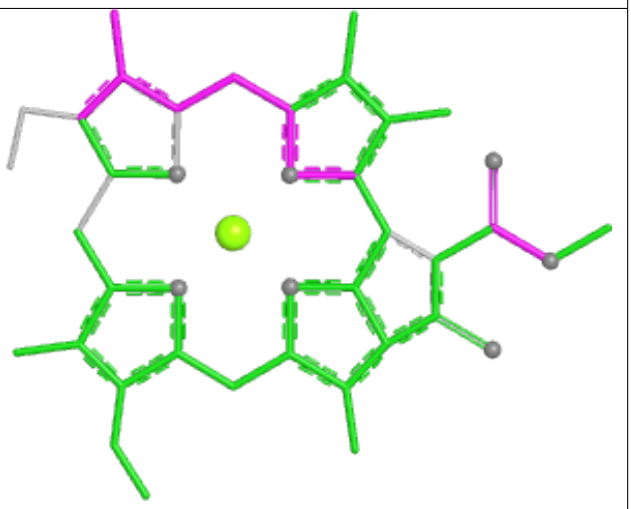
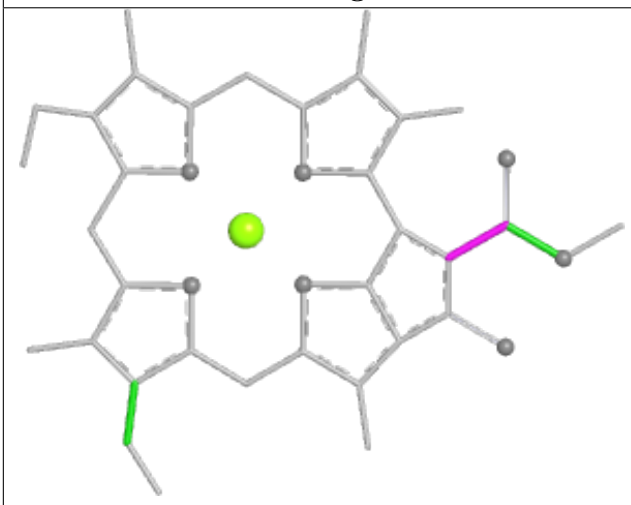
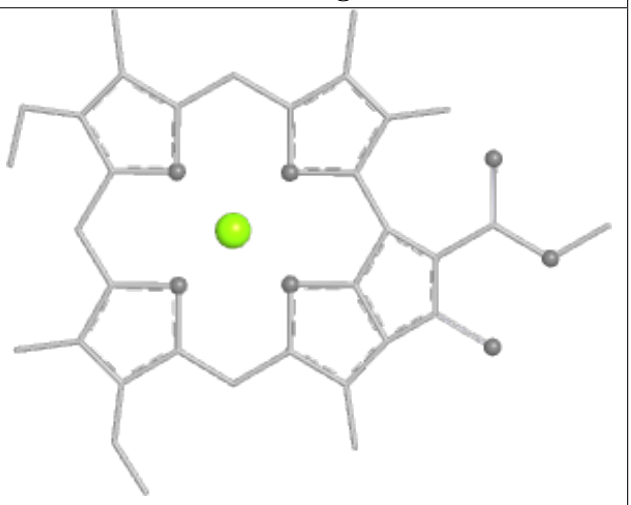


Rings

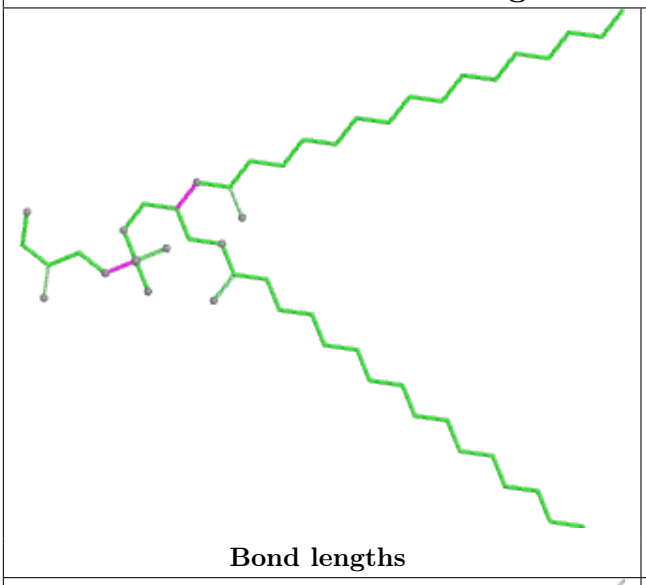
Ligand CLA B 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L2 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

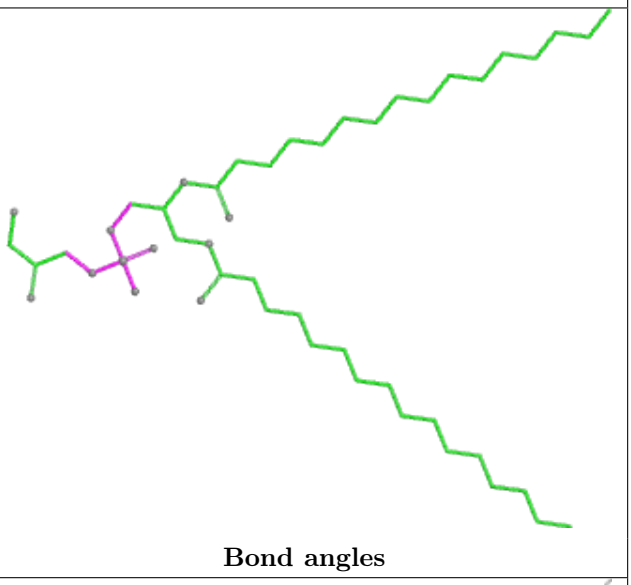
Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

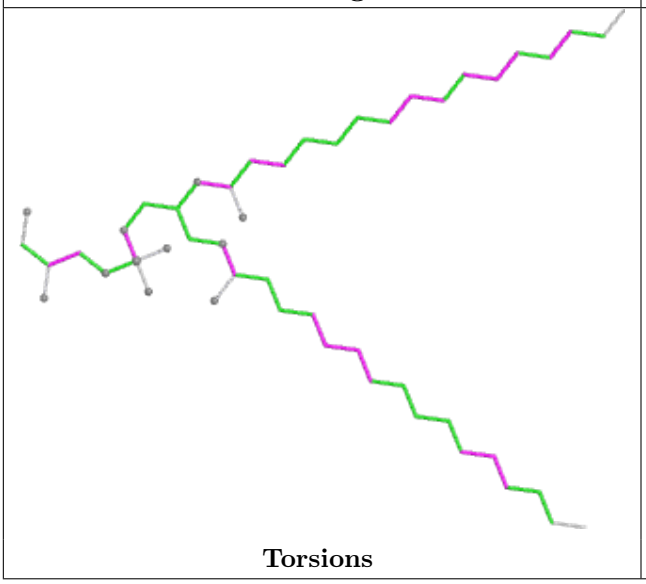
Ligand LHG AA 846



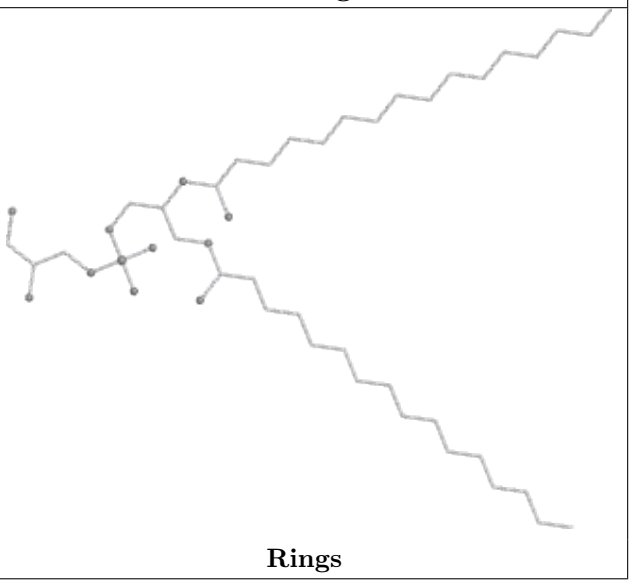
Bond lengths



Bond angles

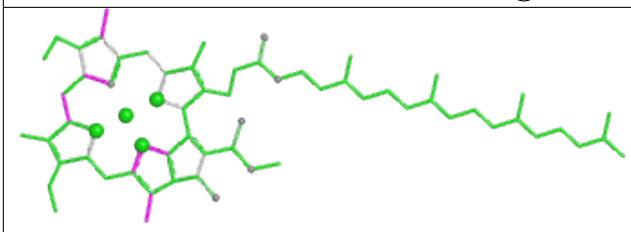


Torsions

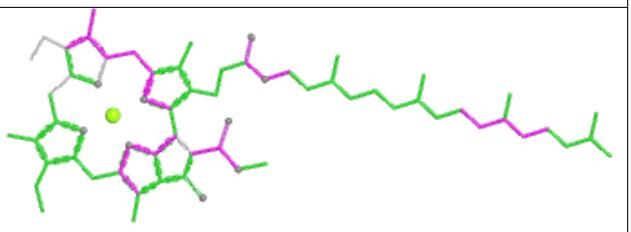


Rings

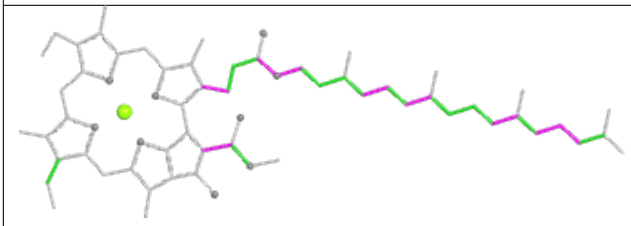
Ligand CLA B2 807



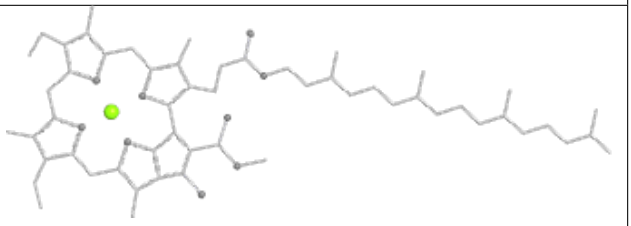
Bond lengths



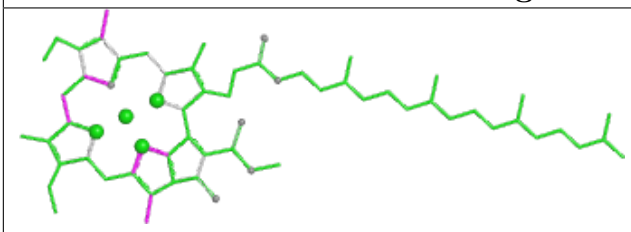
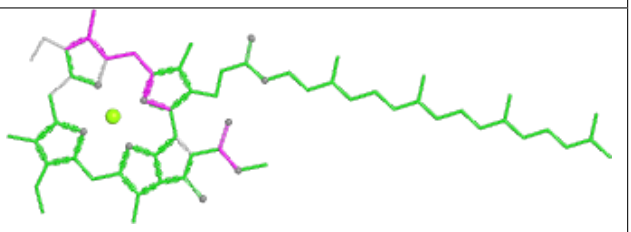
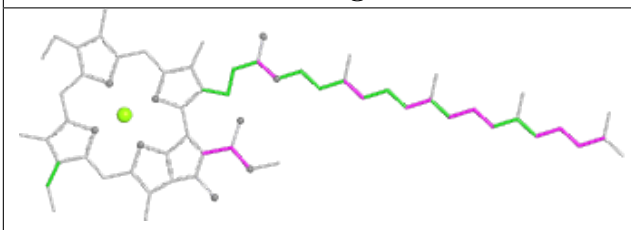
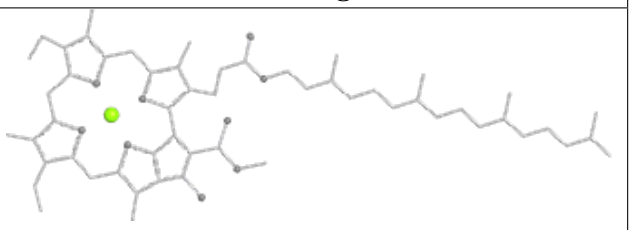
Bond angles

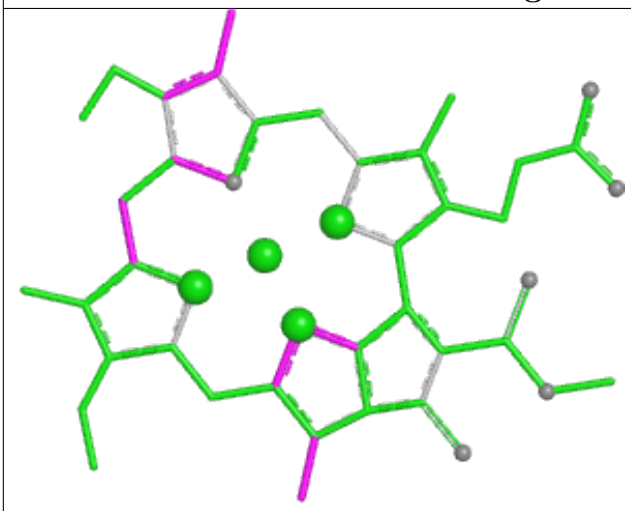
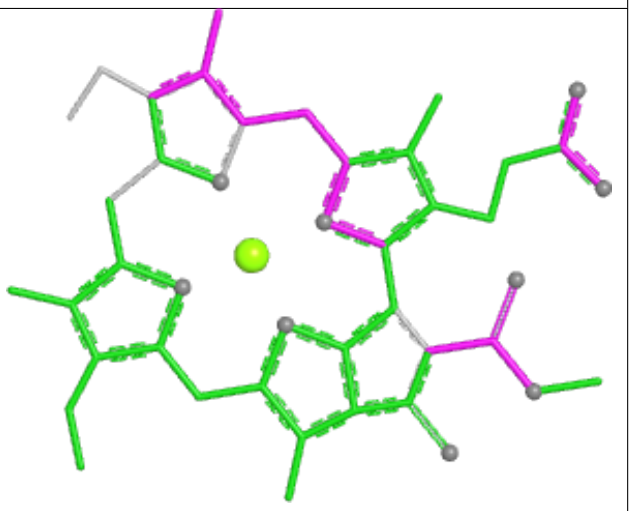
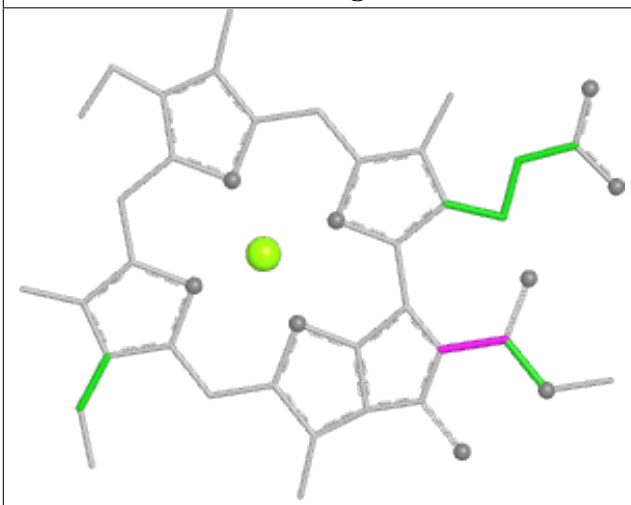
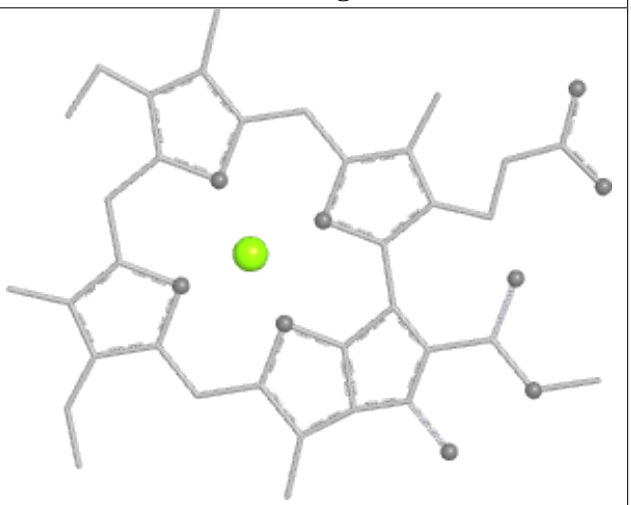


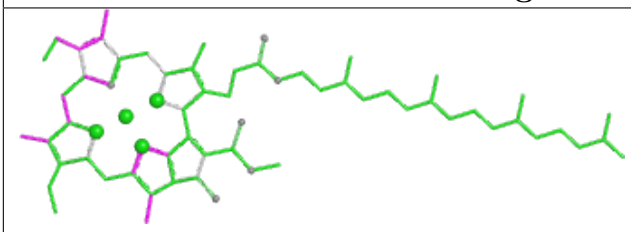
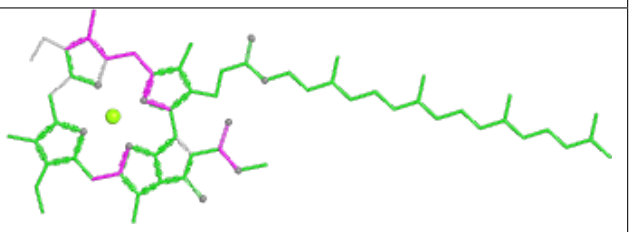
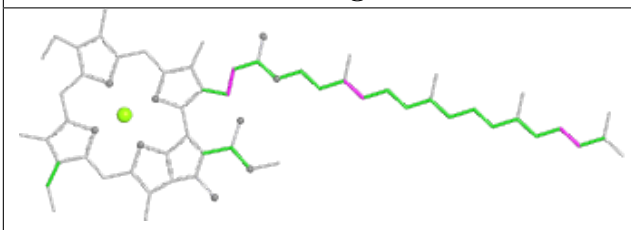
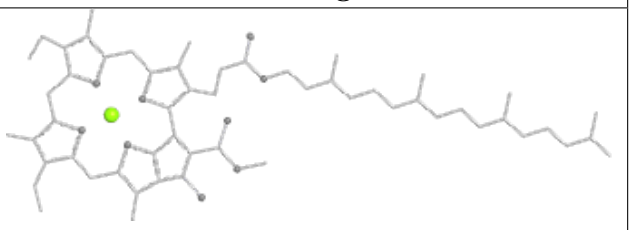
Torsions

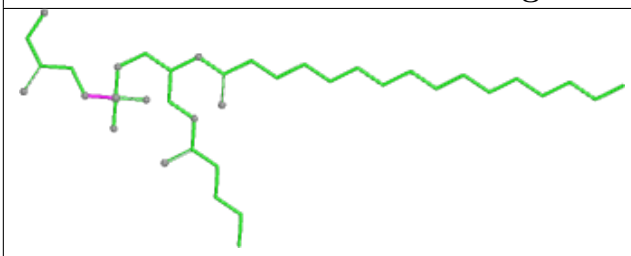
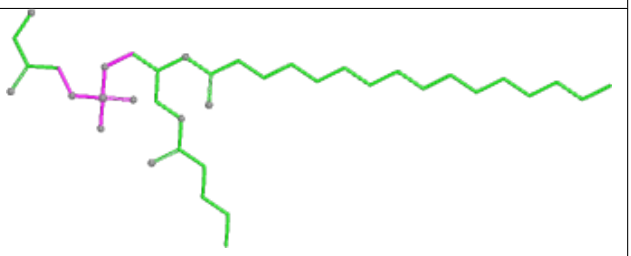
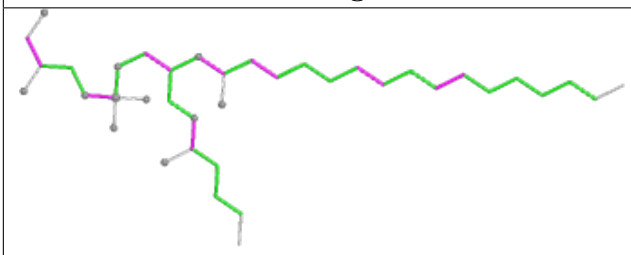
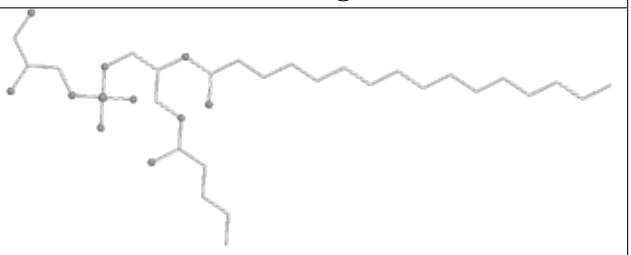


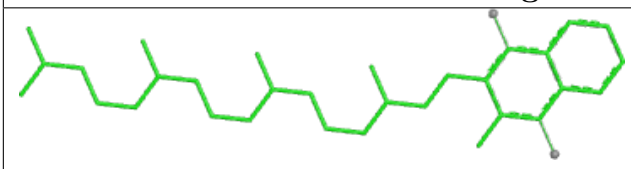
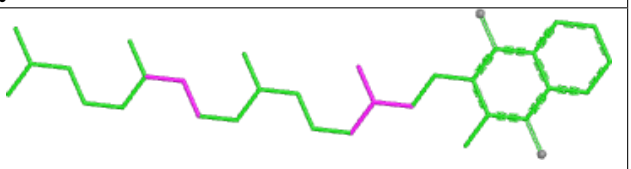
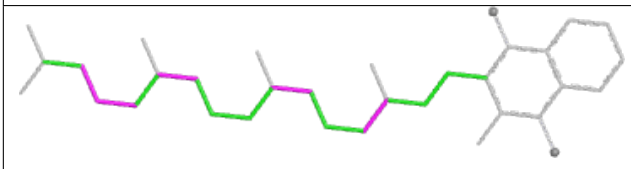
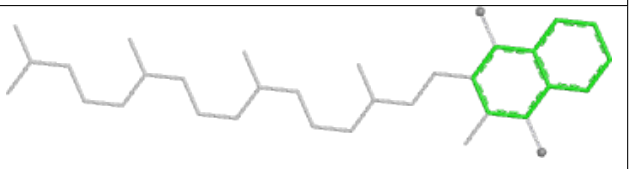
Rings

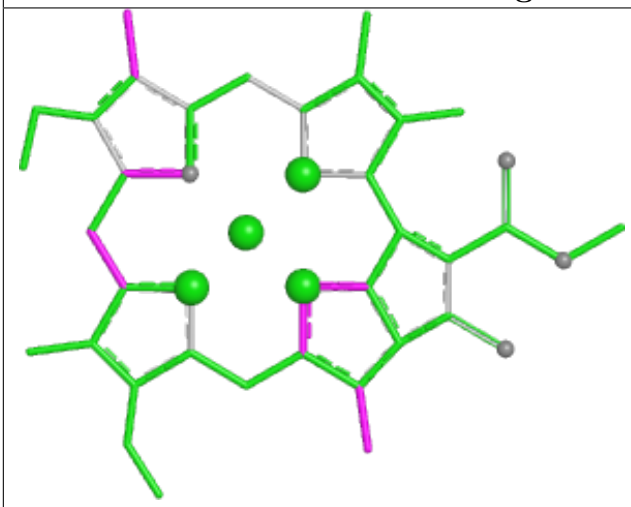
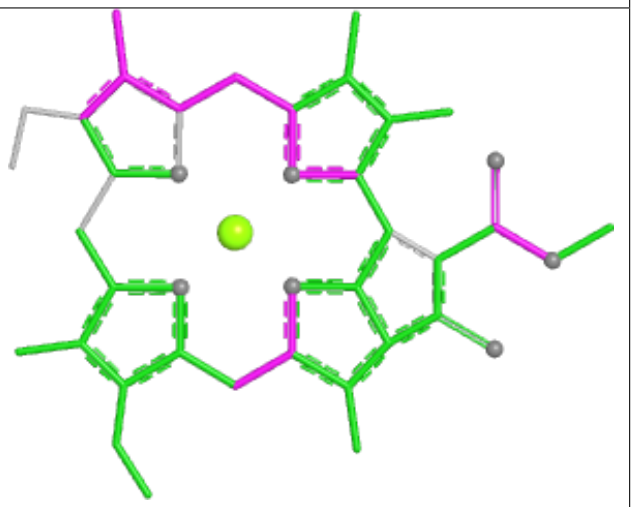
Ligand CLA B1 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PQN A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 812	
	
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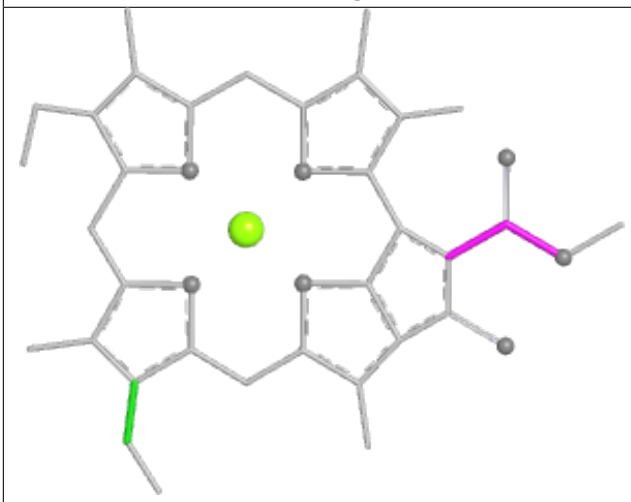
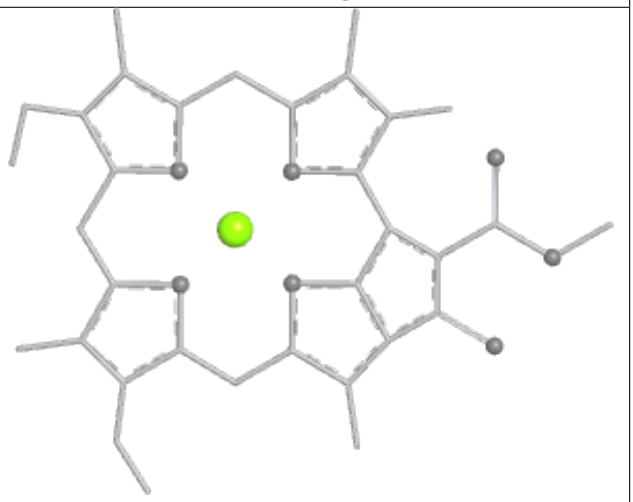
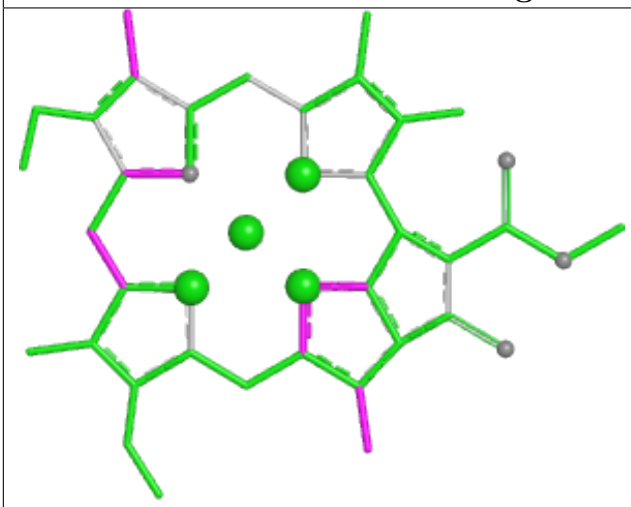
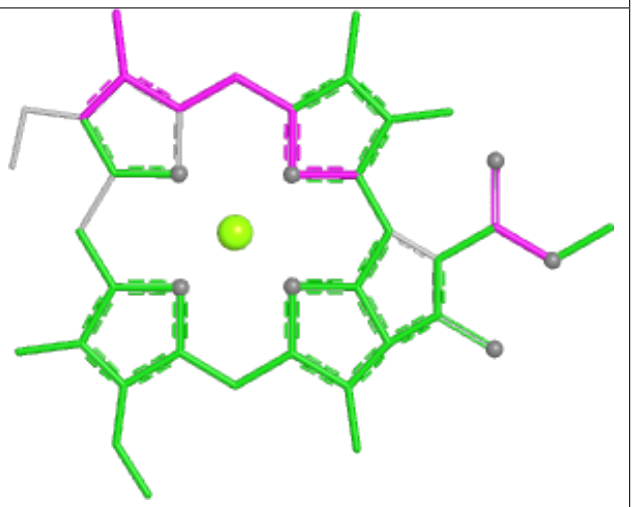
	
Torsions	**Rings**

Ligand CLA B1 818	
	
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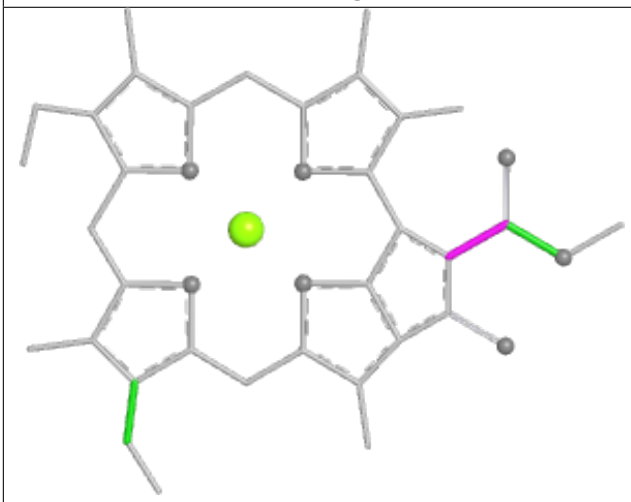
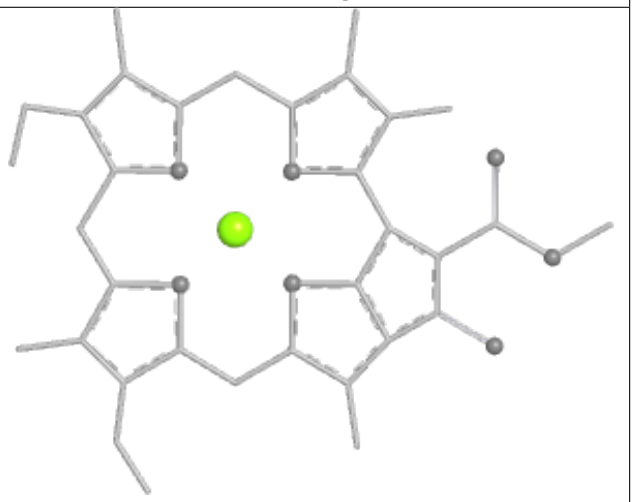
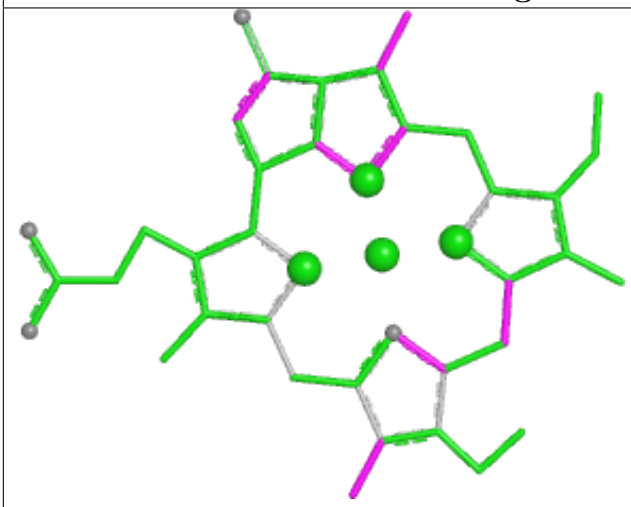
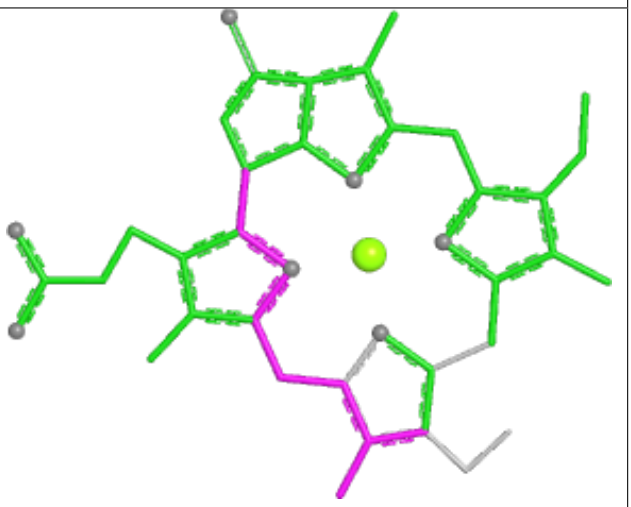
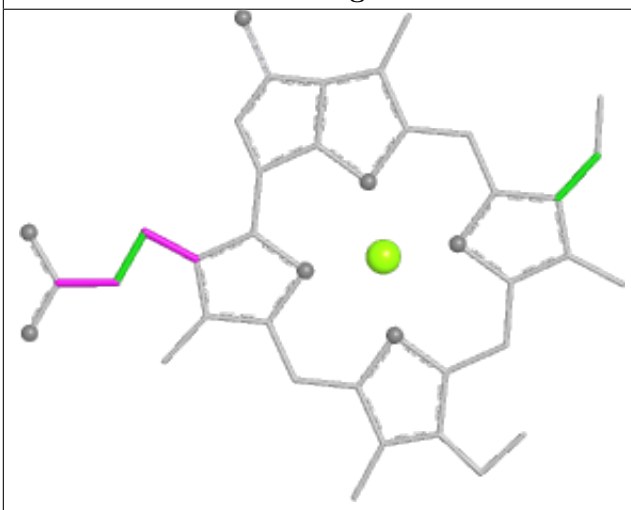
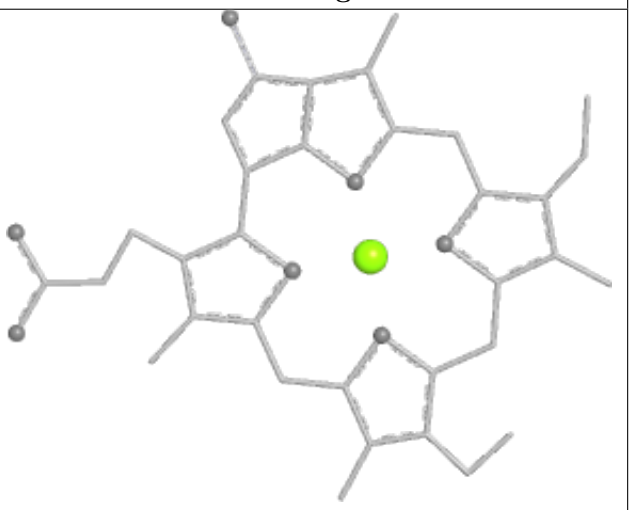
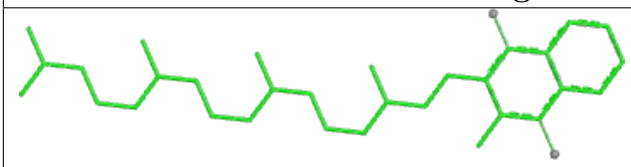
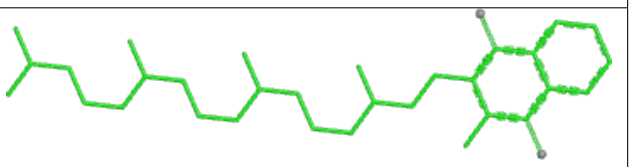
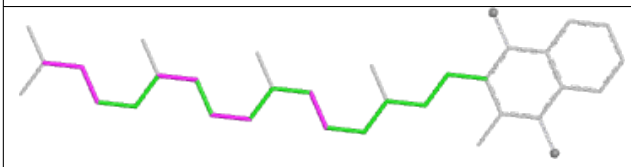
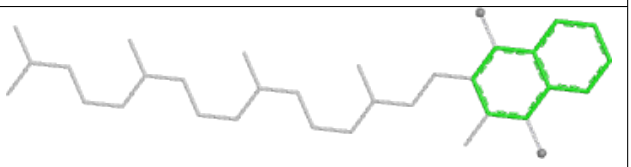
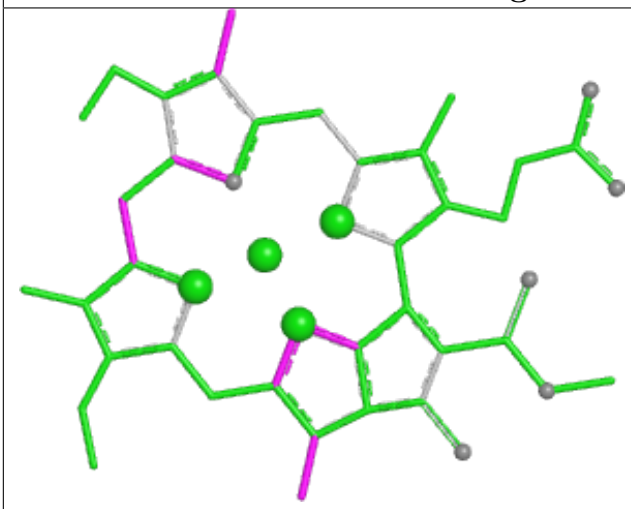
	
Torsions	**Rings**

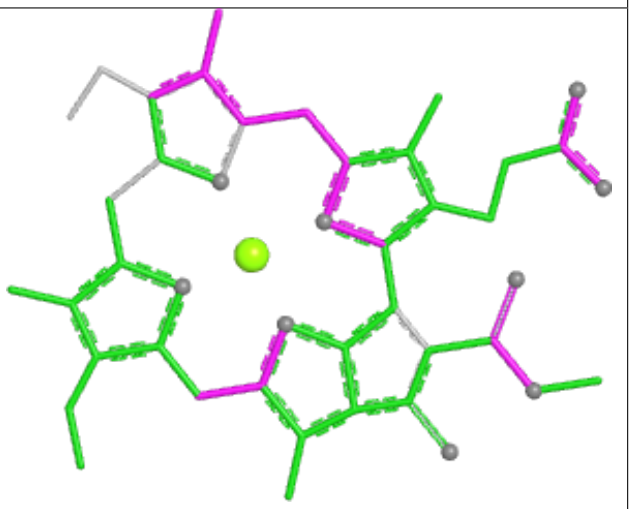
Ligand CLA K2 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN B1 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

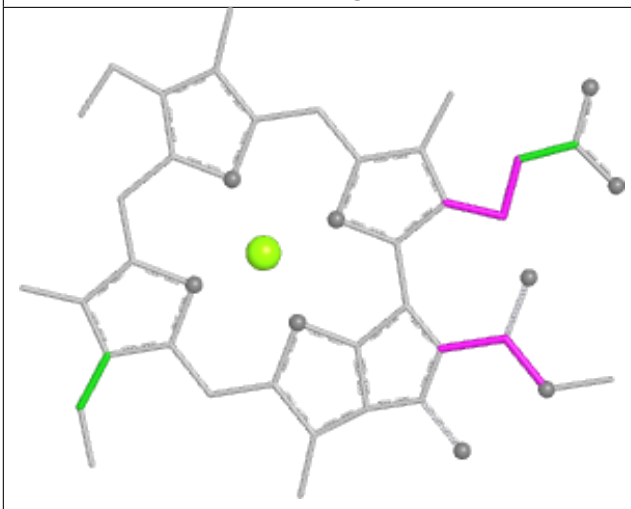
Ligand CLA AA 824



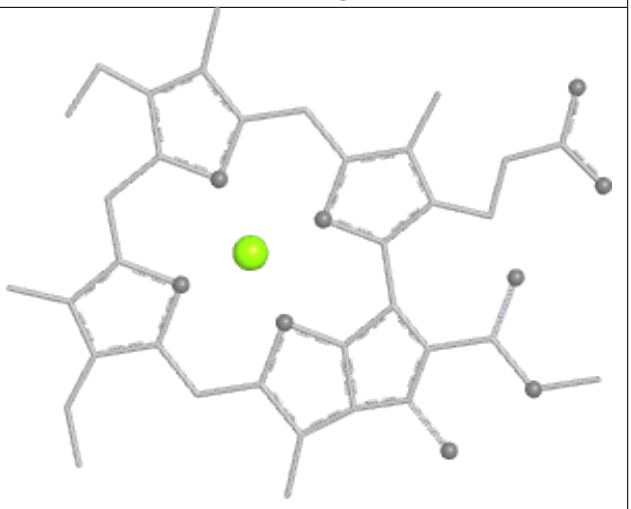
Bond lengths



Bond angles

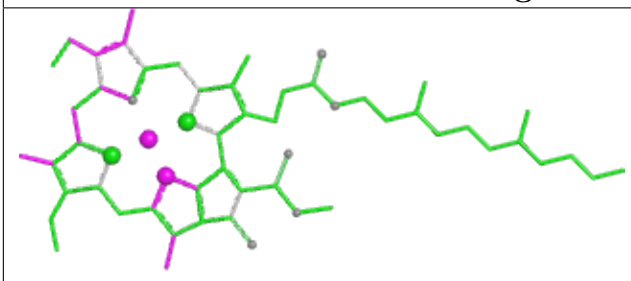


Torsions

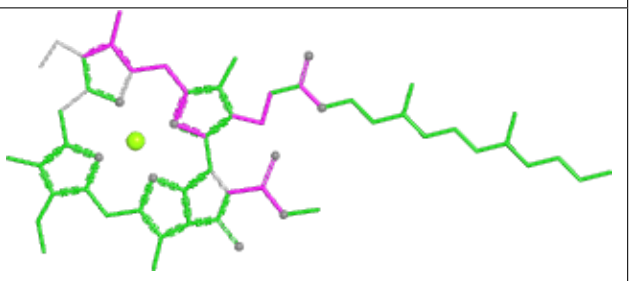


Rings

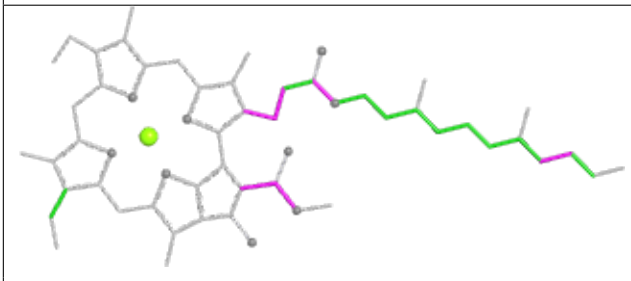
Ligand CLA A2 820



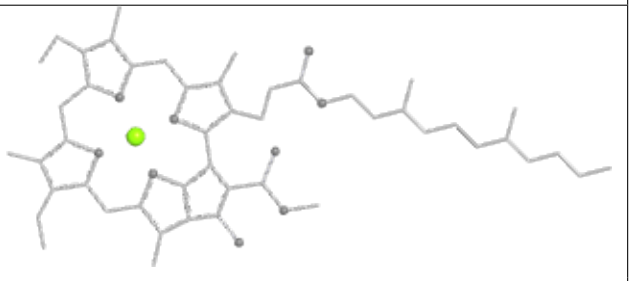
Bond lengths



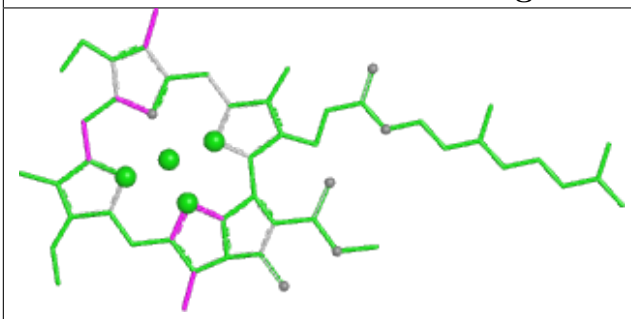
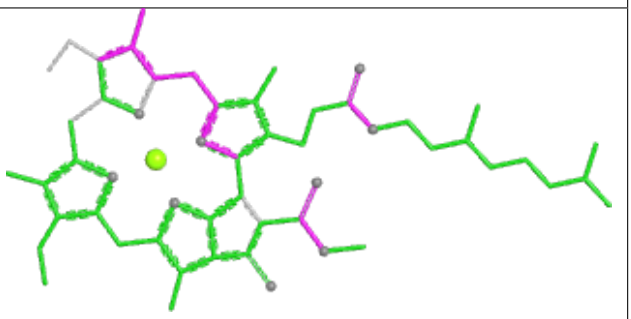
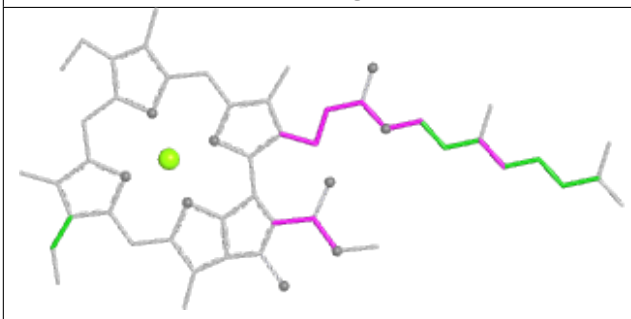
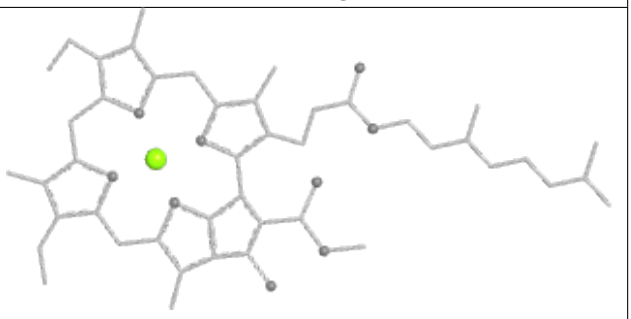
Bond angles

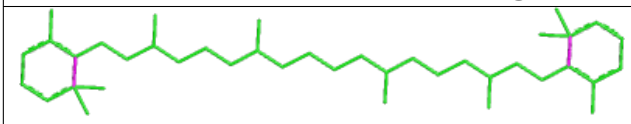
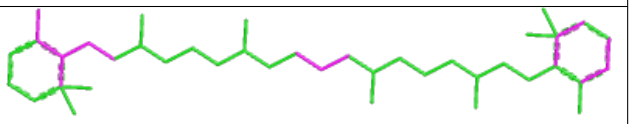
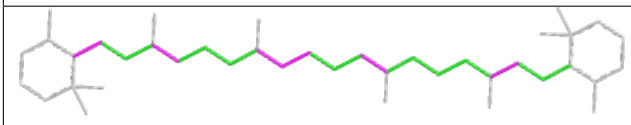
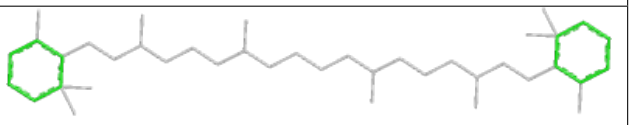


Torsions

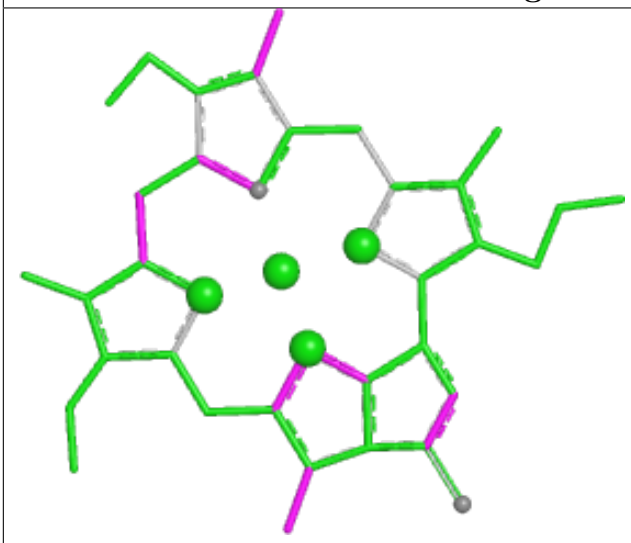


Rings

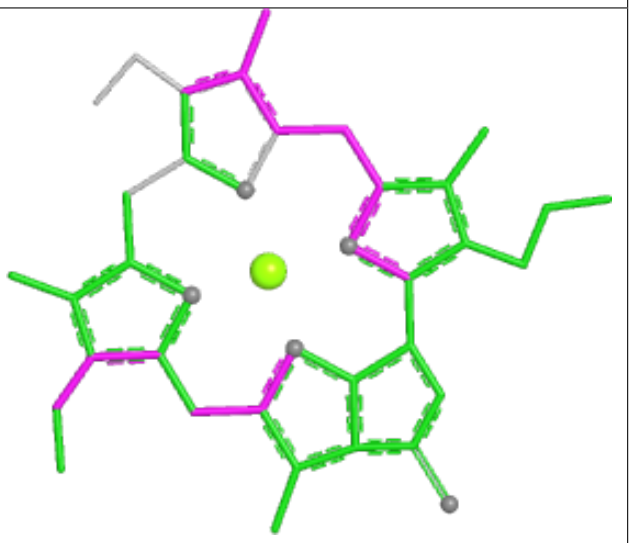
Ligand CLA B2 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BB 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

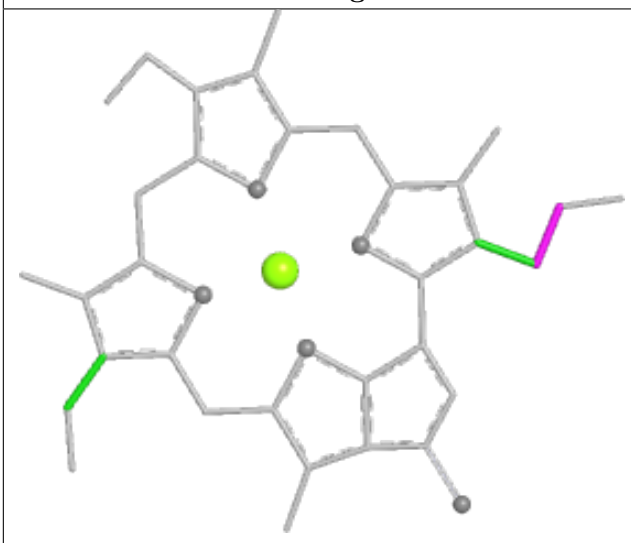
Ligand CLA B 846



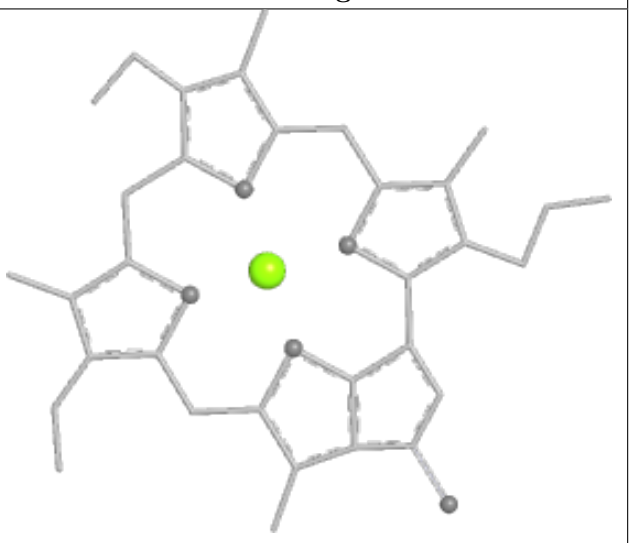
Bond lengths



Bond angles

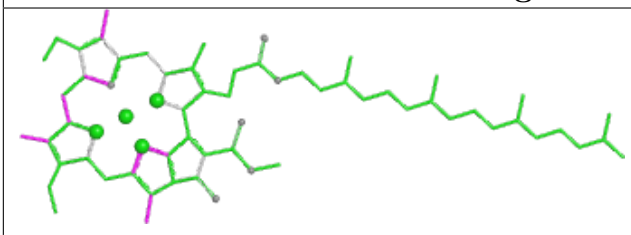


Torsions

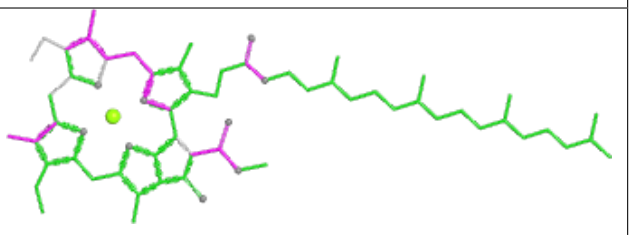


Rings

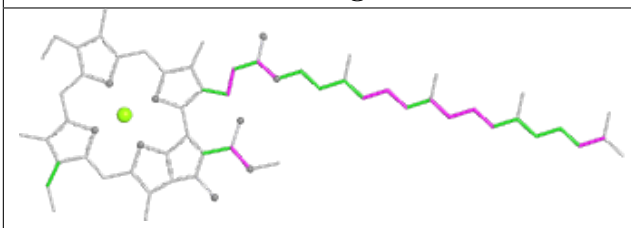
Ligand CLA A1 801



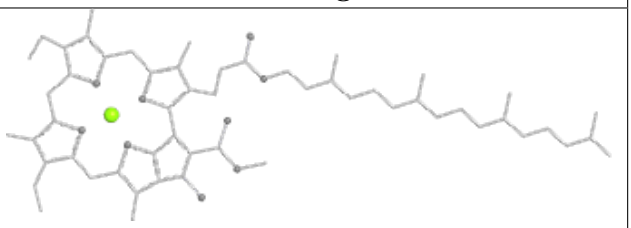
Bond lengths



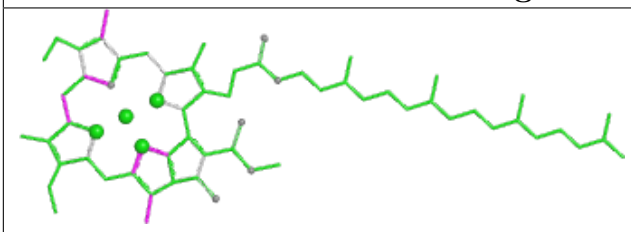
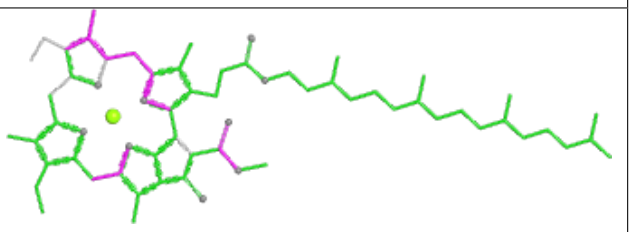
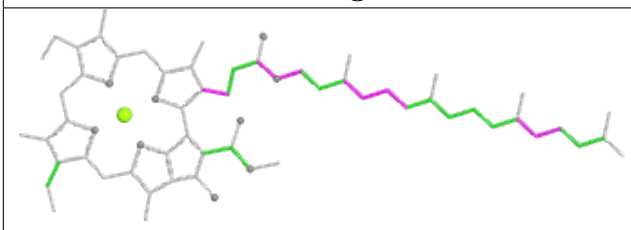
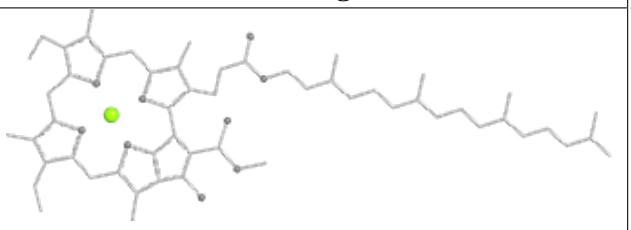
Bond angles

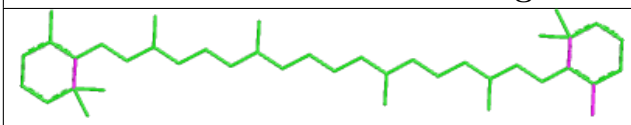
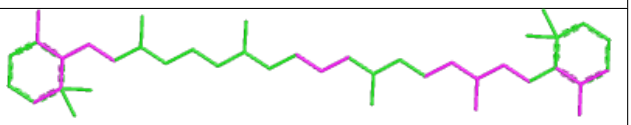
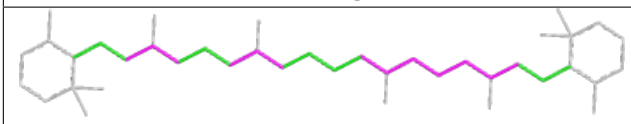
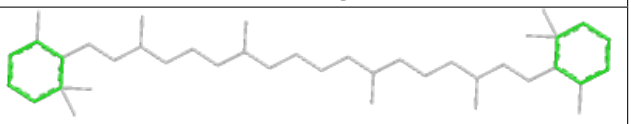


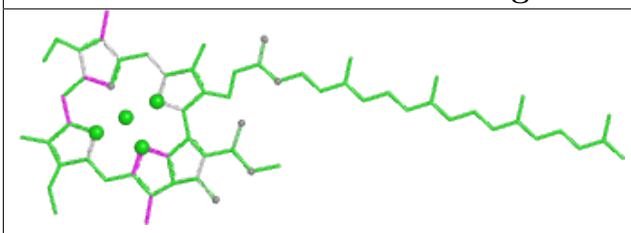
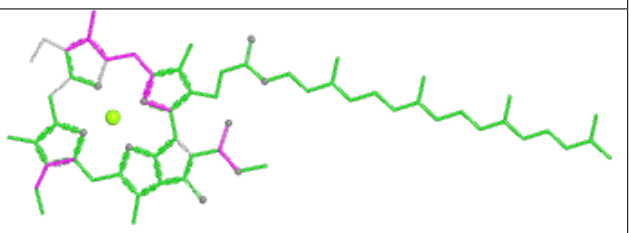
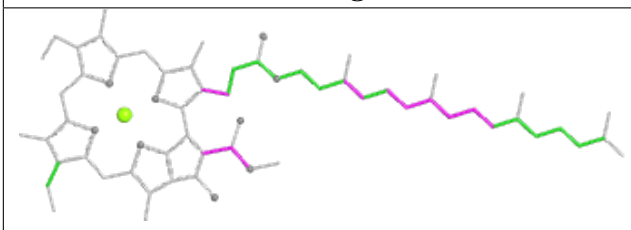
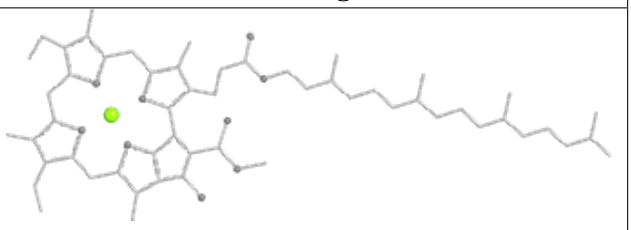
Torsions

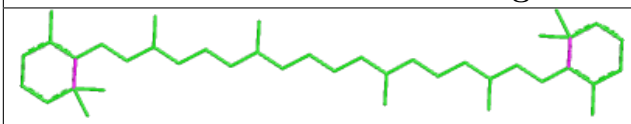
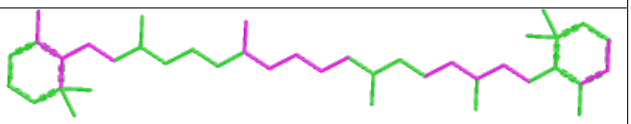
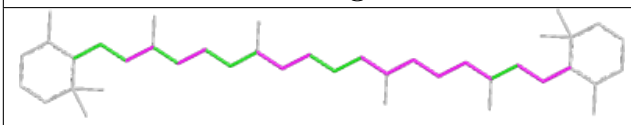
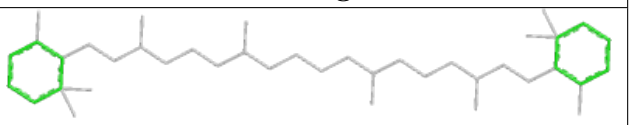


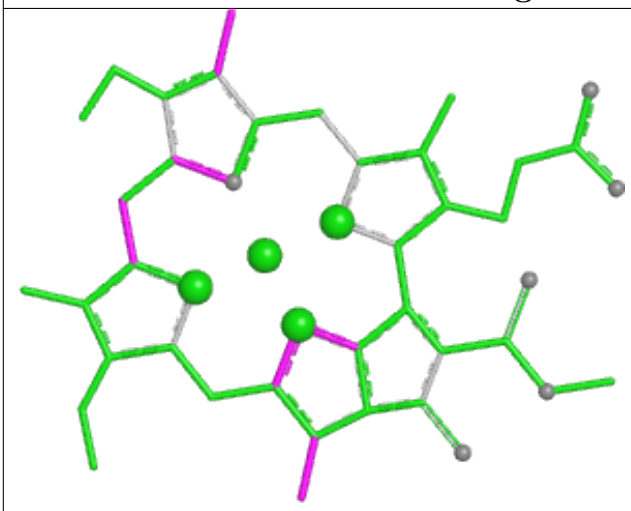
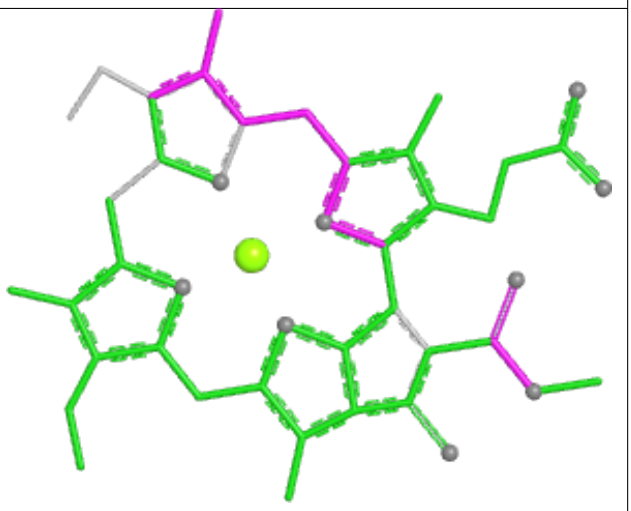
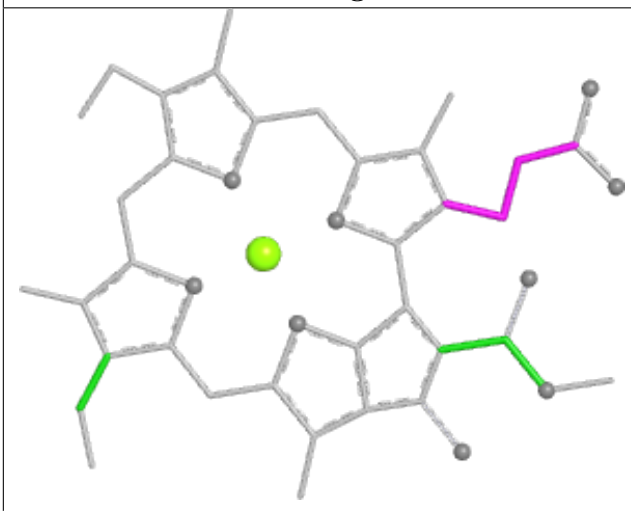
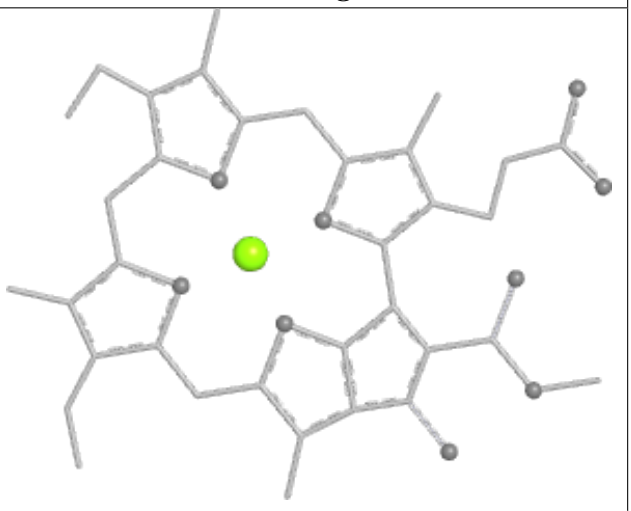
Rings

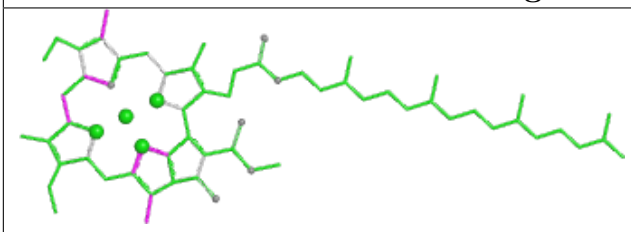
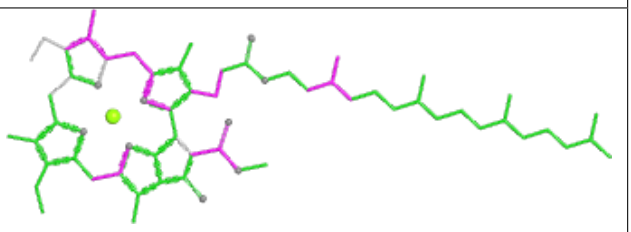
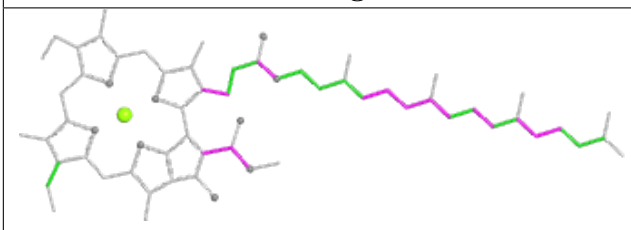
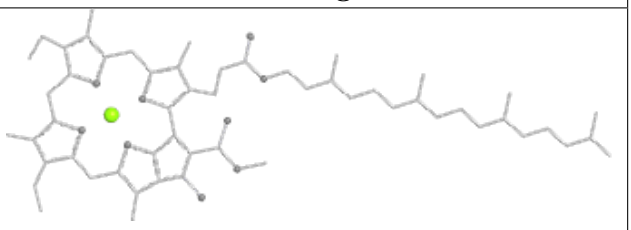
Ligand CLA FF 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

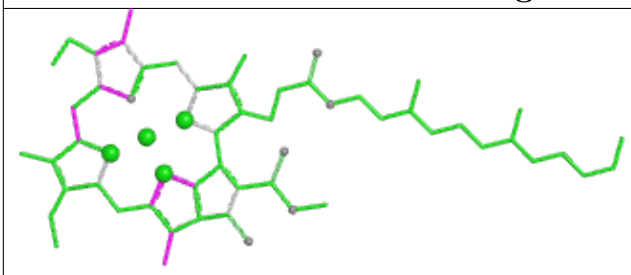
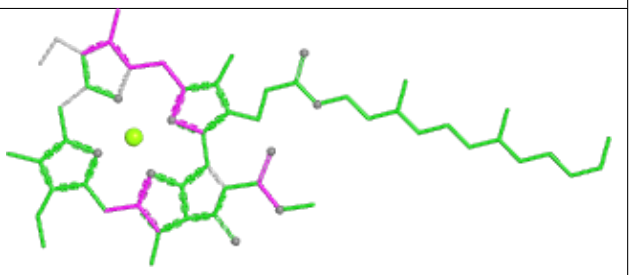
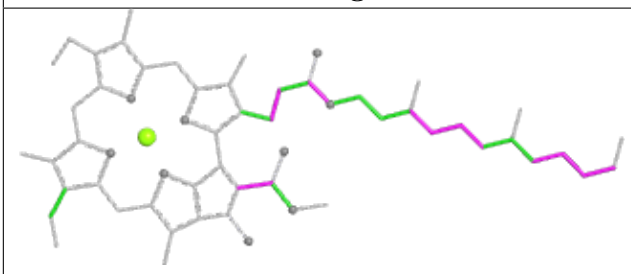
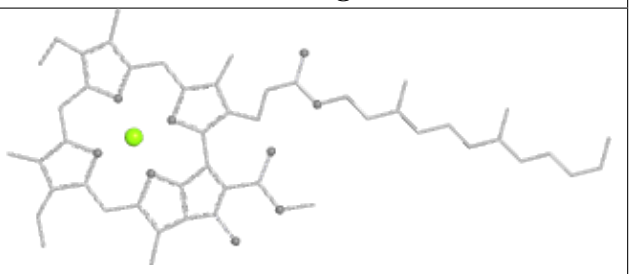
Ligand BCR F1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

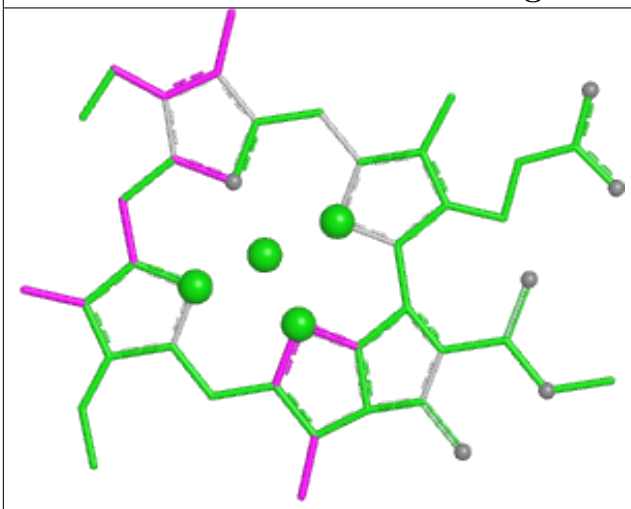
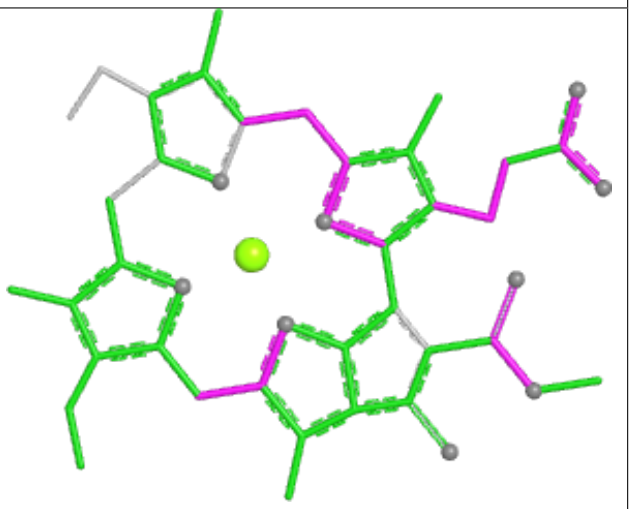
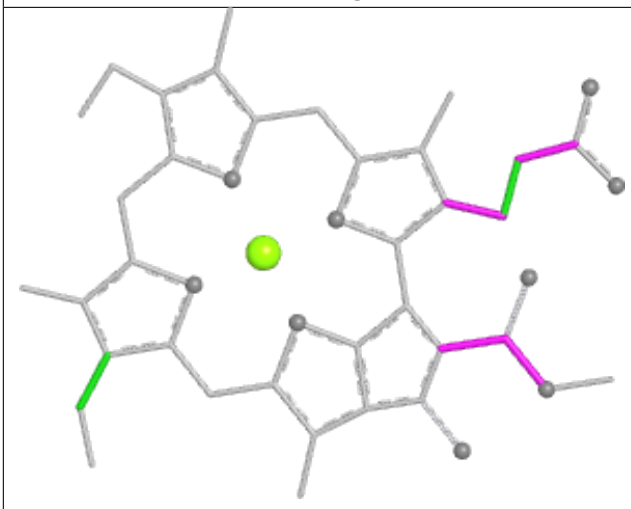
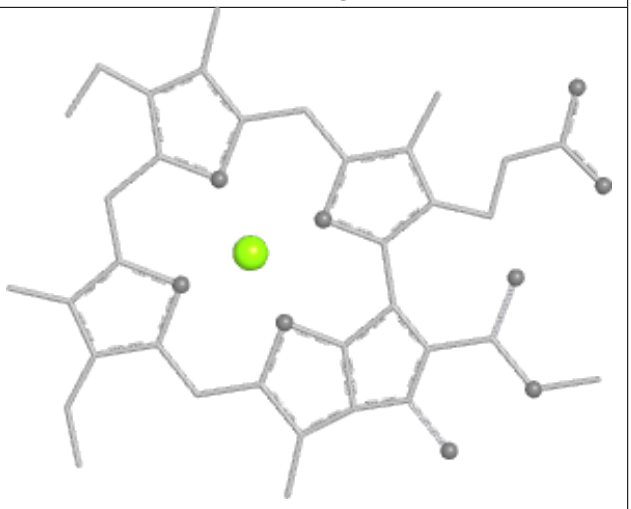
Ligand CLA BB 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

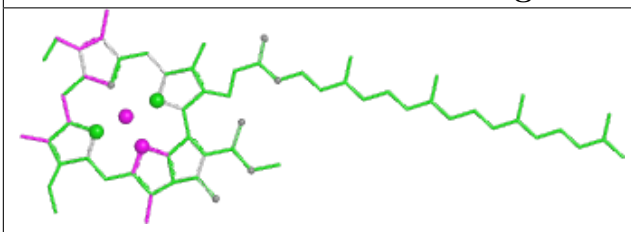
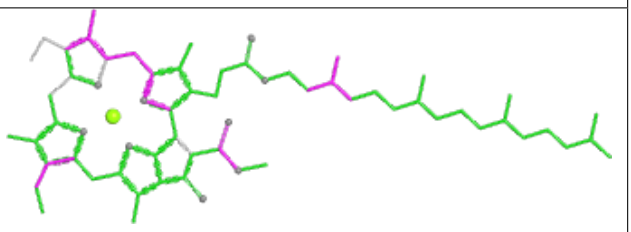
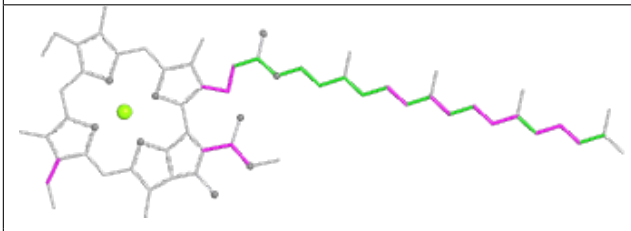
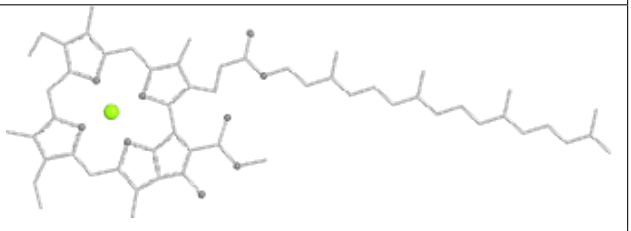
Ligand BCR K2 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

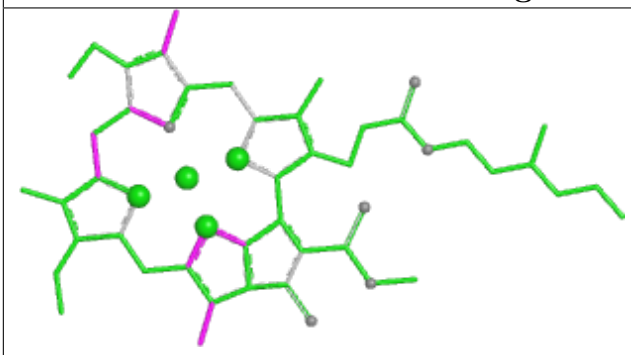
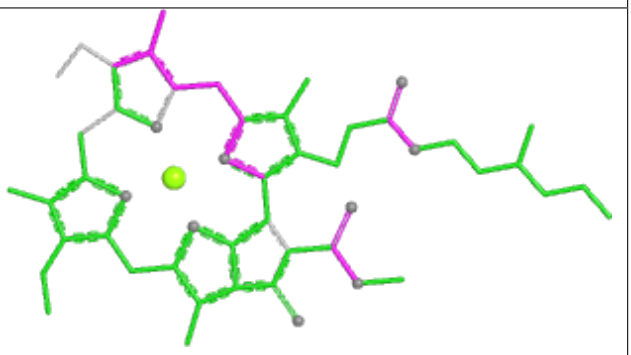
Ligand CLA X1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 838	
	
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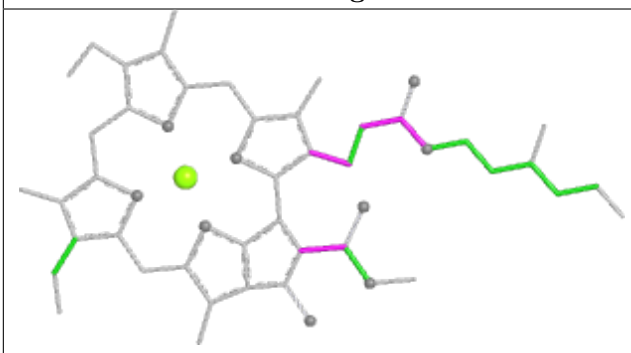	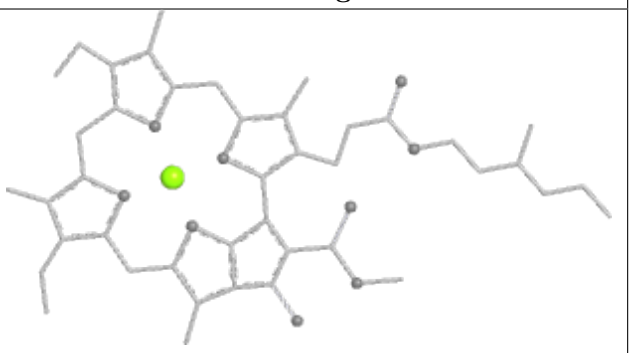
Torsions	**Rings**

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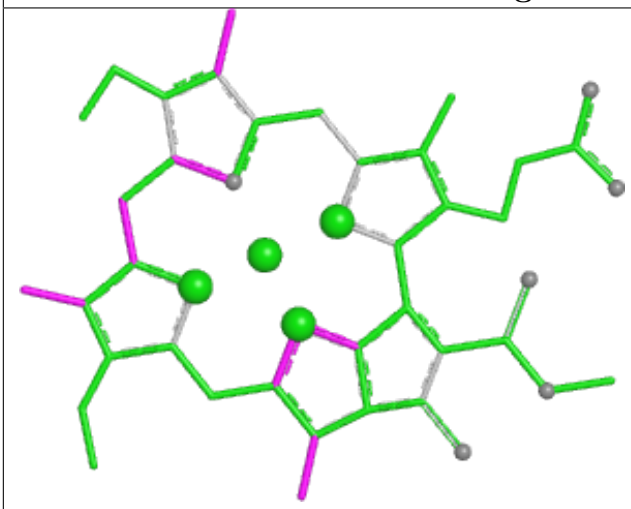
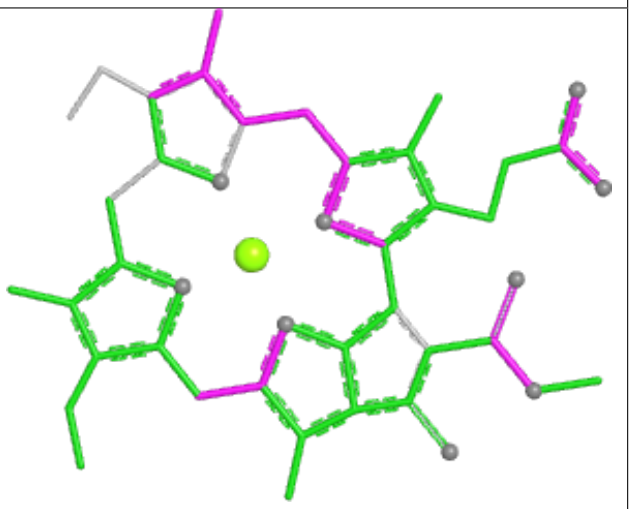
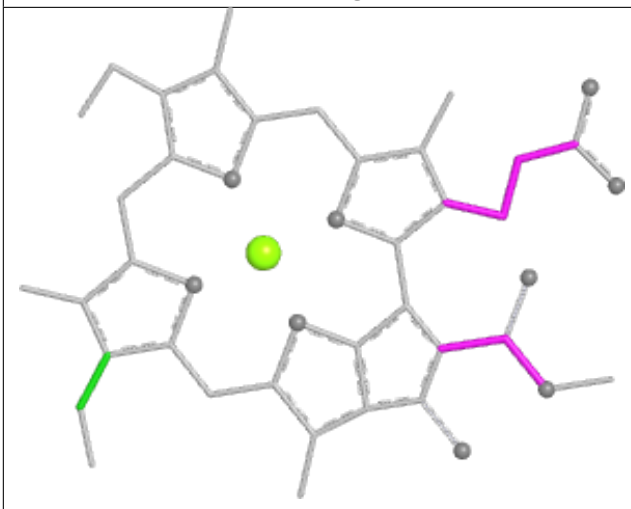
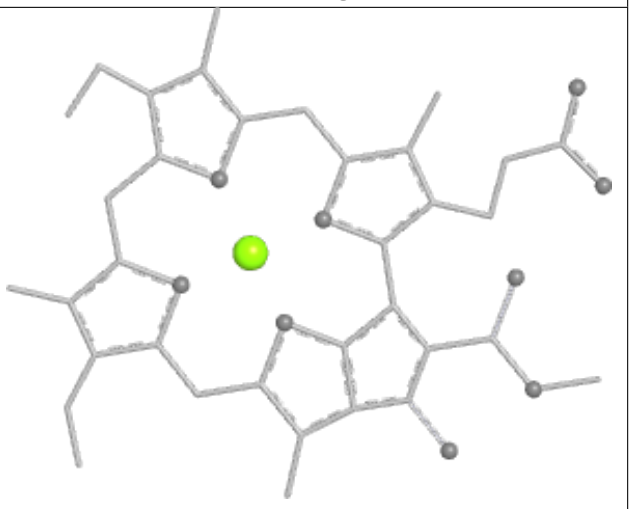
	
Bond lengths	Bond angles
	
Torsions	Rings

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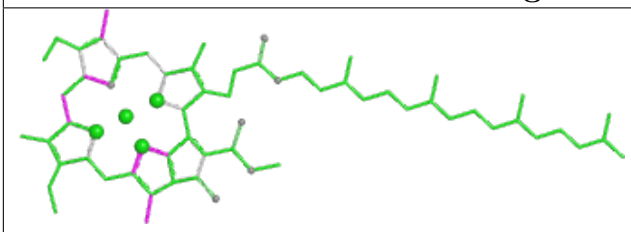
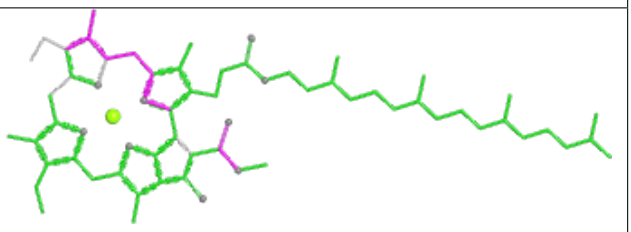
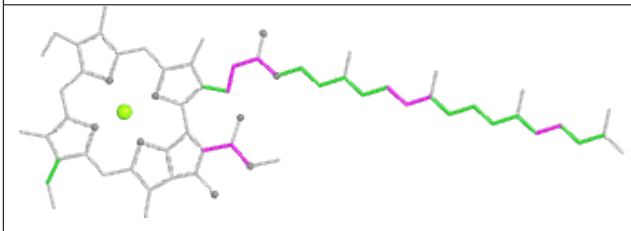
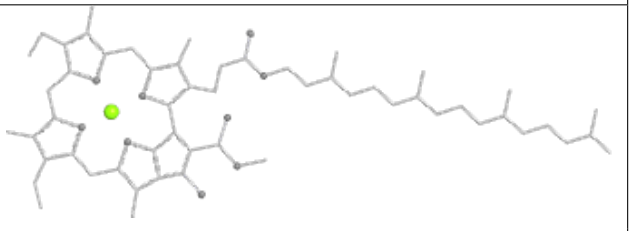
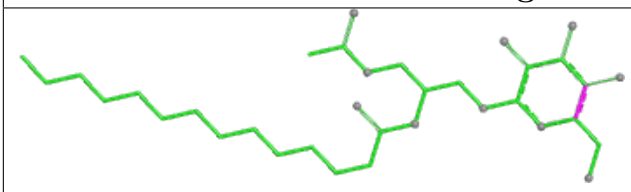
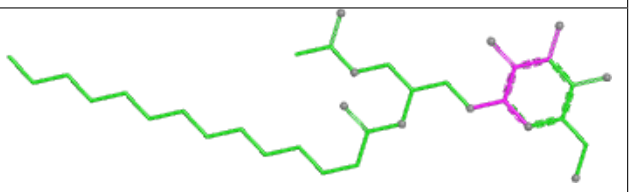
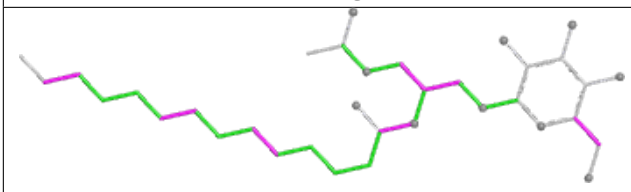
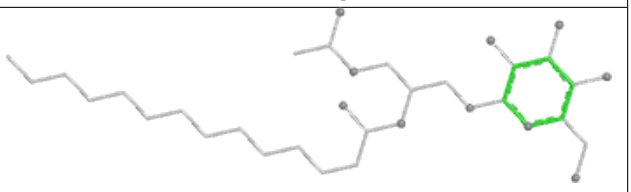
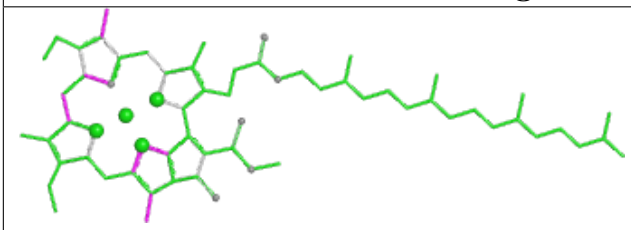
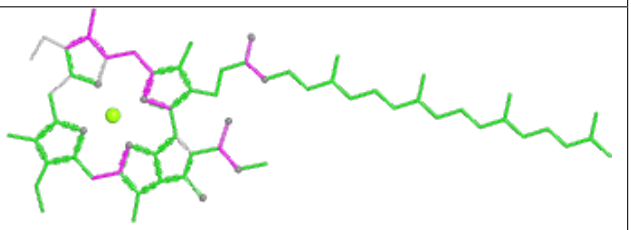
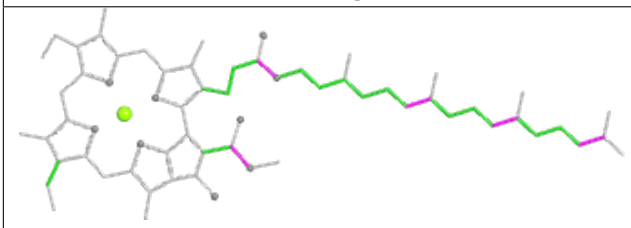
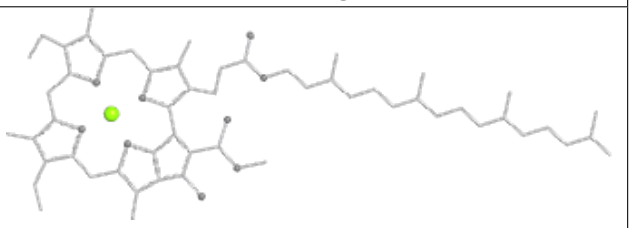
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG I2 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

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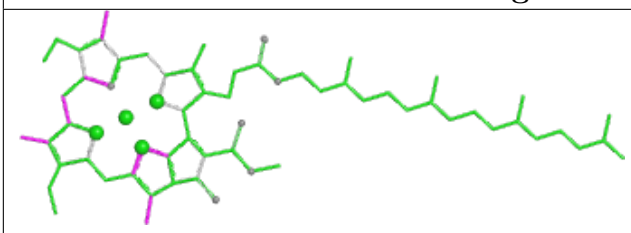
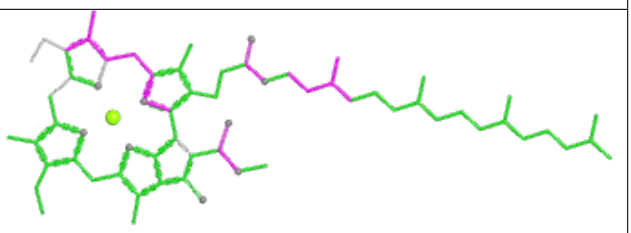
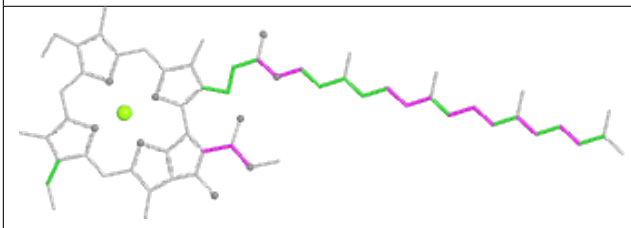
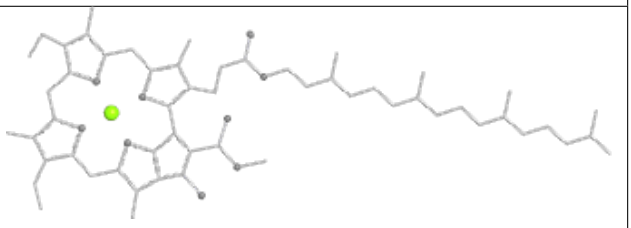
 Bond lengths	 Bond angles
 Torsions	 Rings

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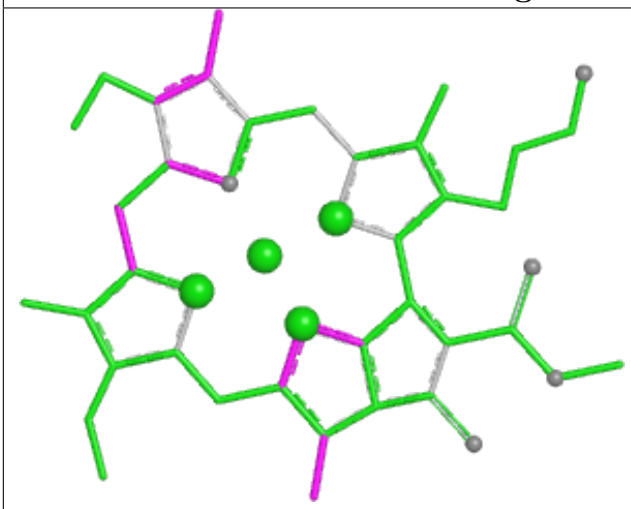
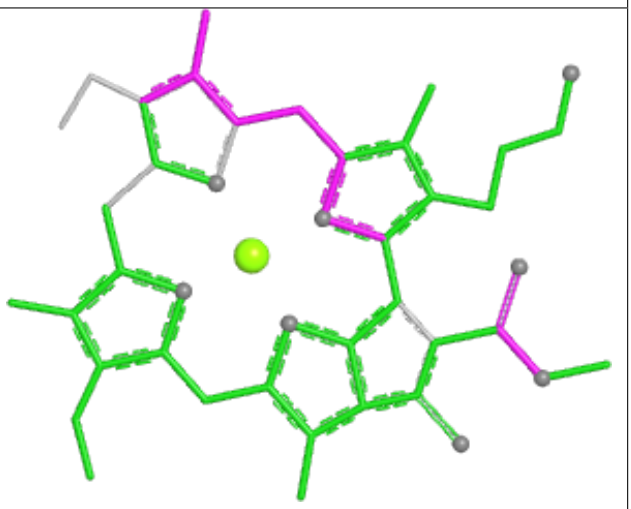
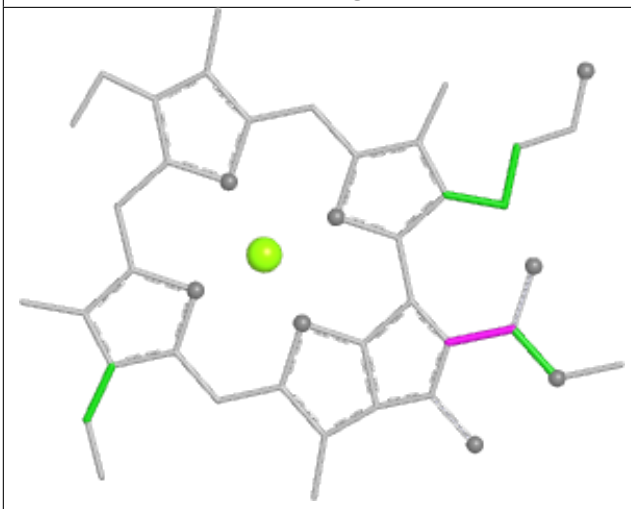
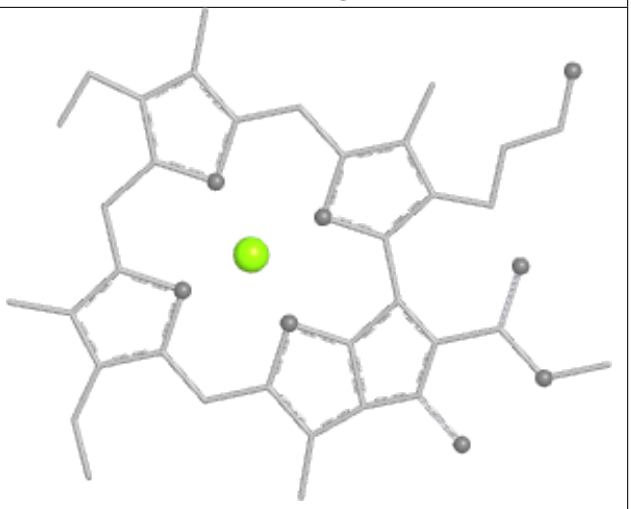
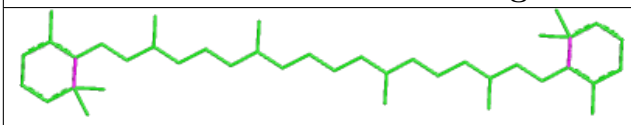
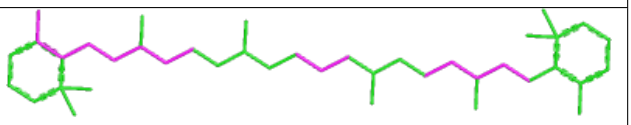
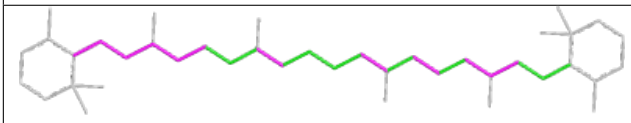
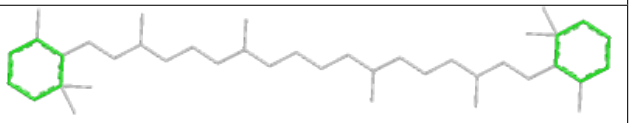
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BB 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

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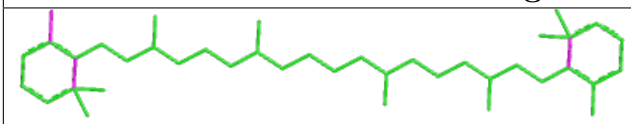
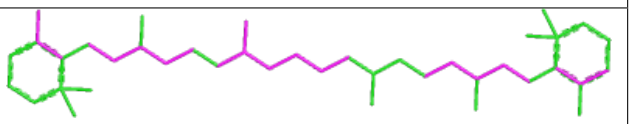
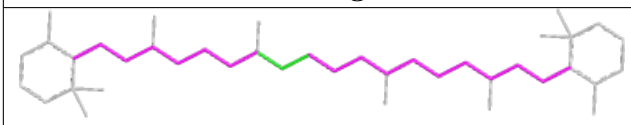
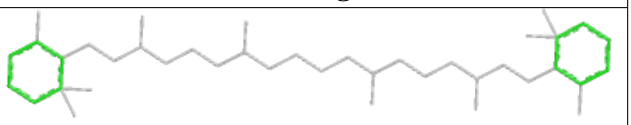
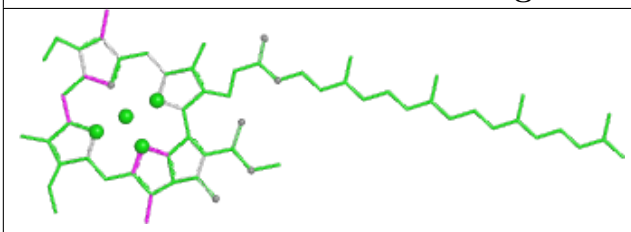
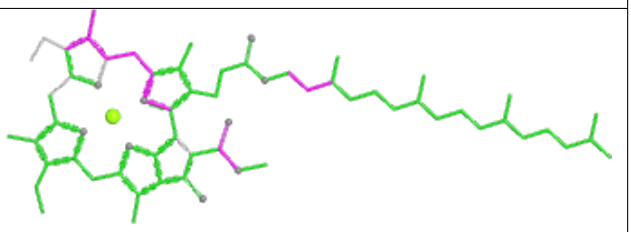
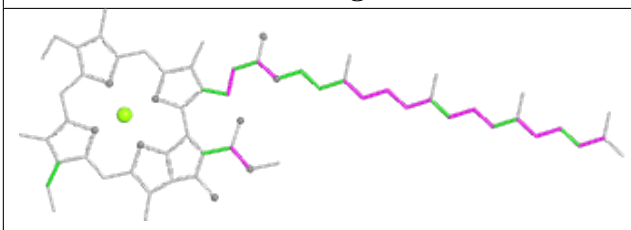
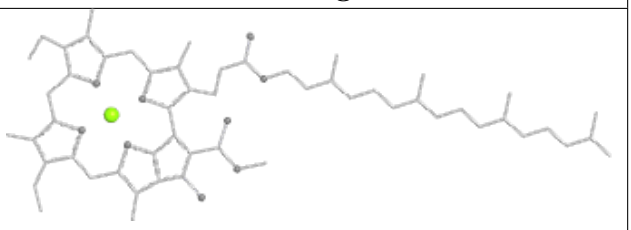
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

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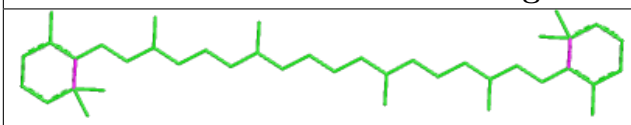
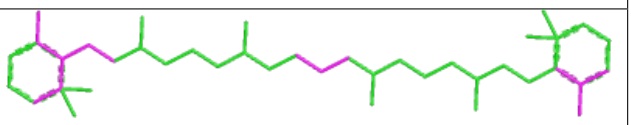
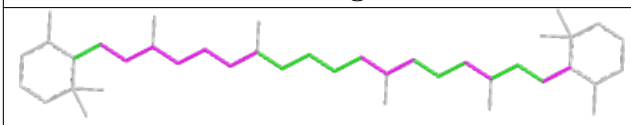
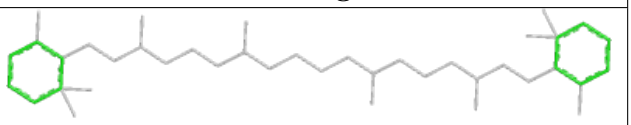
	
Bond lengths	Bond angles
	
Torsions	Rings

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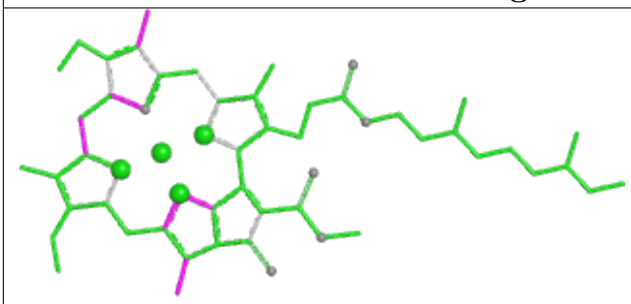
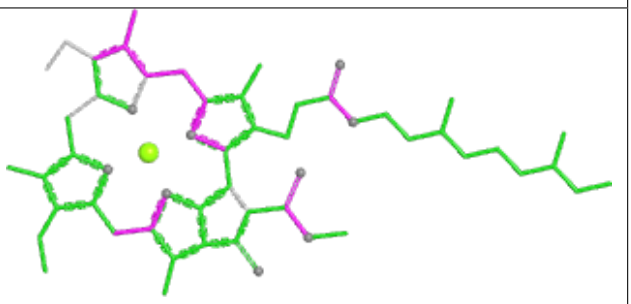
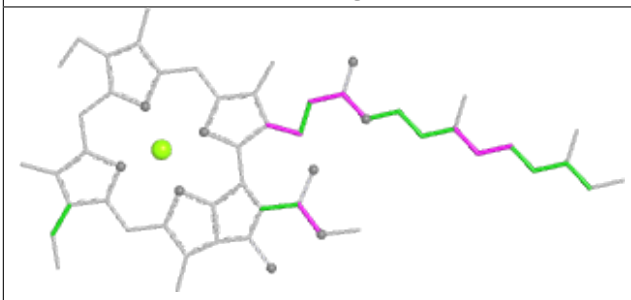
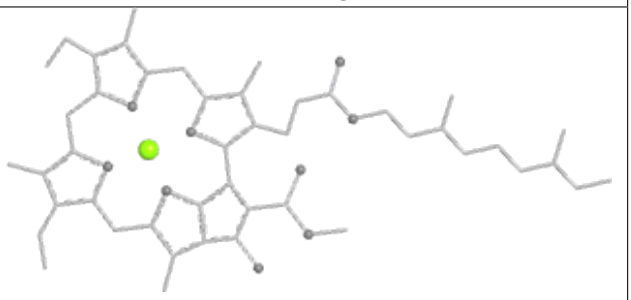
	
Bond lengths	Bond angles
	
Torsions	Rings

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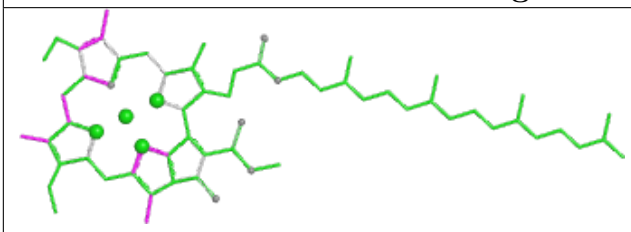
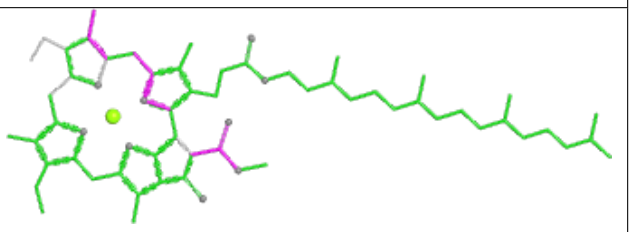
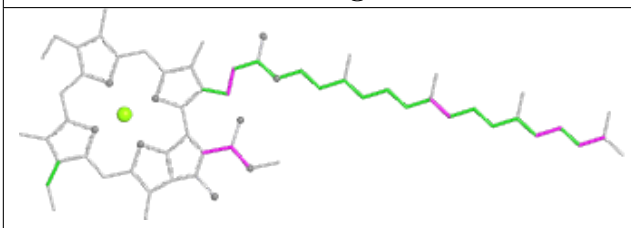
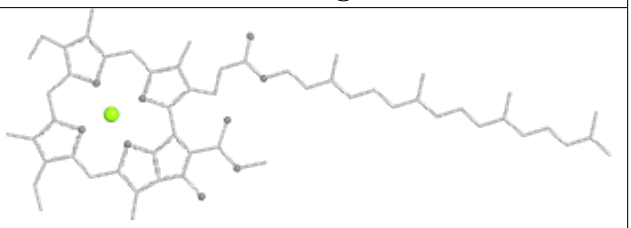
	
Bond lengths	Bond angles
	
Torsions	Rings

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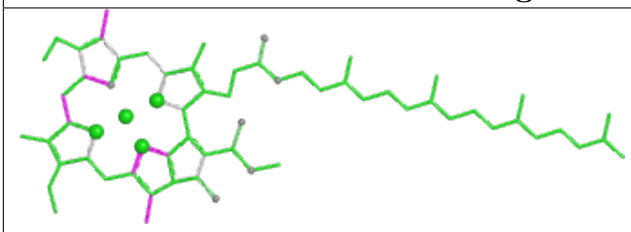
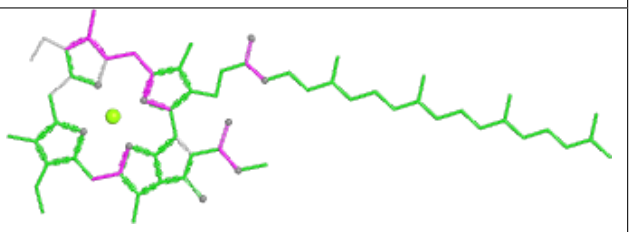
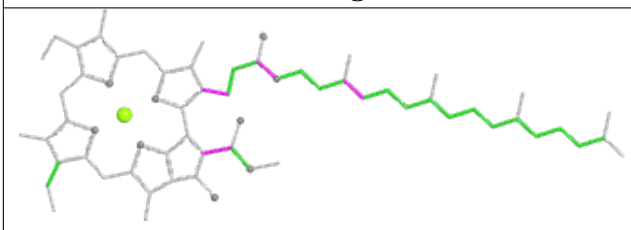
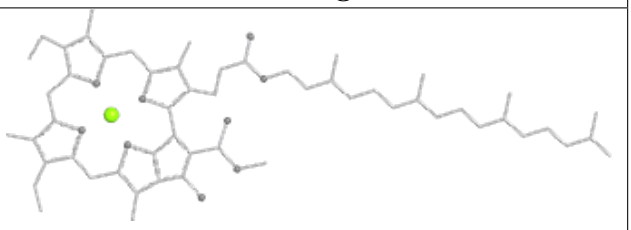
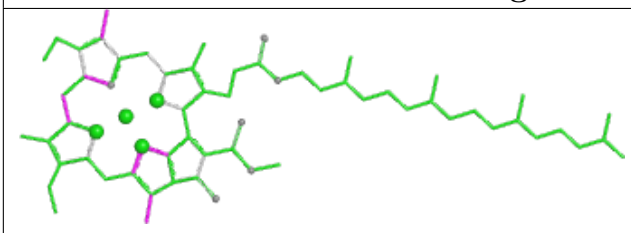
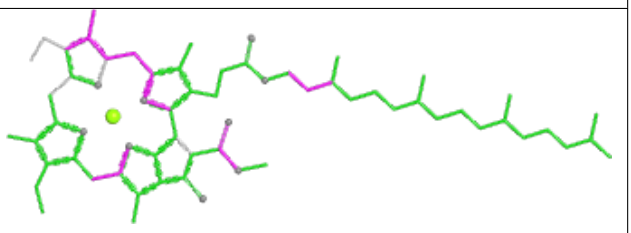
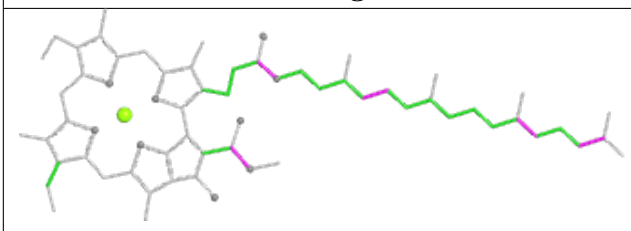
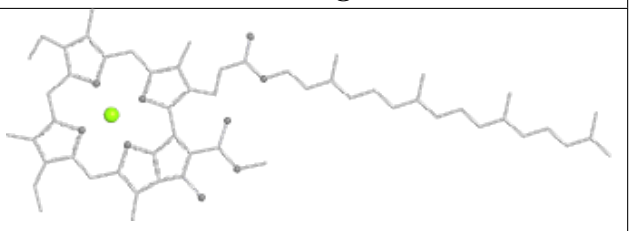
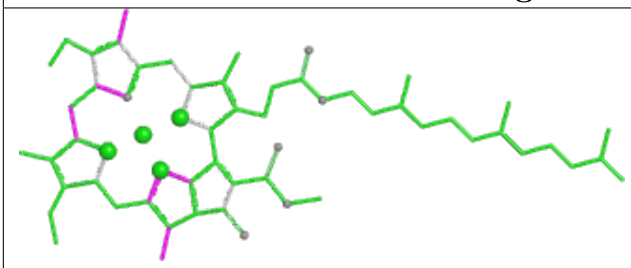
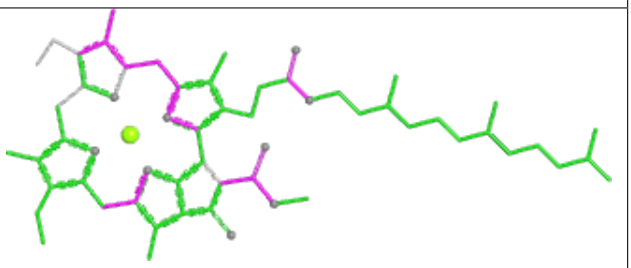
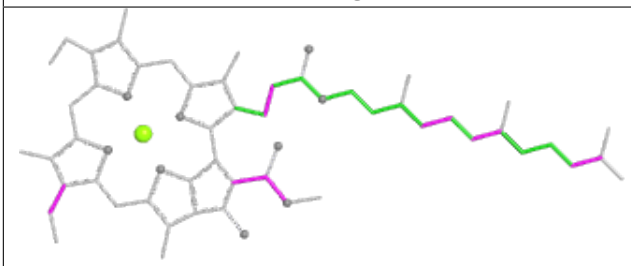
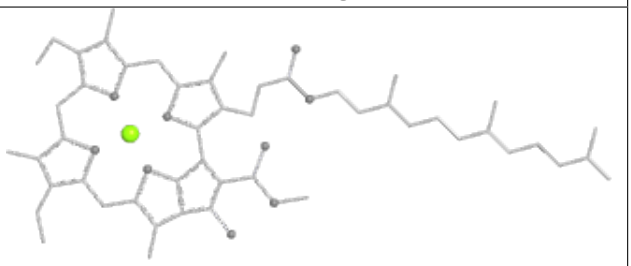
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

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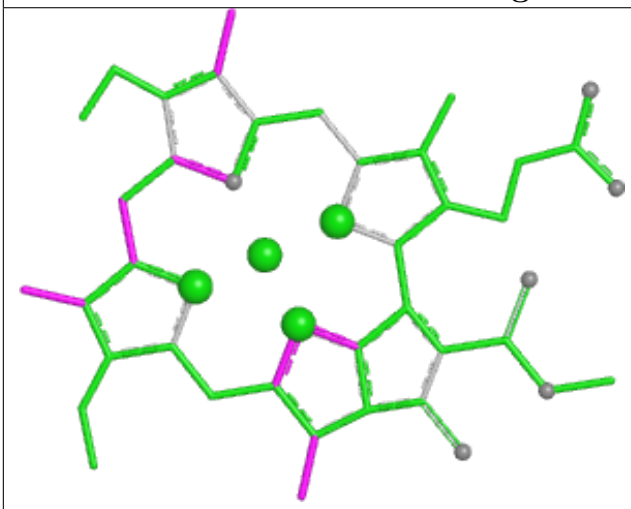
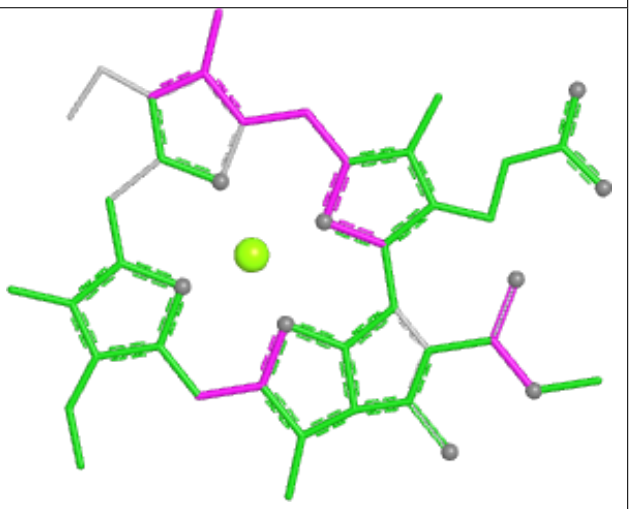
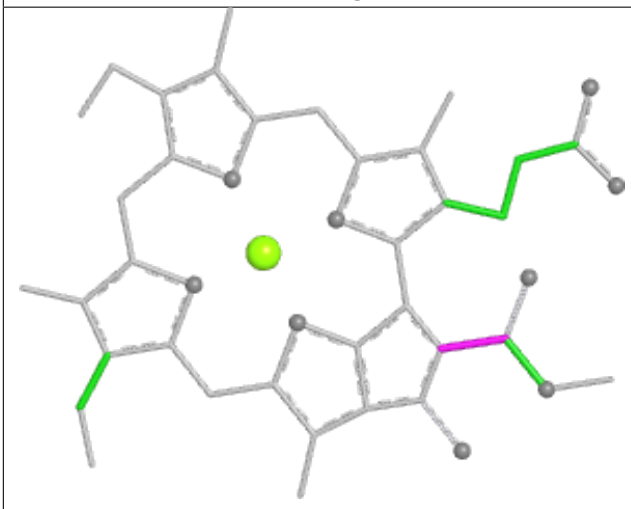
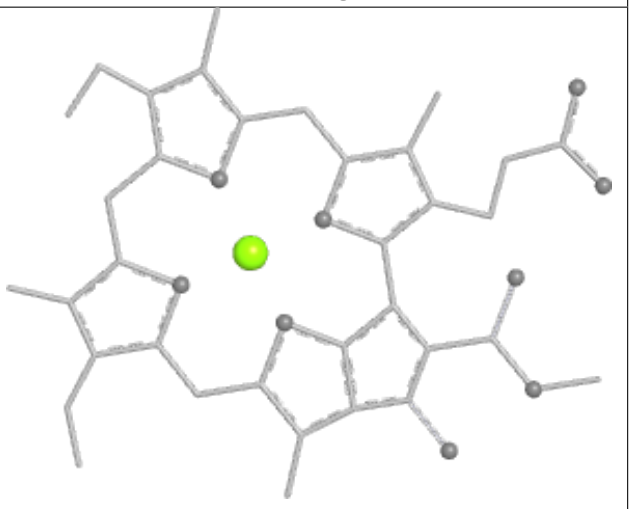
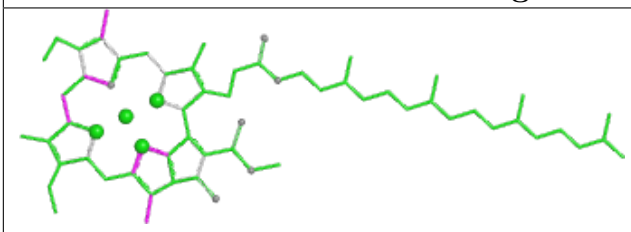
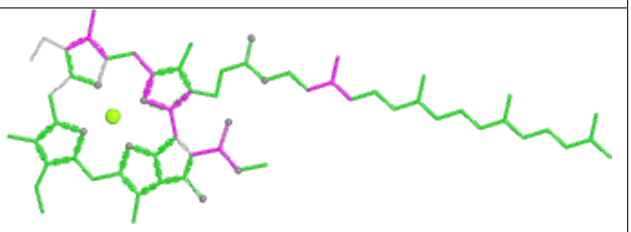
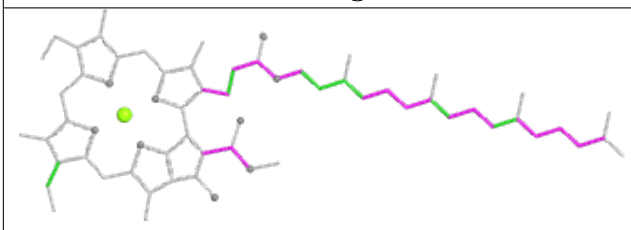
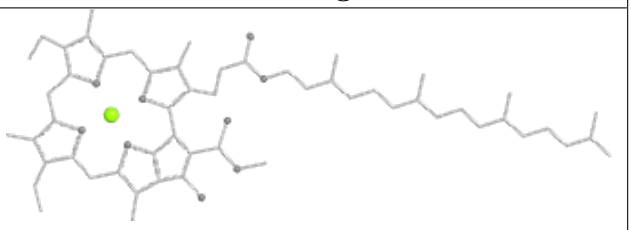
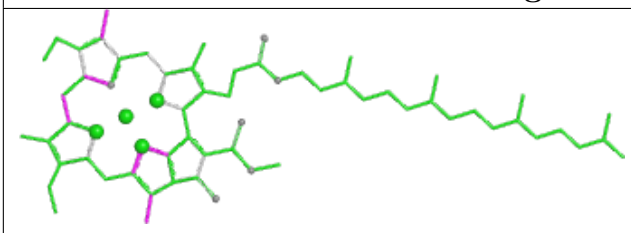
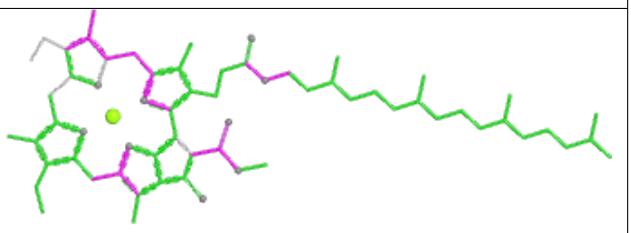
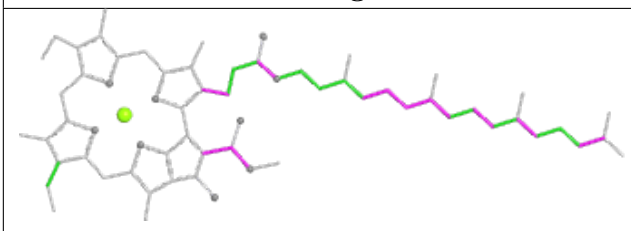
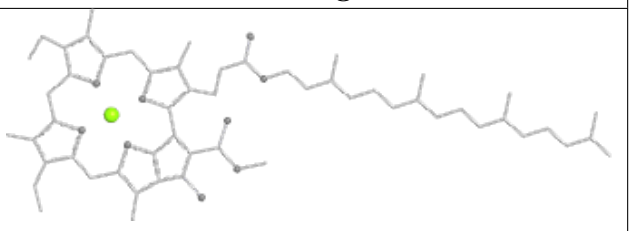
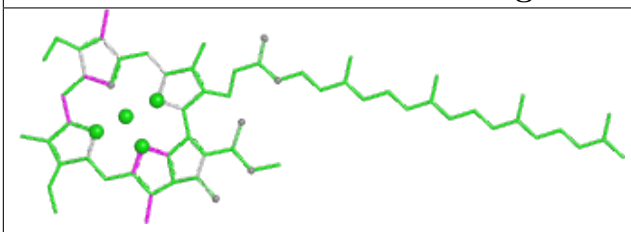
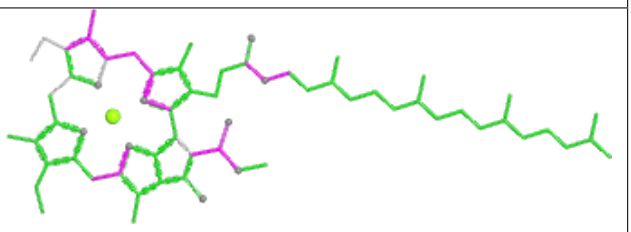
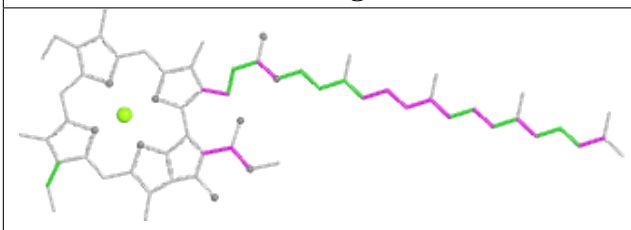
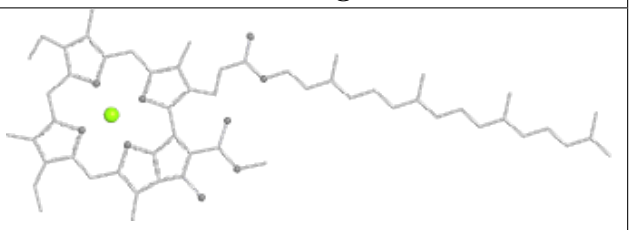
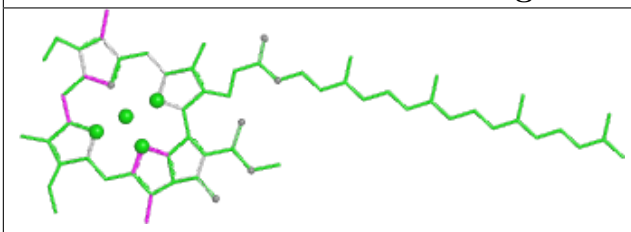
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

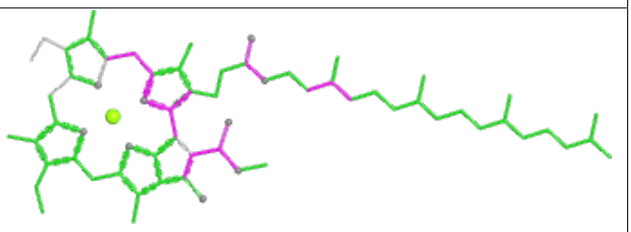
Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

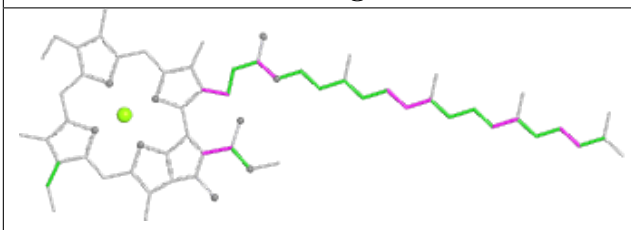
Ligand CLA B2 833



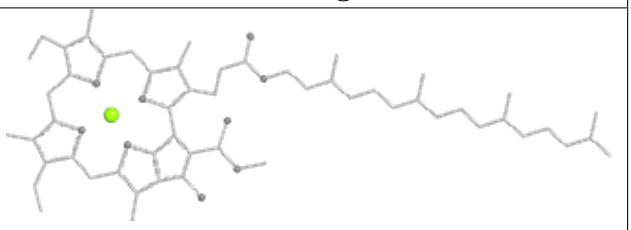
Bond lengths



Bond angles

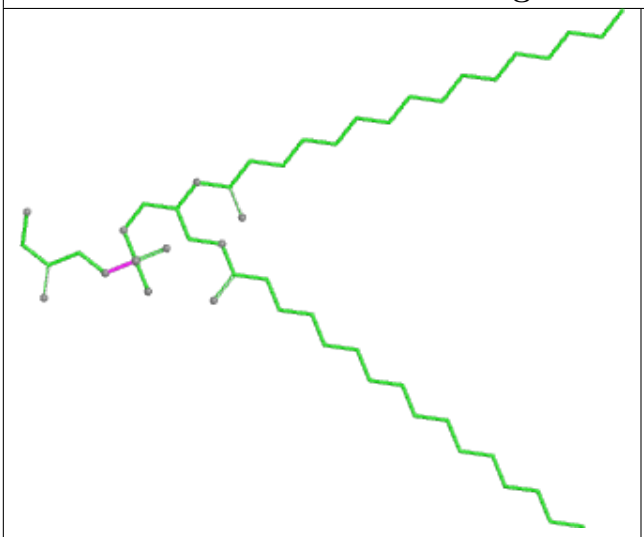


Torsions



Rings

Ligand LHG A2 845



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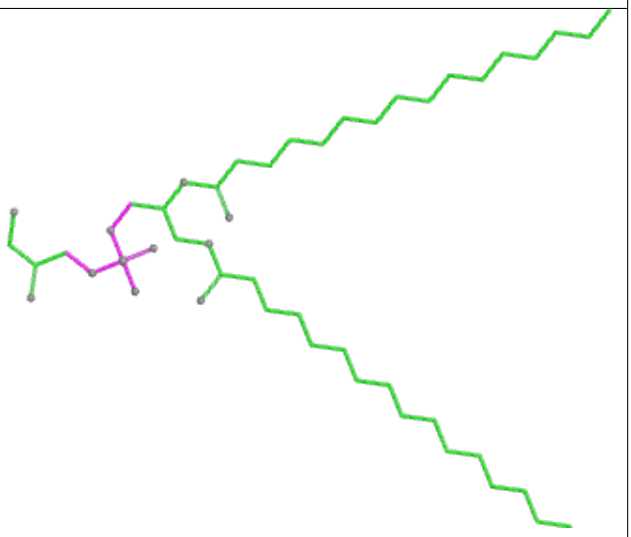
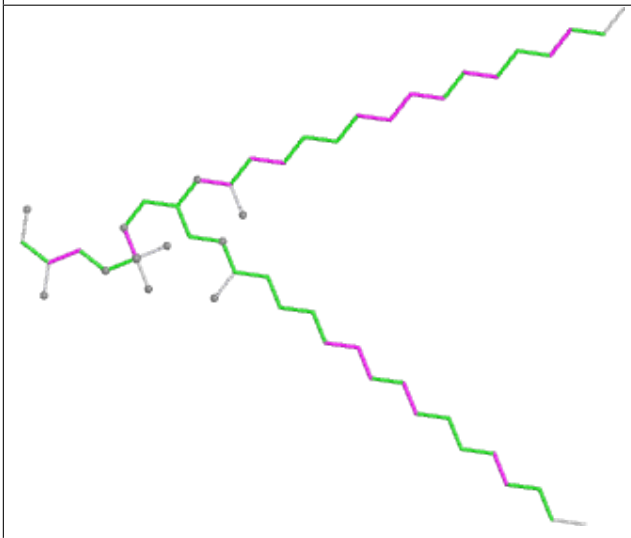


Bond angles



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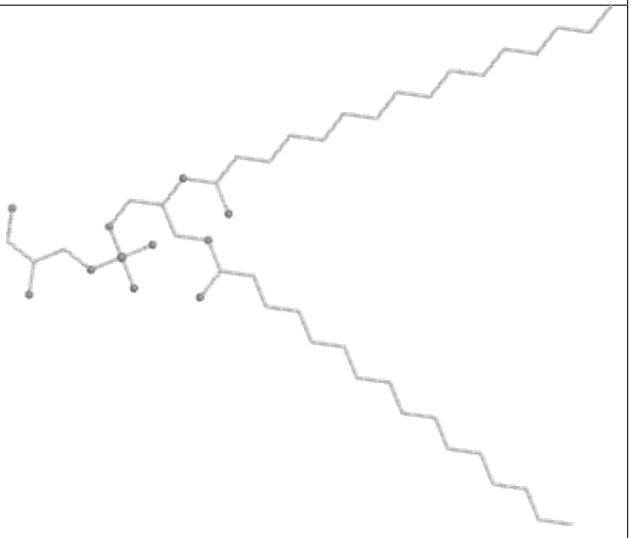
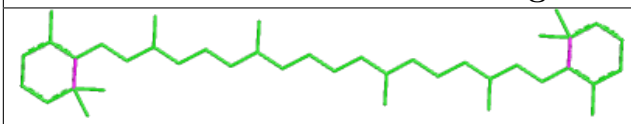


Rings

Ligand BCR I 102



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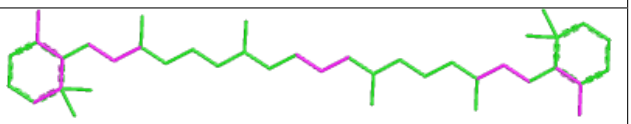
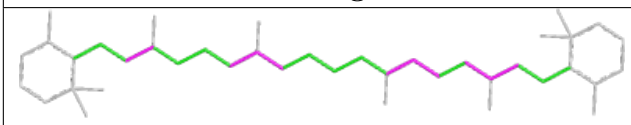
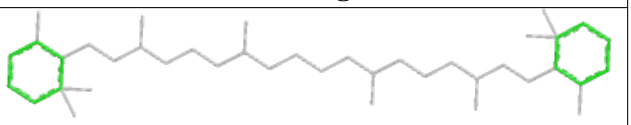


Bond angles

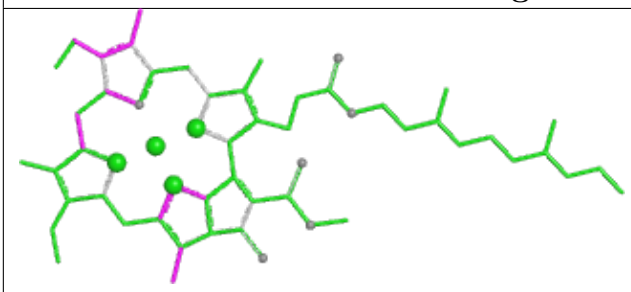


Torsions

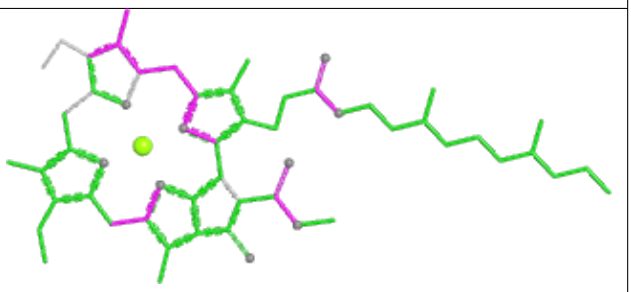


Rings

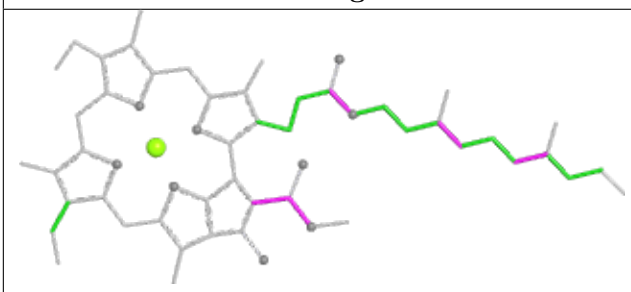
Ligand CLA BB 816



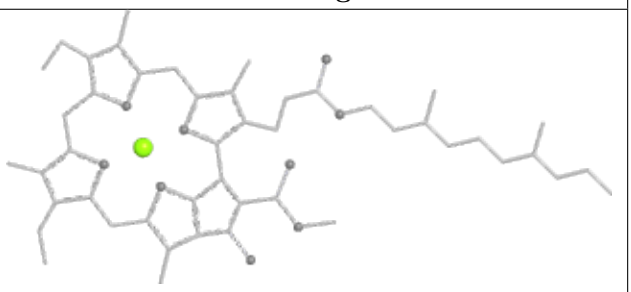
Bond lengths



Bond angles

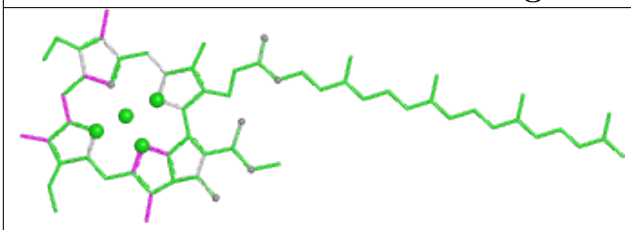


Torsions

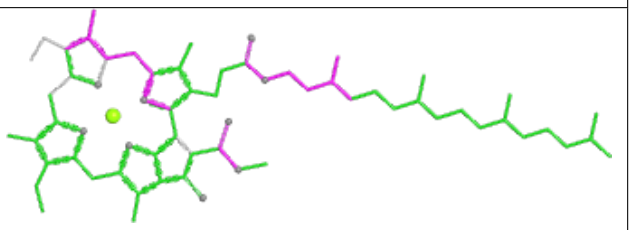


Rings

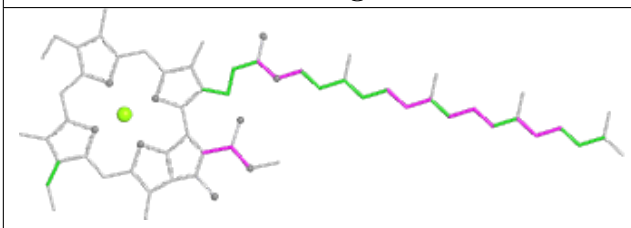
Ligand CLA B 806



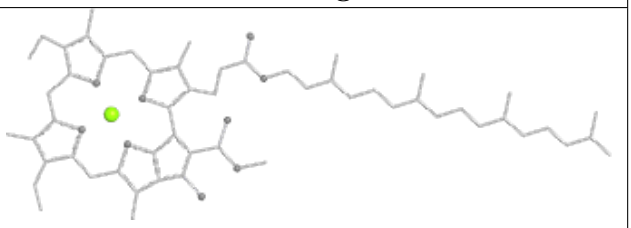
Bond lengths



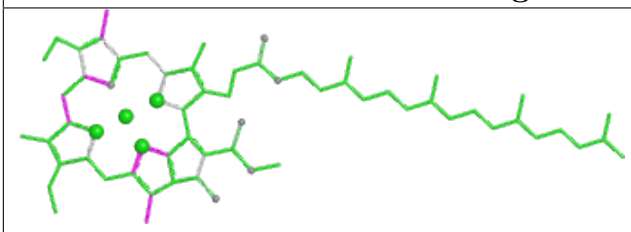
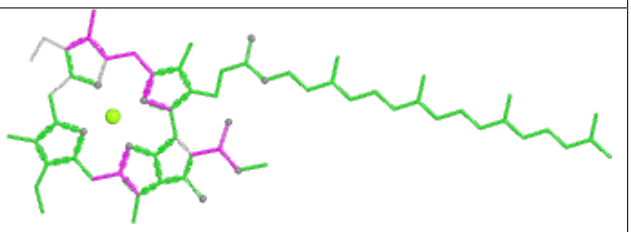
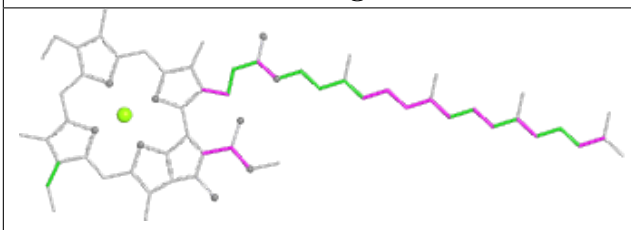
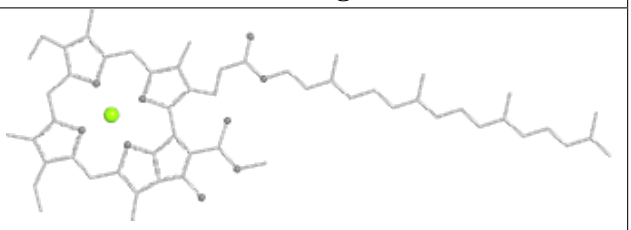
Bond angles

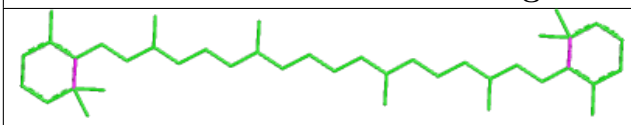
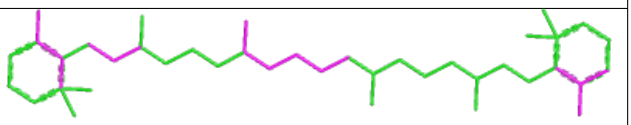
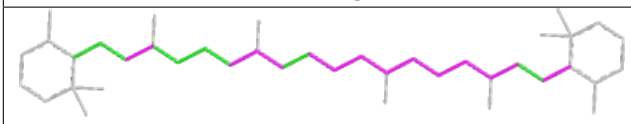
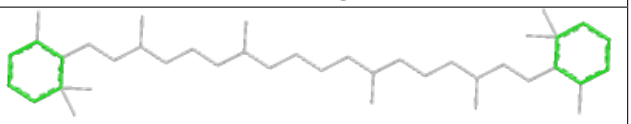


Torsions

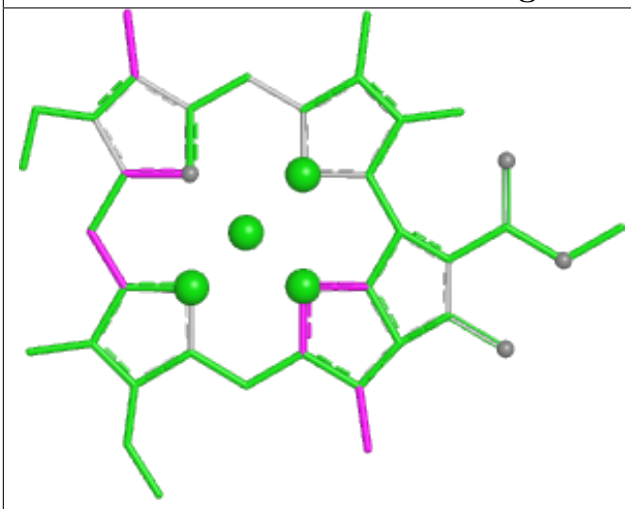


Rings

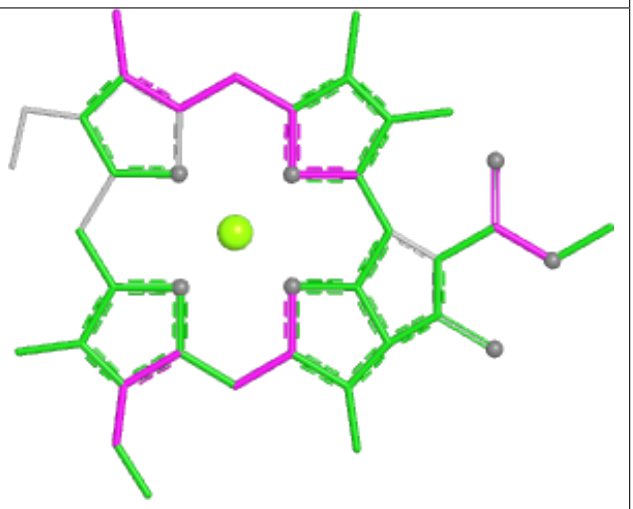
Ligand CLA BB 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

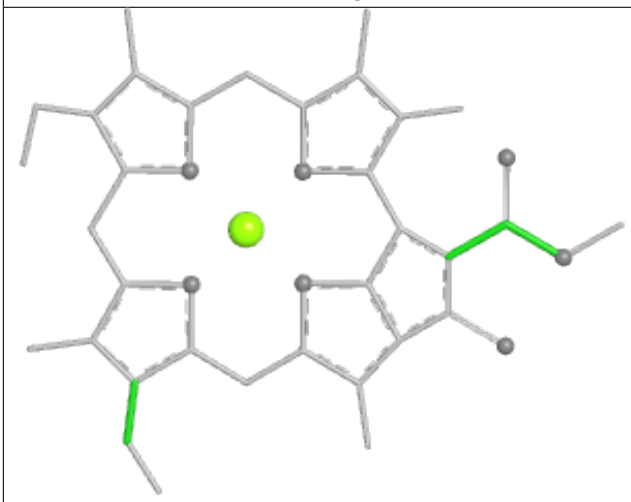
Ligand CLA JJ 103



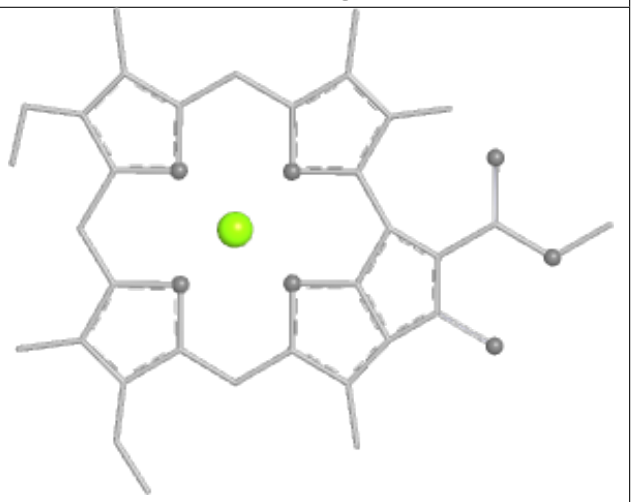
Bond lengths



Bond angles

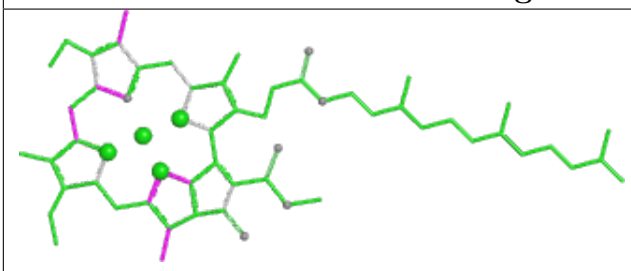


Torsions

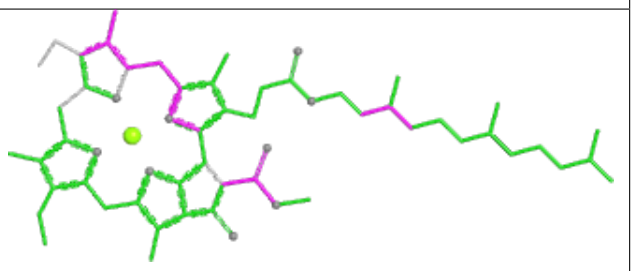


Rings

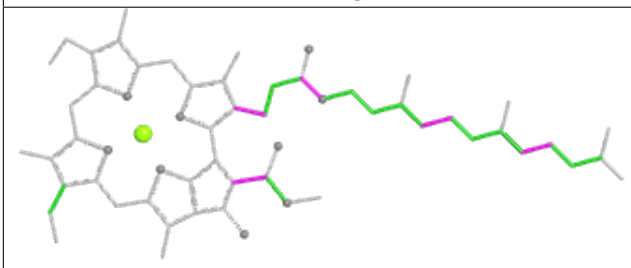
Ligand CLA A2 805



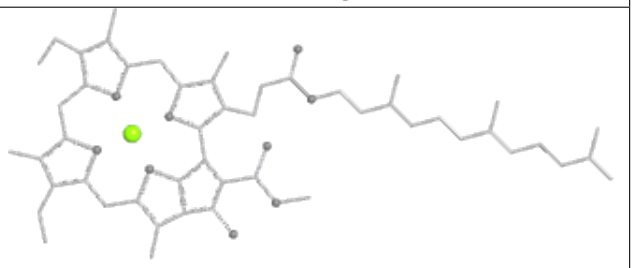
Bond lengths



Bond angles

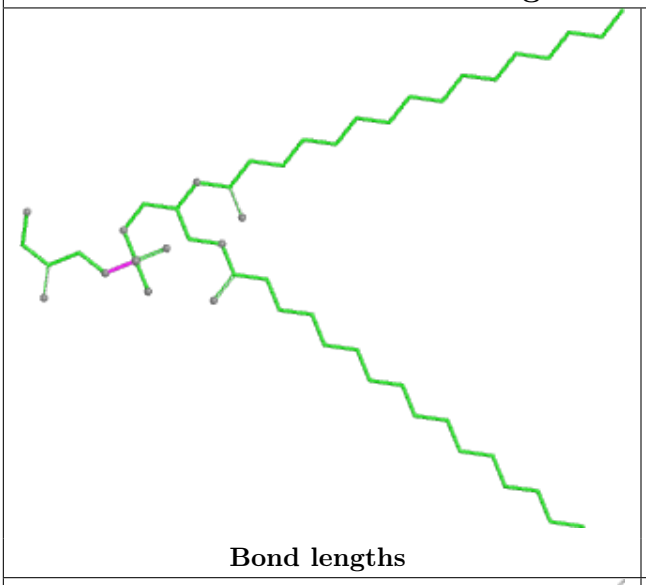


Torsions

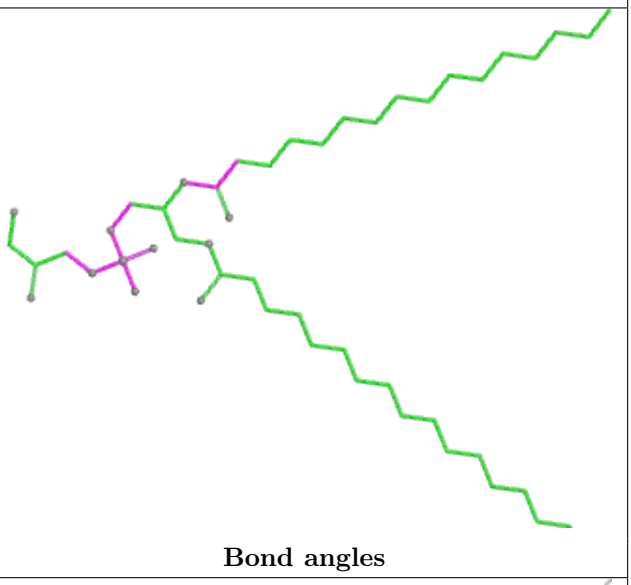


Rings

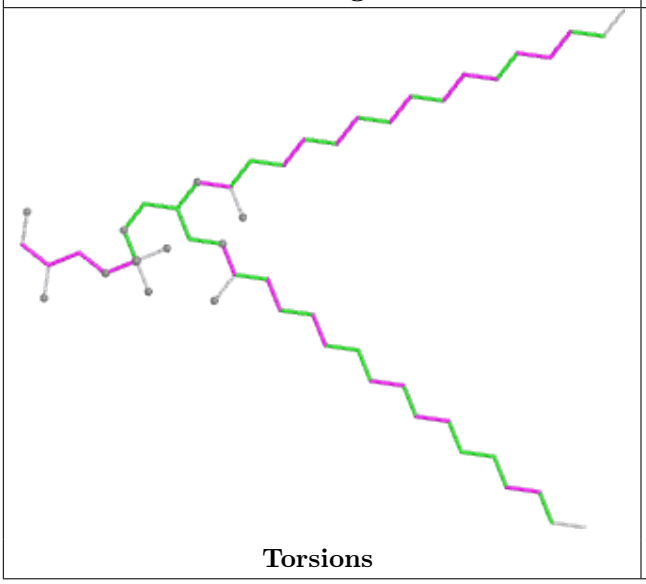
Ligand LHG B 853



Bond lengths



Bond angles



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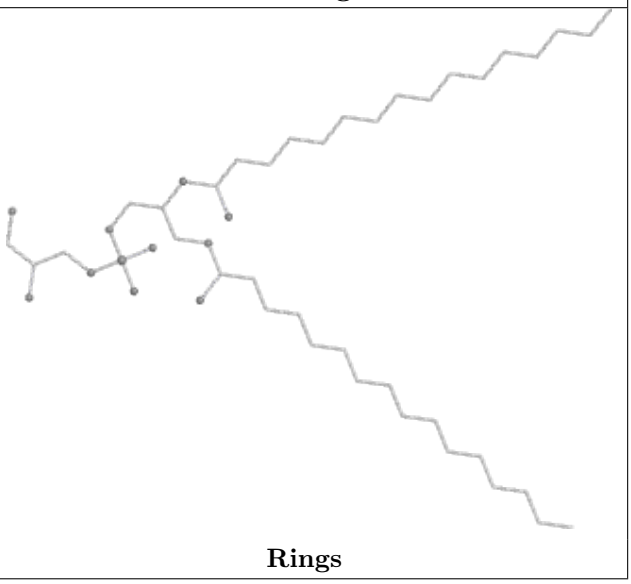
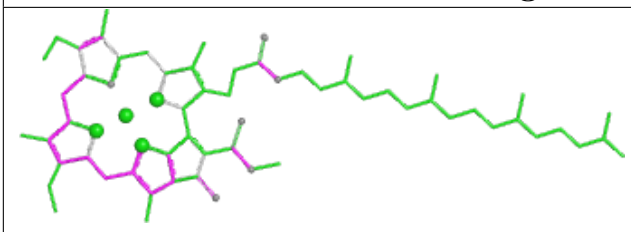
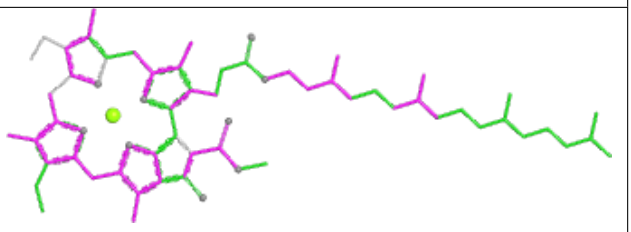


Rings

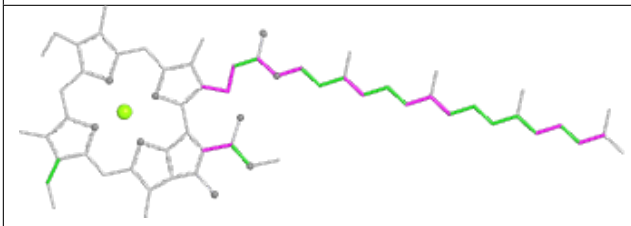
Ligand CL0 A1 802



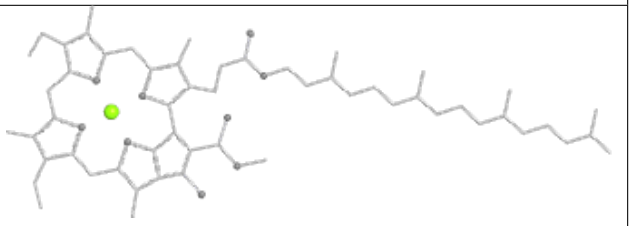
Bond lengths



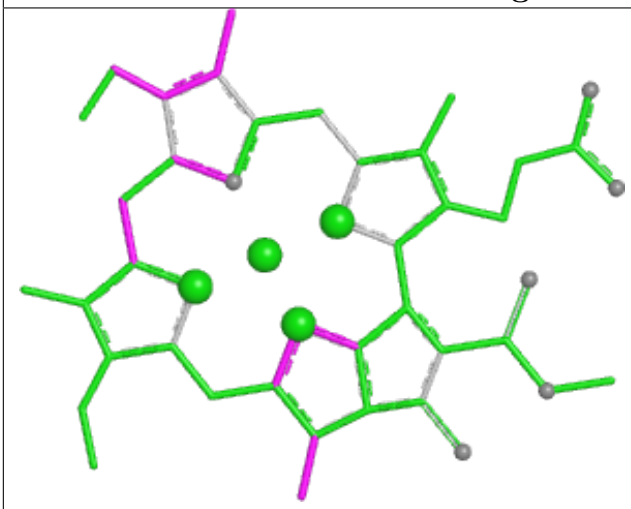
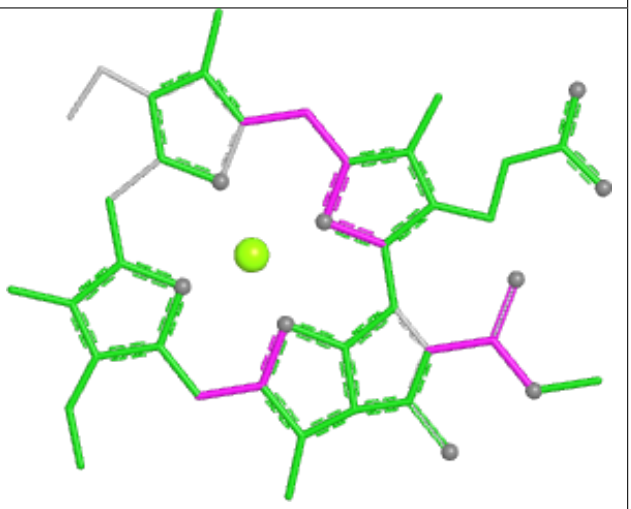
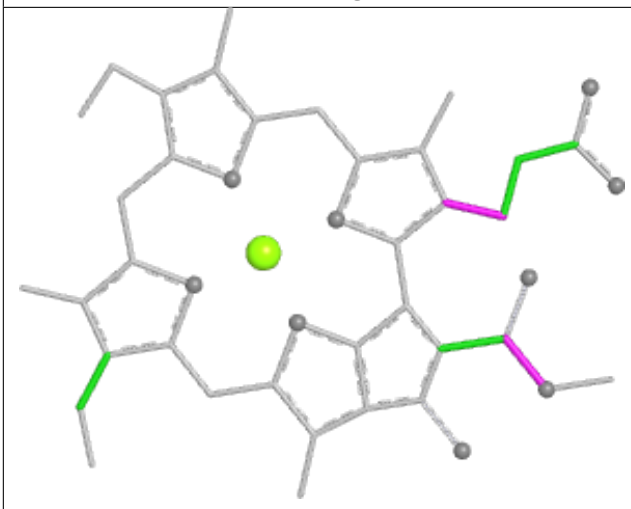
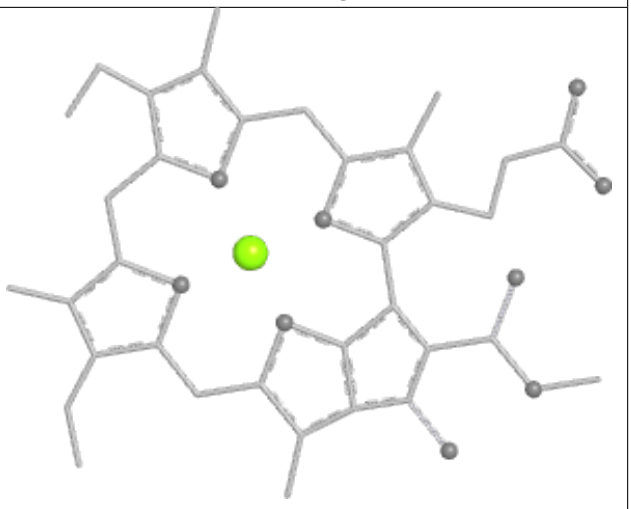
Bond angles

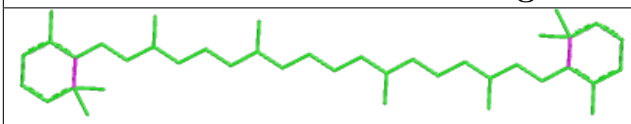
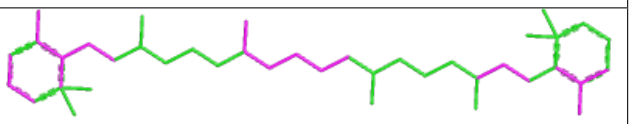
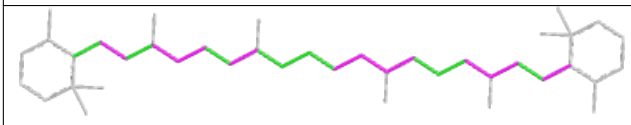
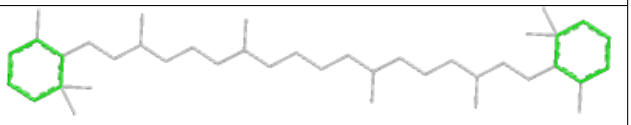


Torsions

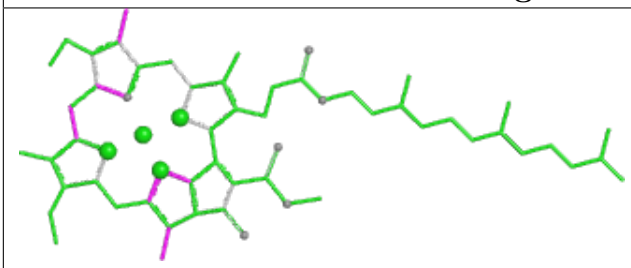


Rings

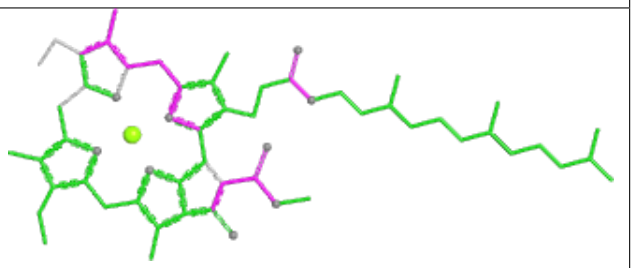
Ligand CLA BB 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J2 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

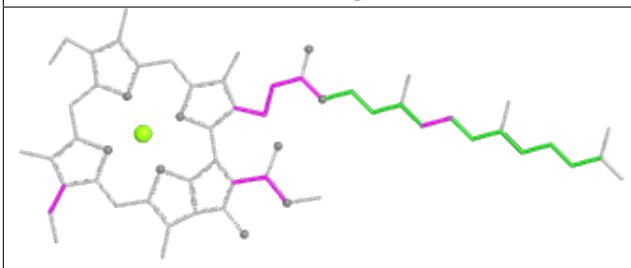
Ligand CLA FF 301



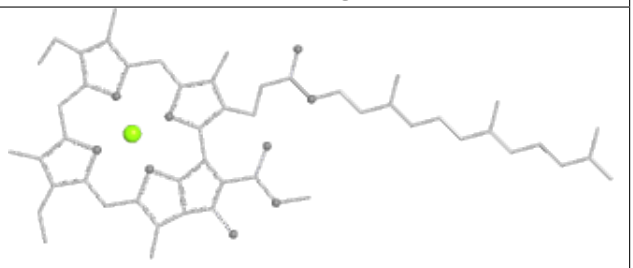
Bond lengths



Bond angles

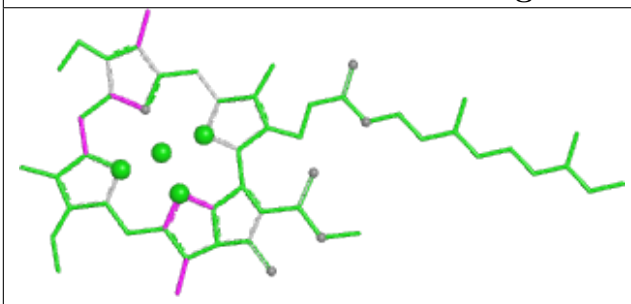


Torsions

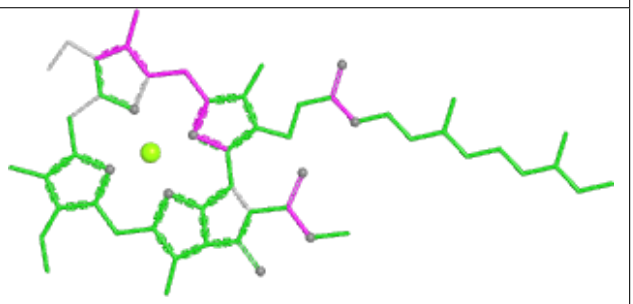


Rings

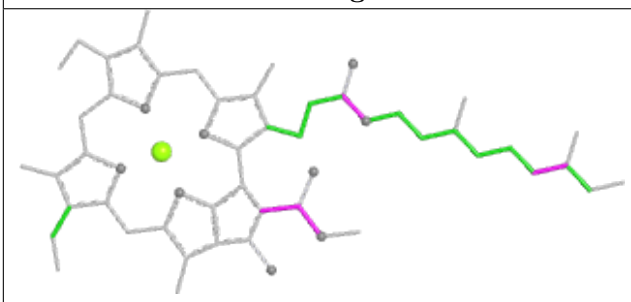
Ligand CLA B2 831



Bond lengths



Bond angles



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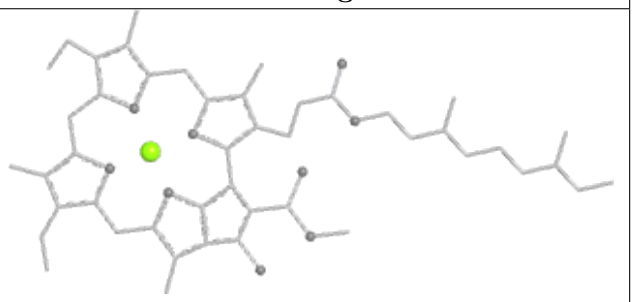
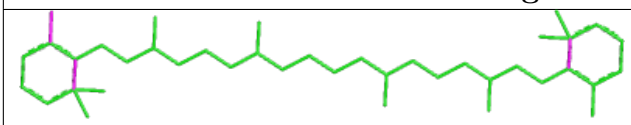
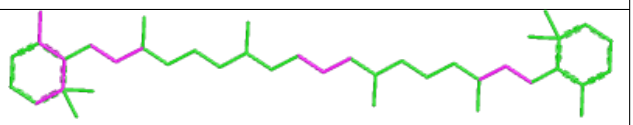


Rings

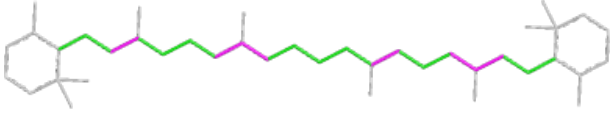
Ligand BCR II 102



Bond lengths



Bond angles



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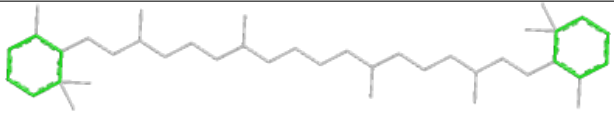
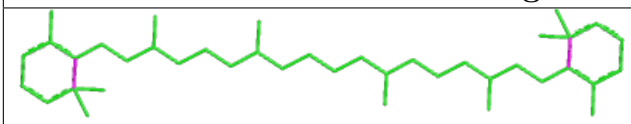
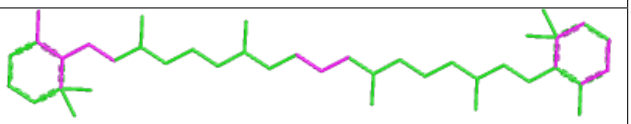
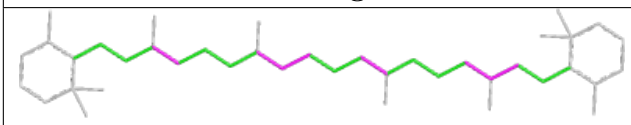
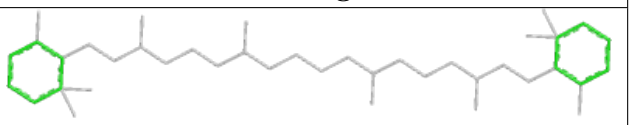
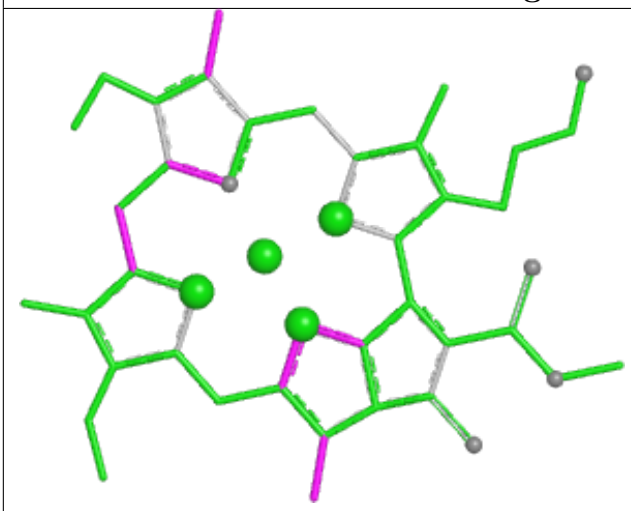
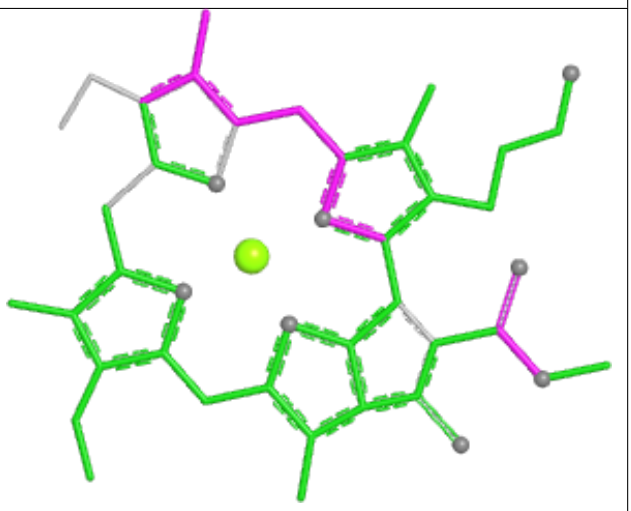
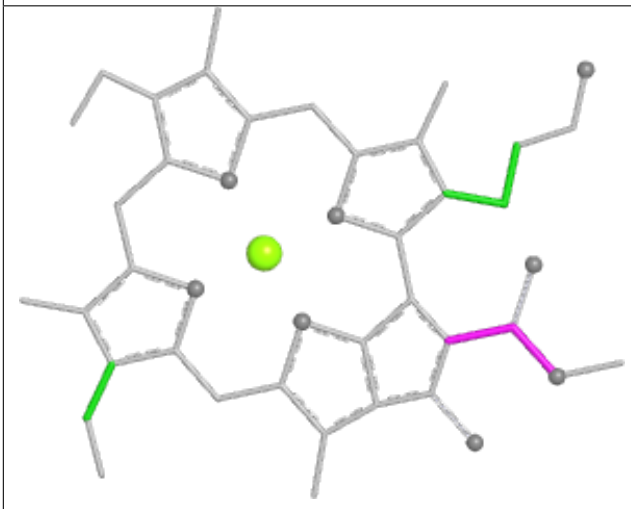
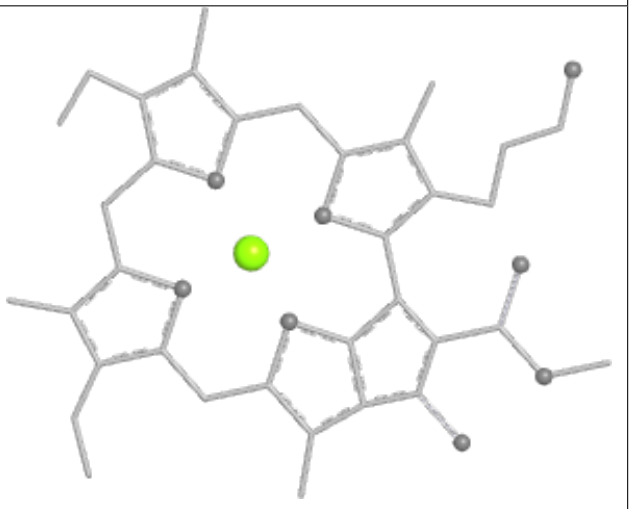
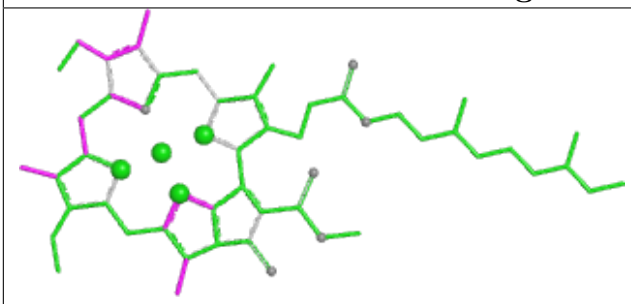
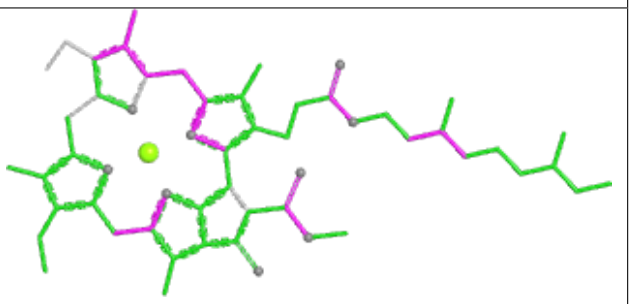
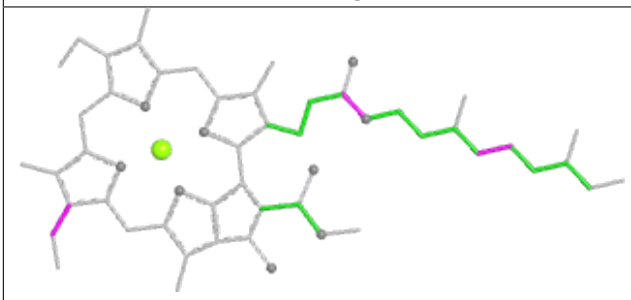
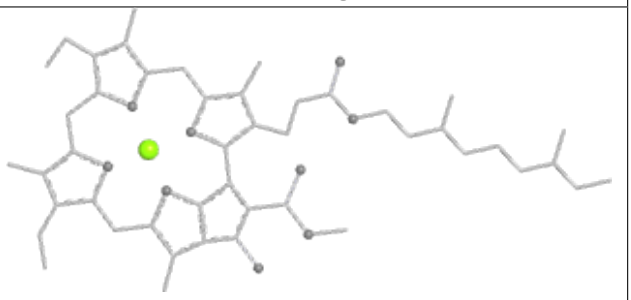
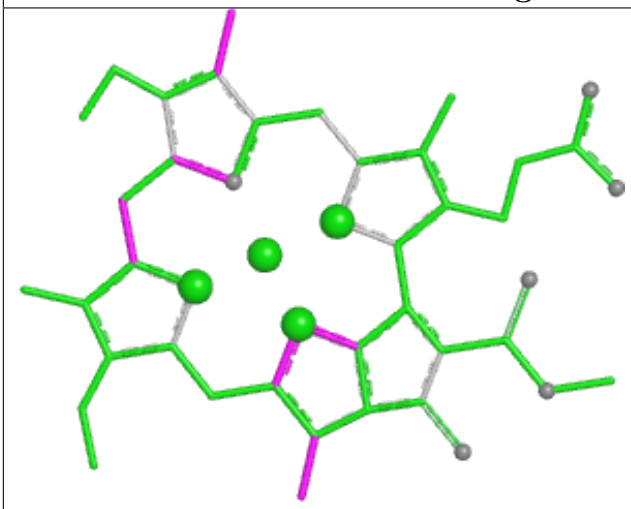
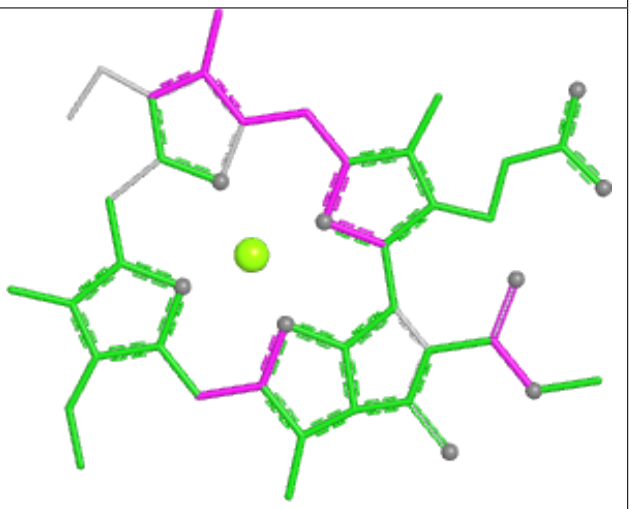
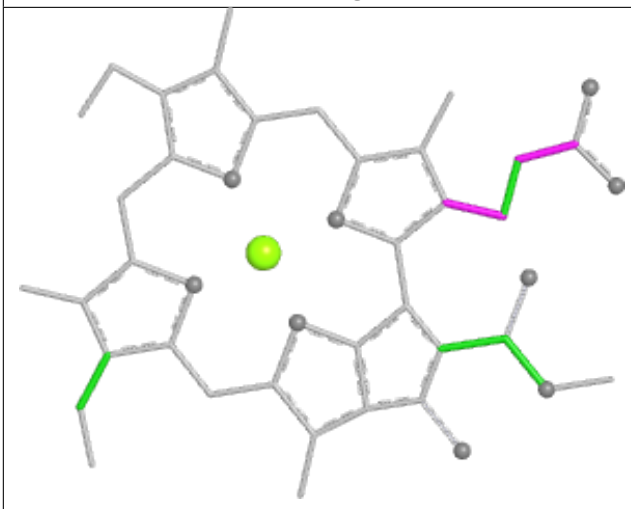
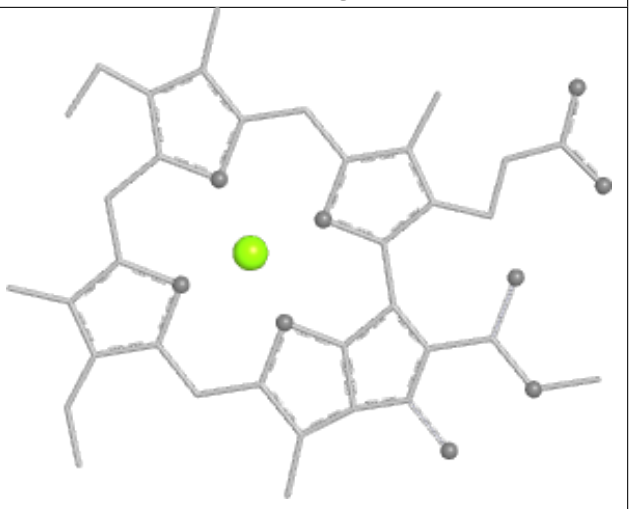


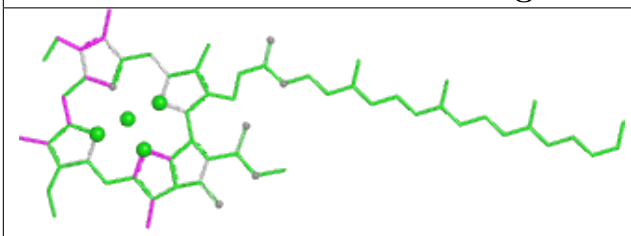
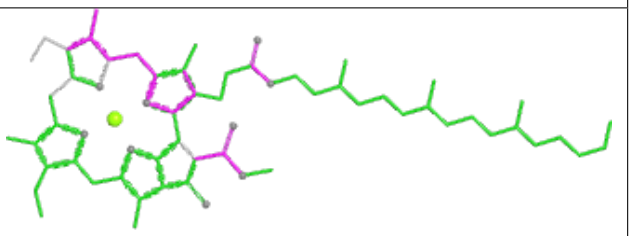
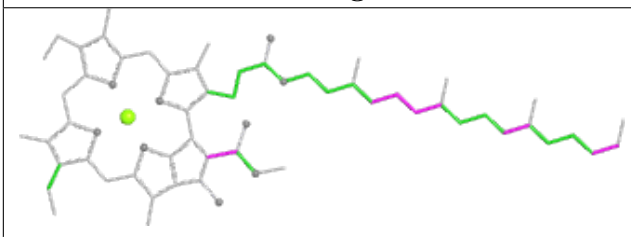
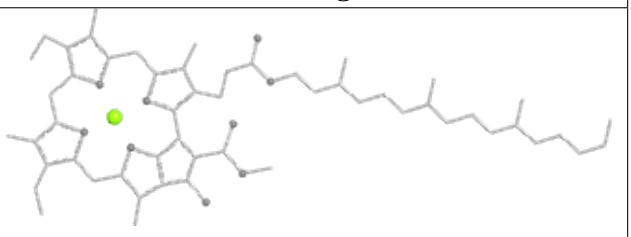
Rings

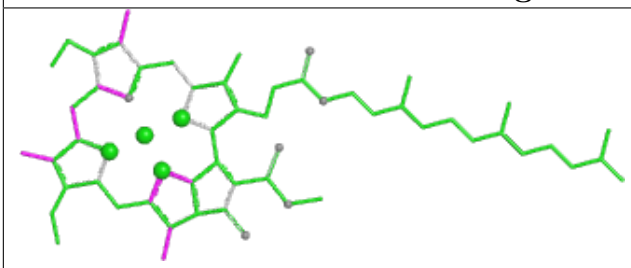
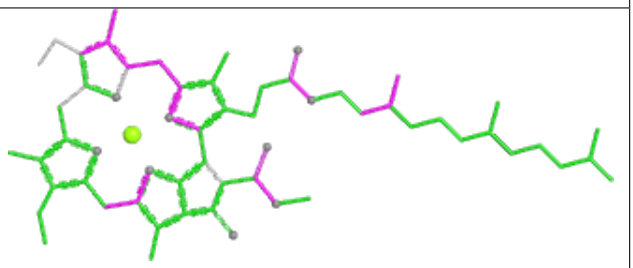
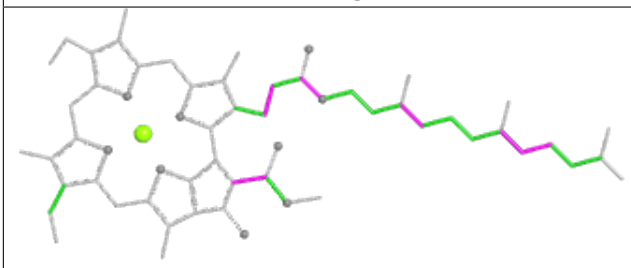
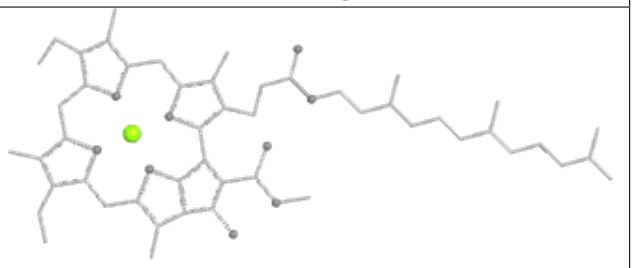
Ligand BCR B 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

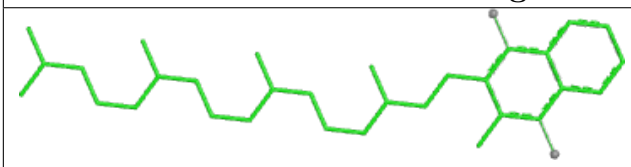
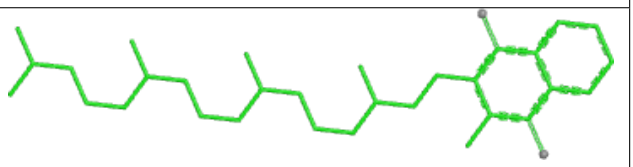
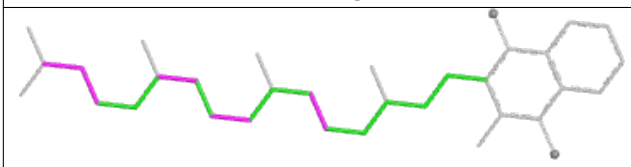
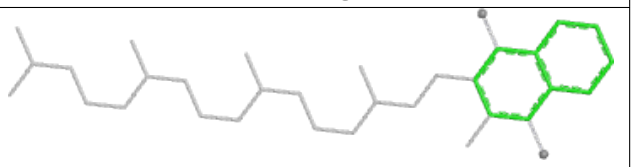
Ligand CLA A 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 829	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A1 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B1 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN BB 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

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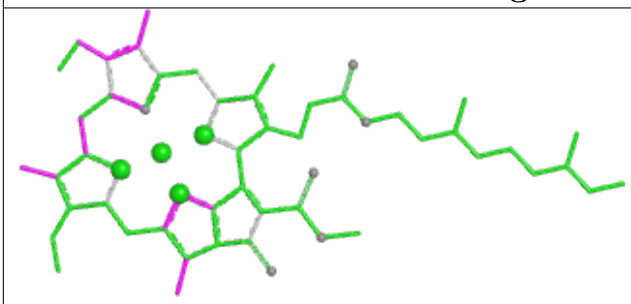
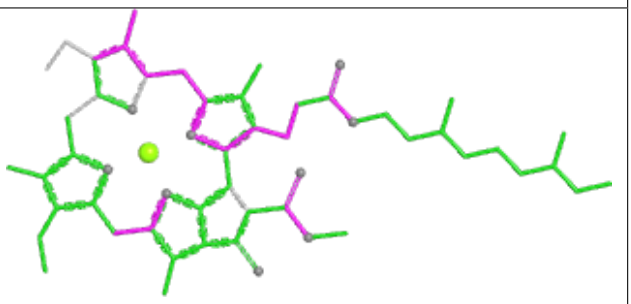
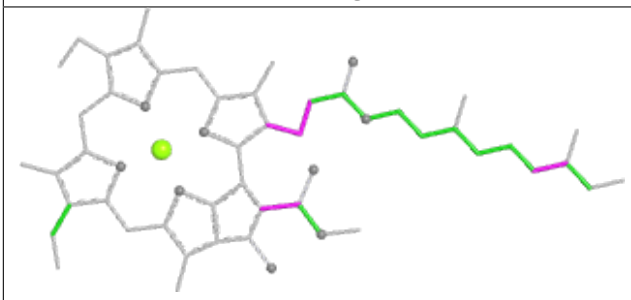
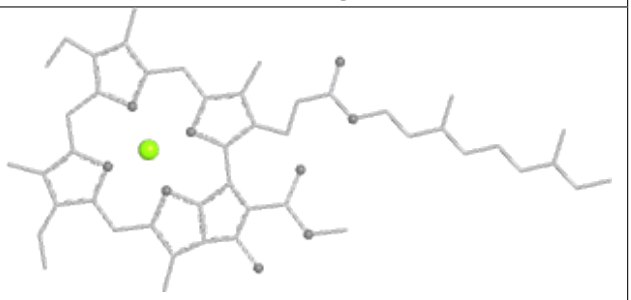
	
Bond lengths	Bond angles
	
Torsions	Rings

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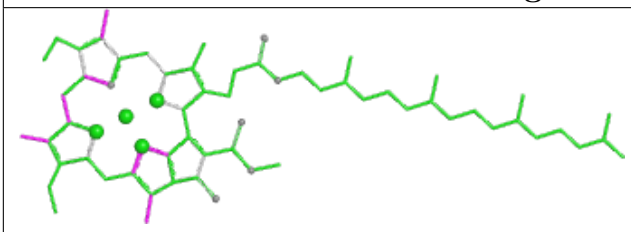
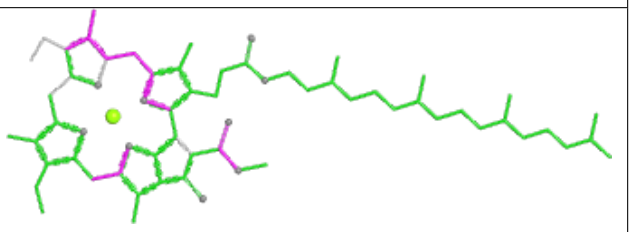
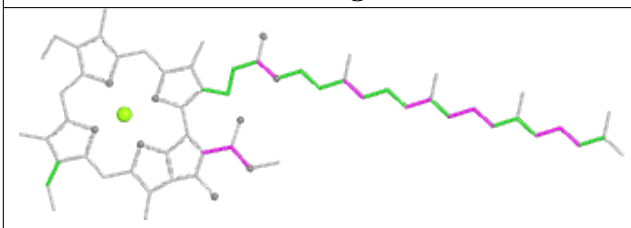
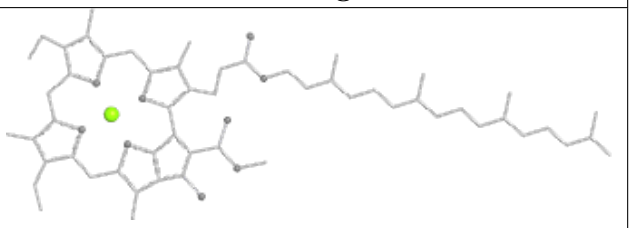
	
Bond lengths	Bond angles
	
Torsions	Rings

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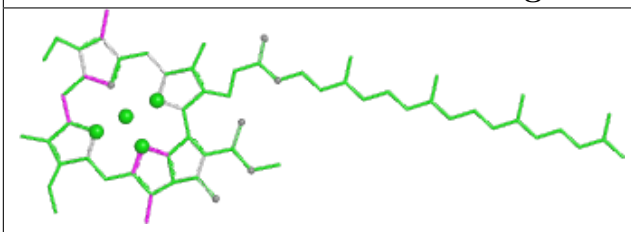
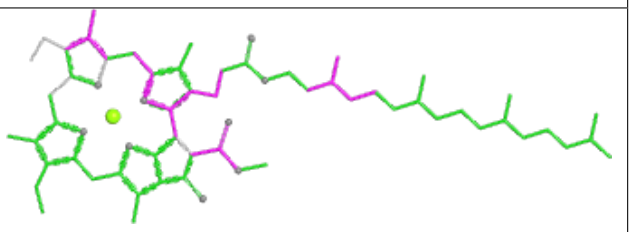
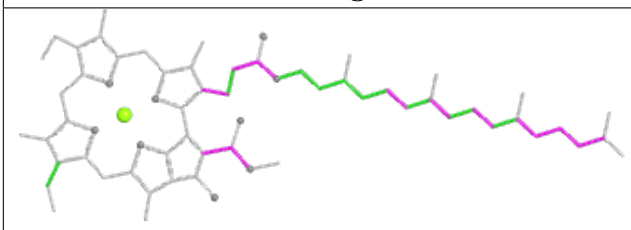
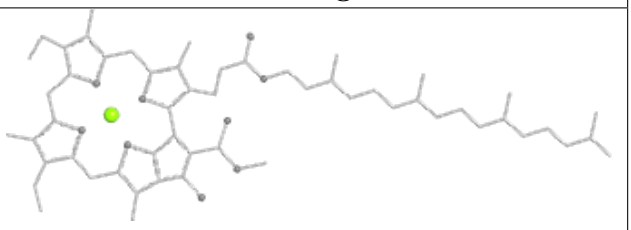
 Bond lengths	 Bond angles
 Torsions	 Rings

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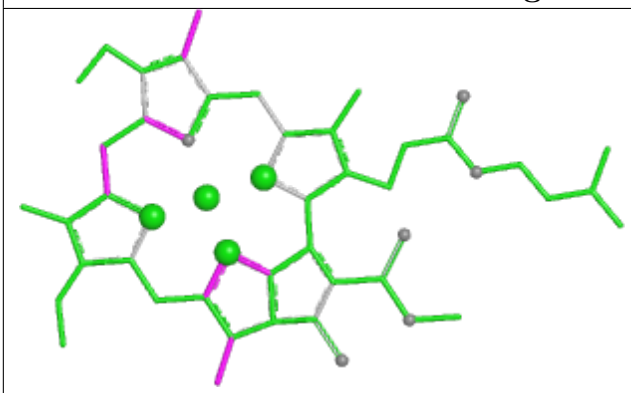
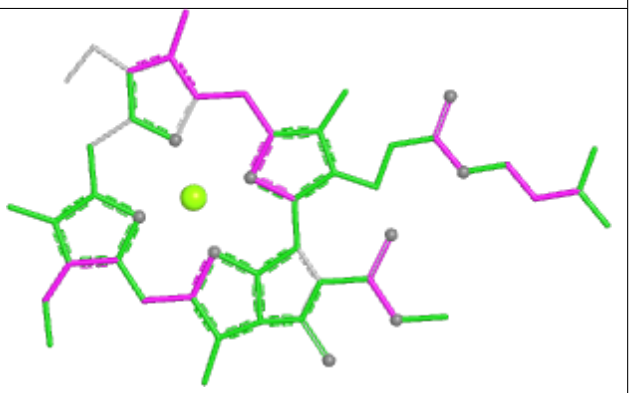
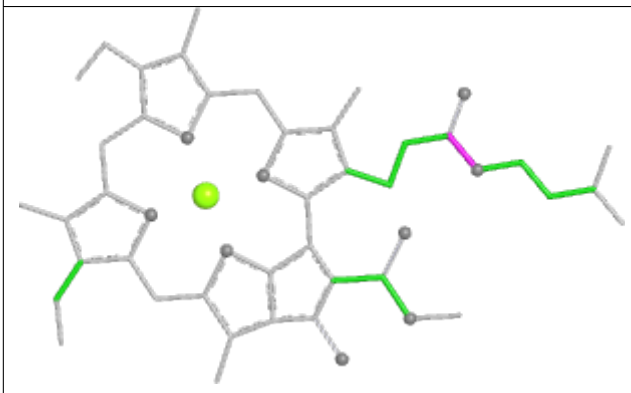
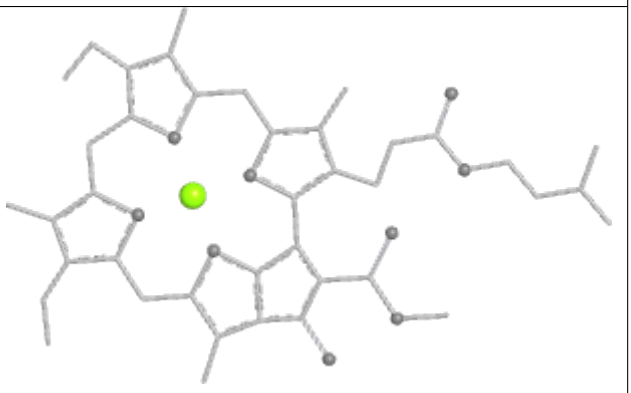
 Bond lengths	 Bond angles
 Torsions	 Rings

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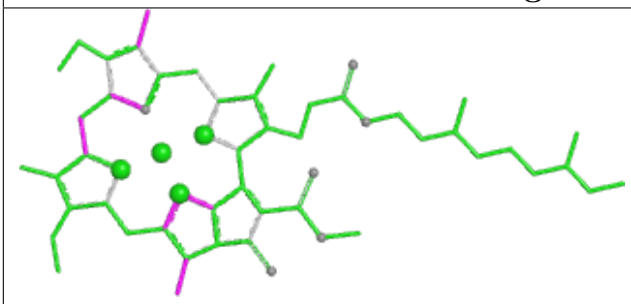
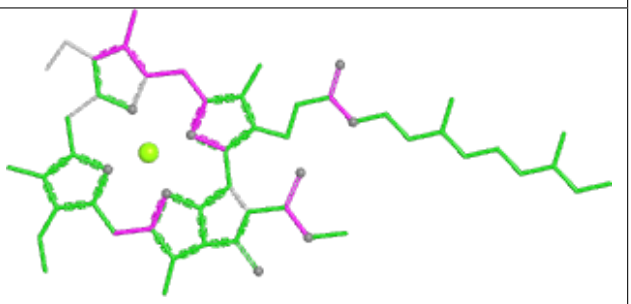
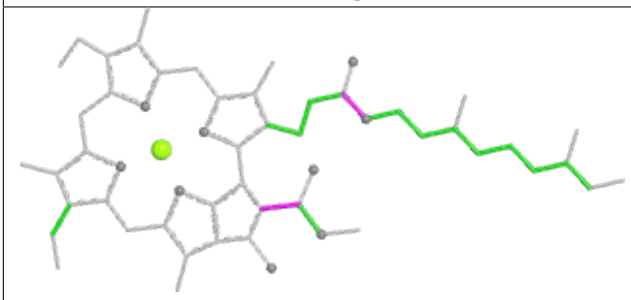
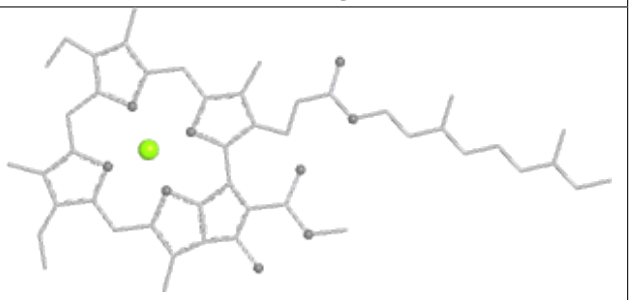
	
Bond lengths	Bond angles
	
Torsions	Rings

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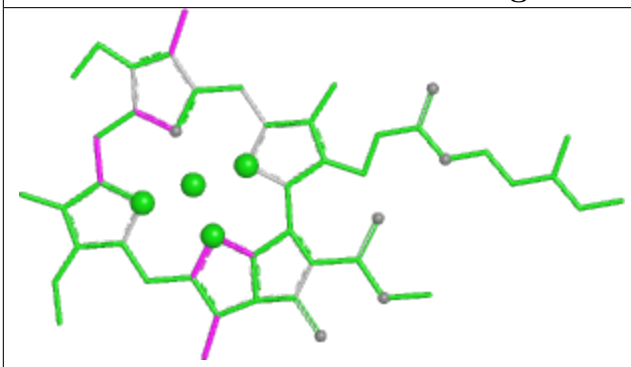
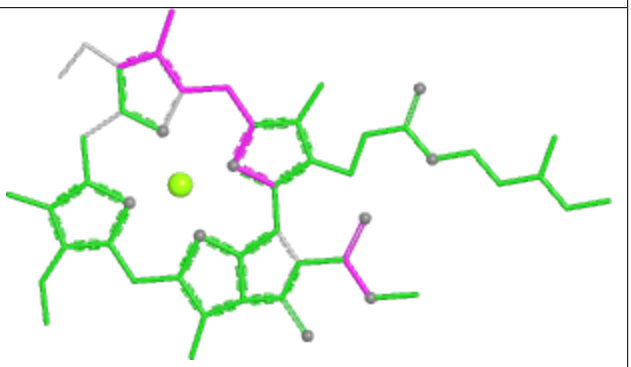
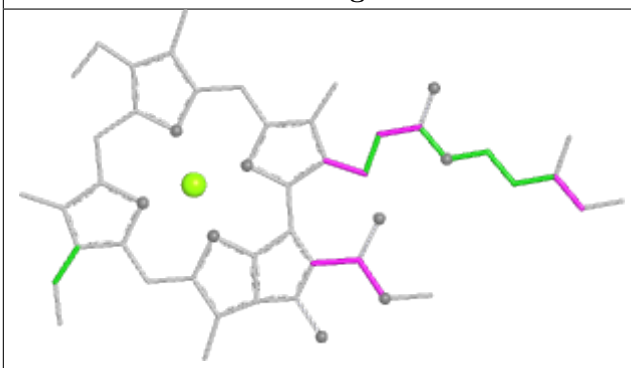
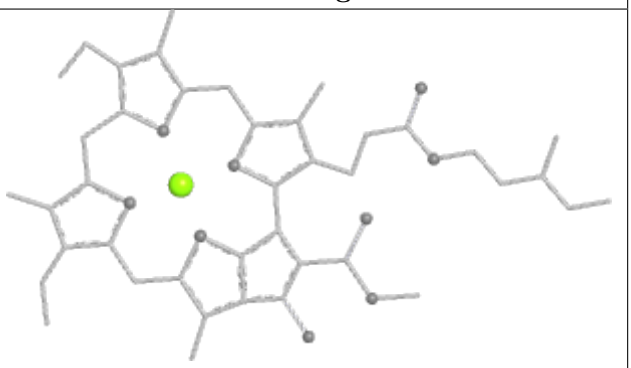
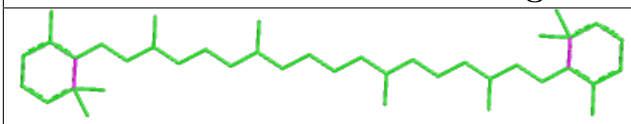
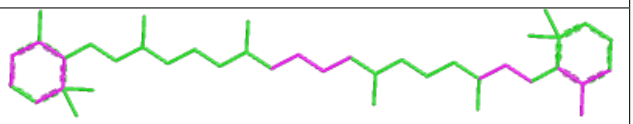
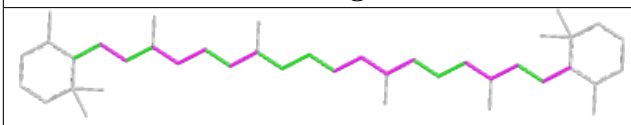
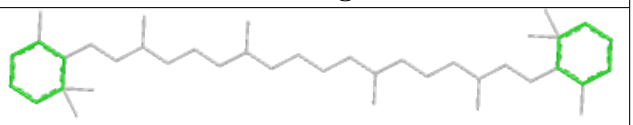
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 104

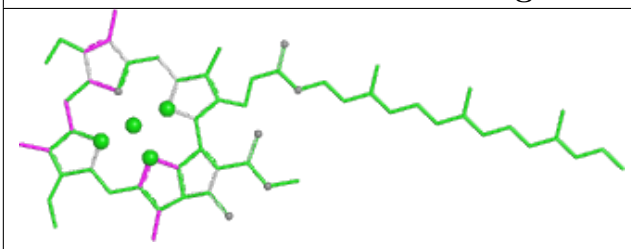

Bond lengths

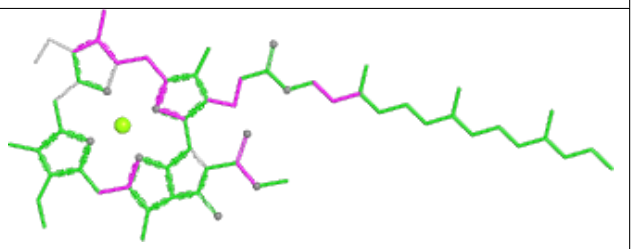

Bond angles

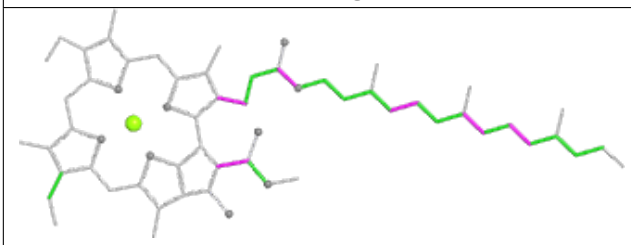

Torsions

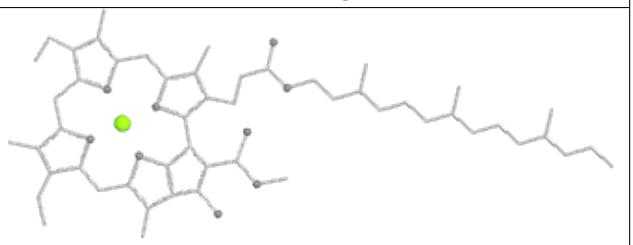

Rings

Ligand CLA B2 804

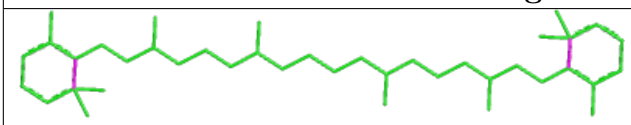

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR L 205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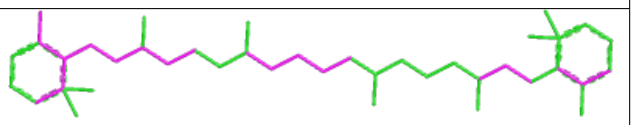
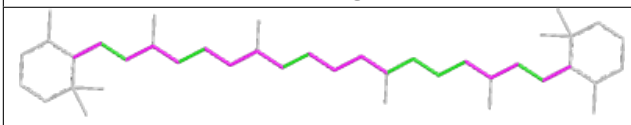
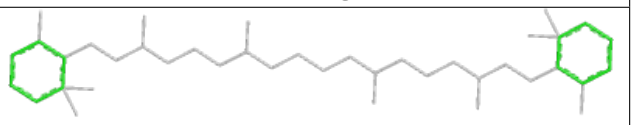
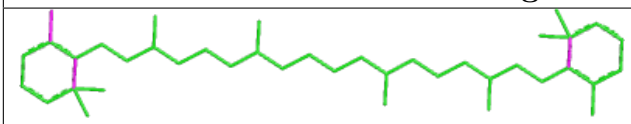
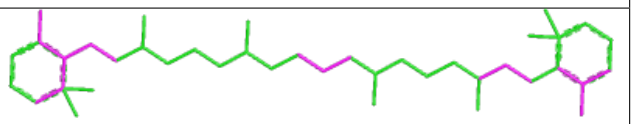

Bond angles

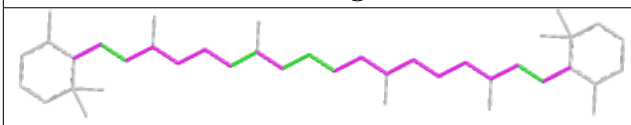

Torsions

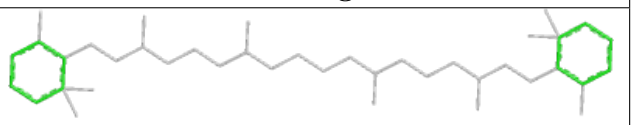

Rings

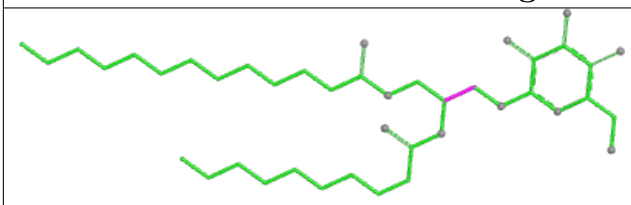
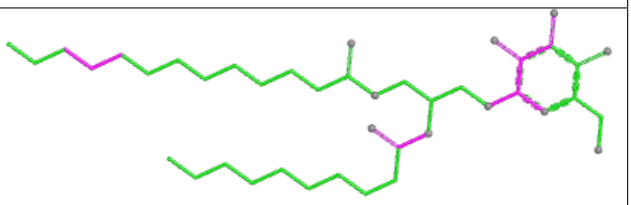
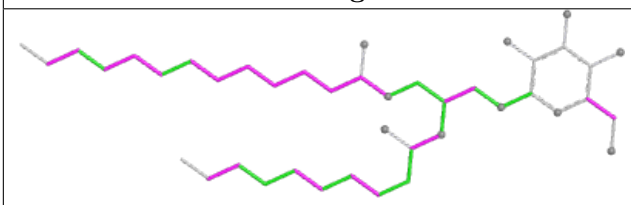
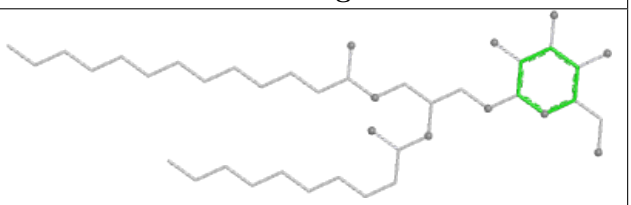
Ligand BCR K 103

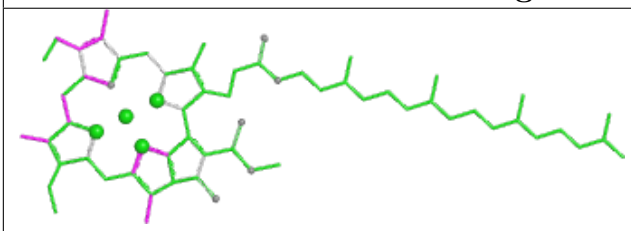
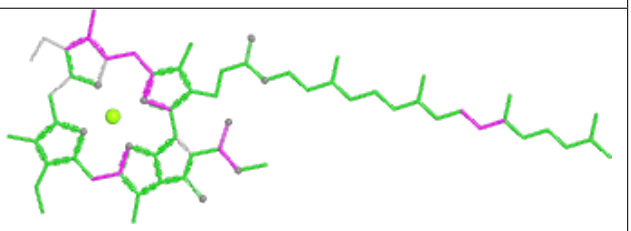
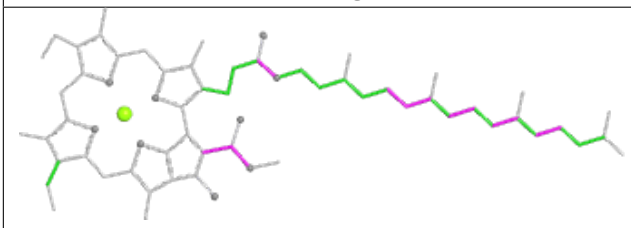
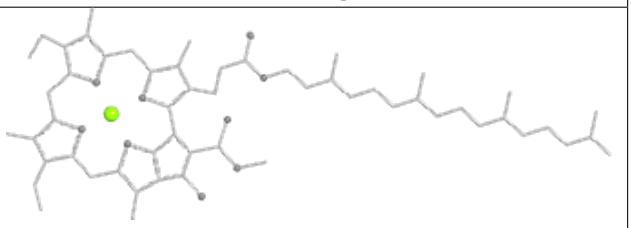

Bond lengths


Bond angles


Torsions


Rings

Ligand LMG II 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

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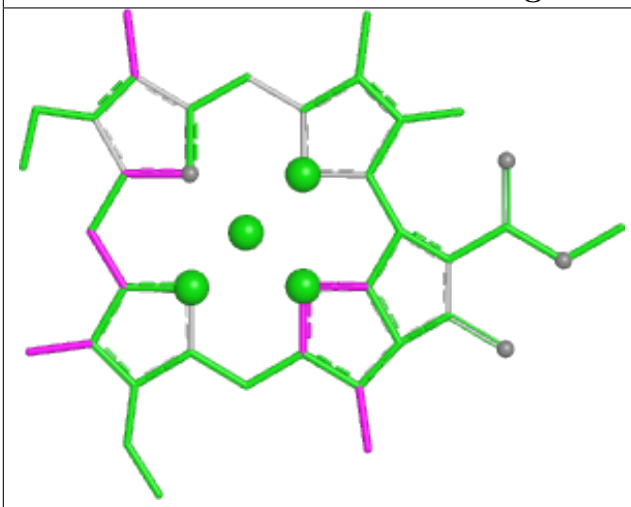
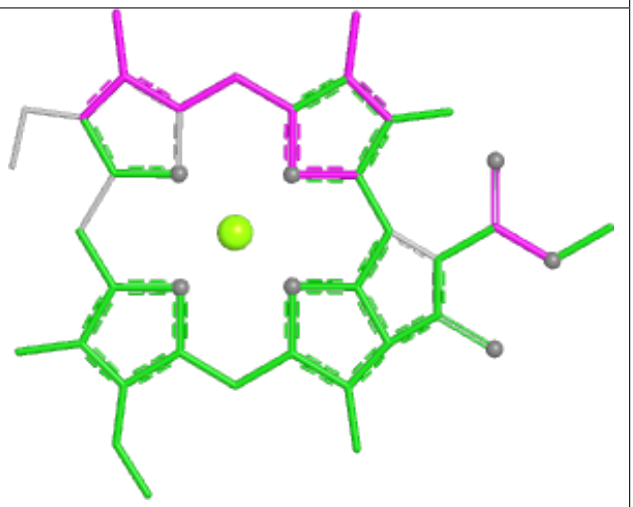
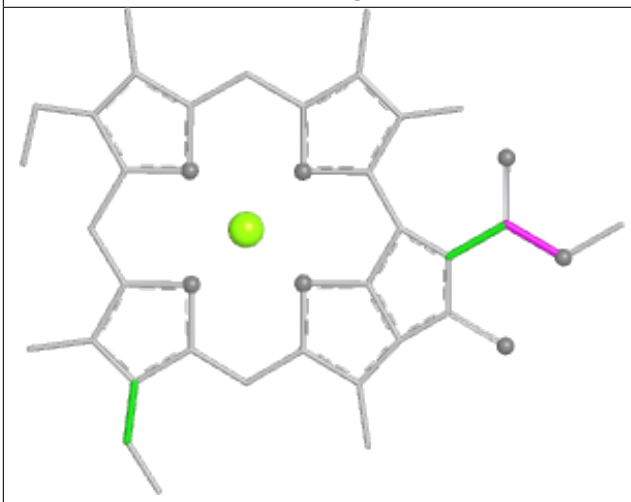
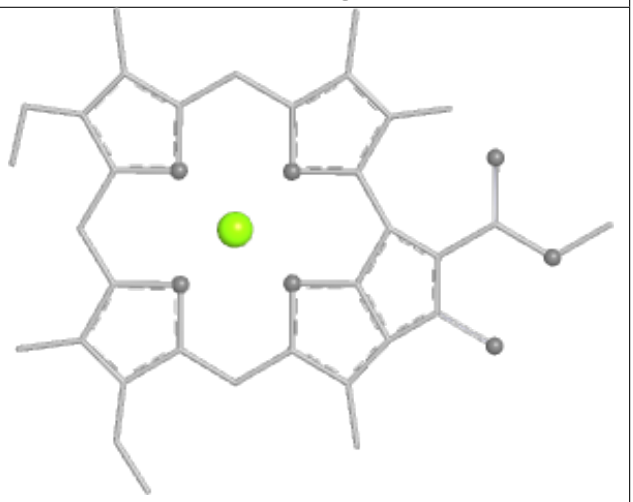
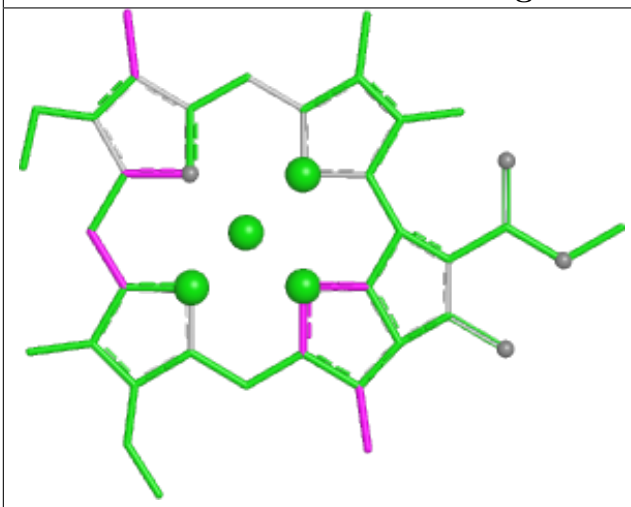
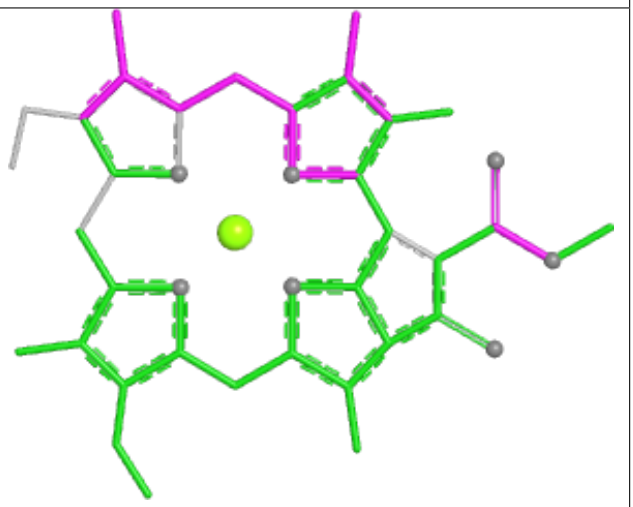
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

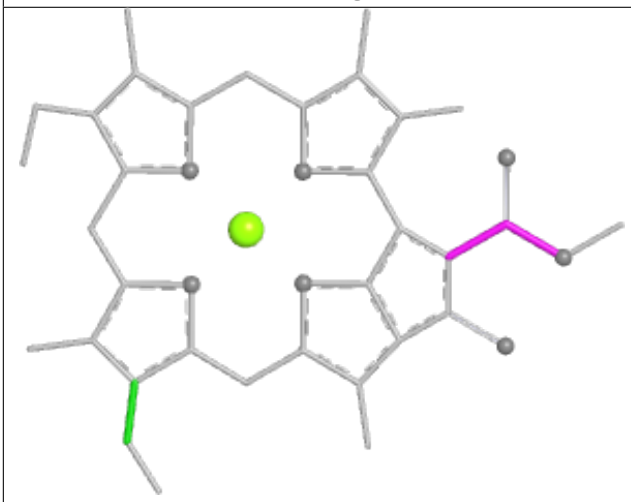
Ligand CLA B1 819



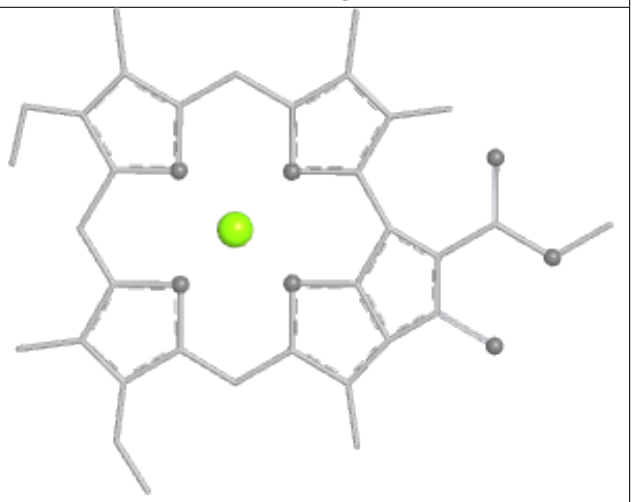
Bond lengths



Bond angles

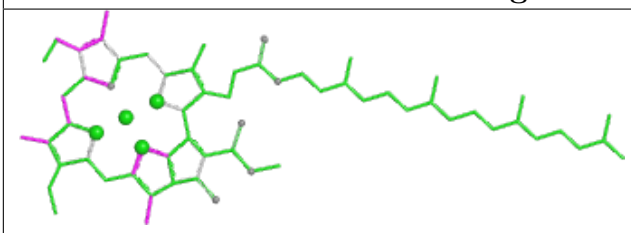


Torsions



Rings

Ligand CLA AA 801



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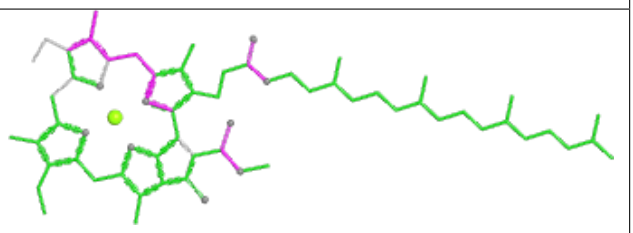
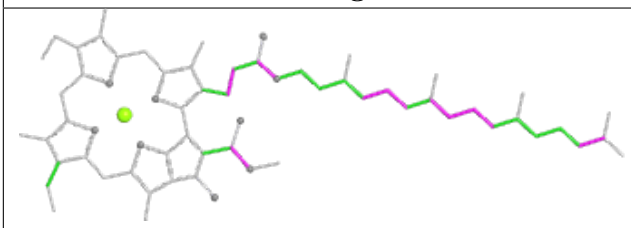
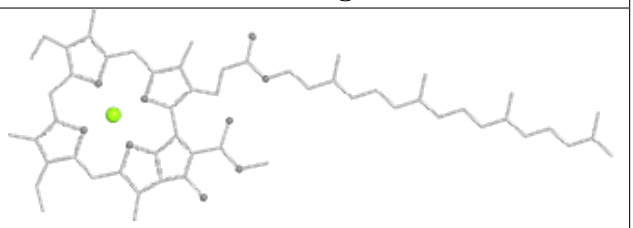


Bond angles

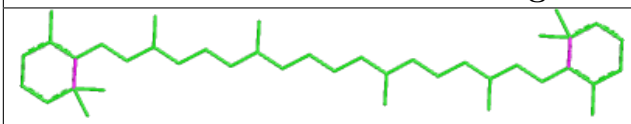


Torsions



Rings

Ligand BCR I 101



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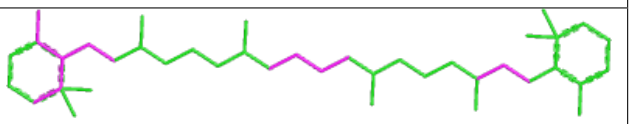
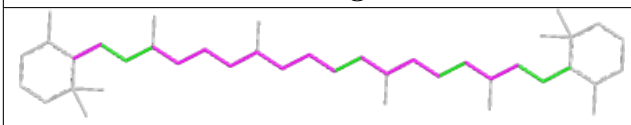


Bond angles



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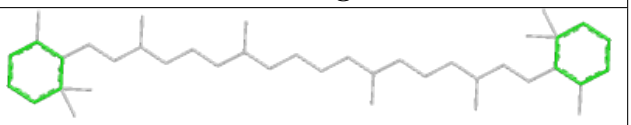
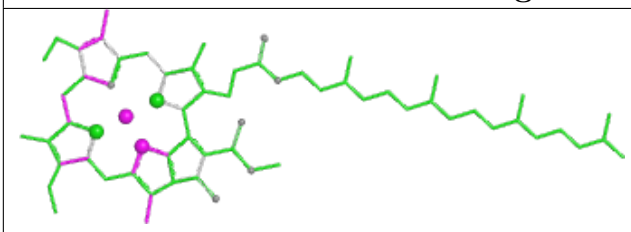


Rings

Ligand CLA A1 842



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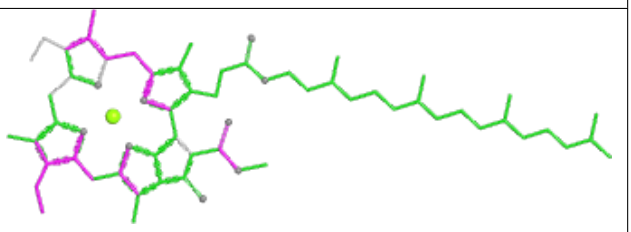
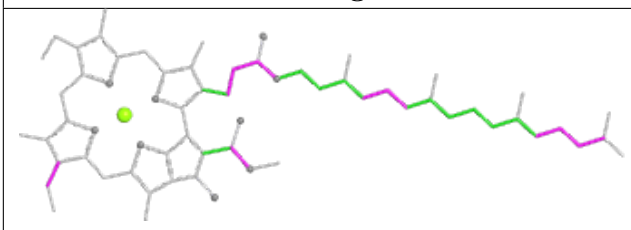
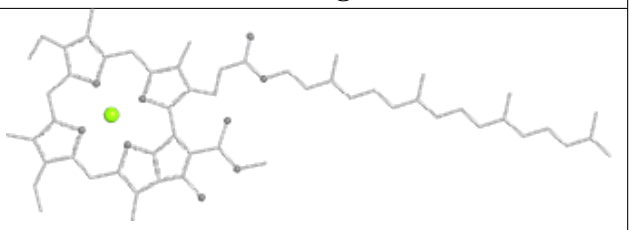


Bond angles

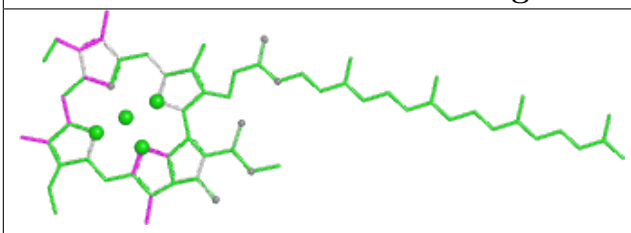


Torsions



Rings

Ligand CLA BB 855



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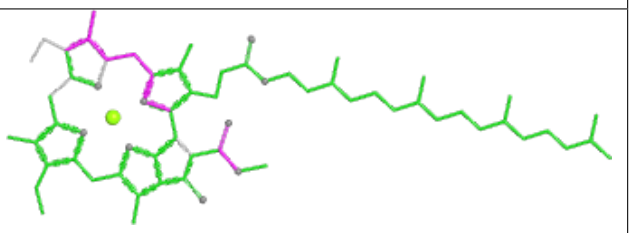
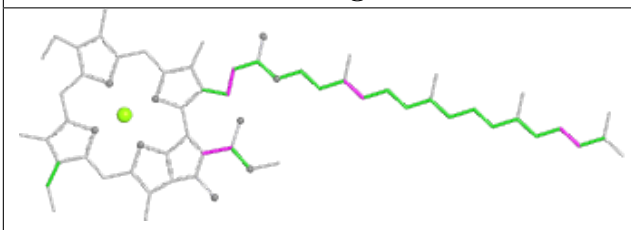


Bond angles



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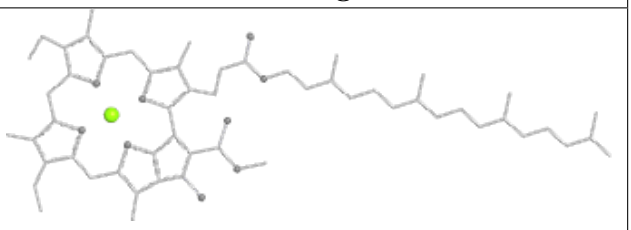
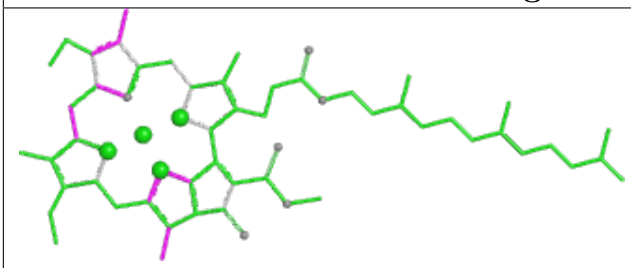
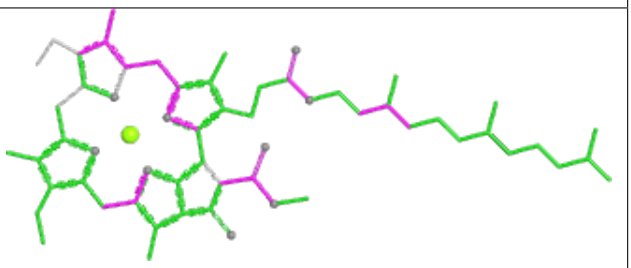
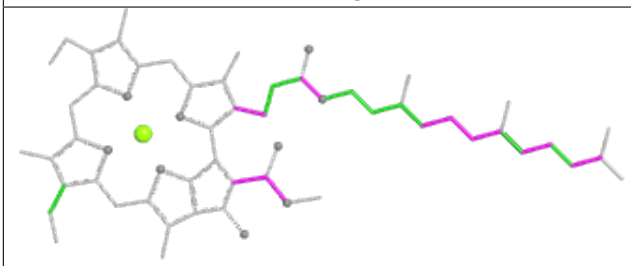
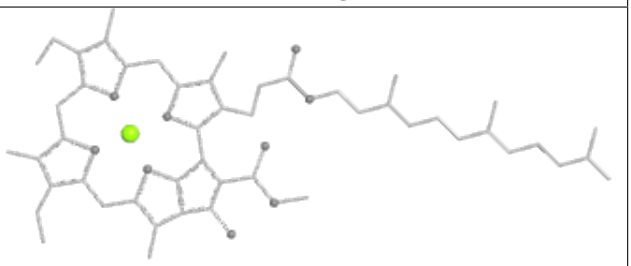


Rings

Ligand CLA A 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

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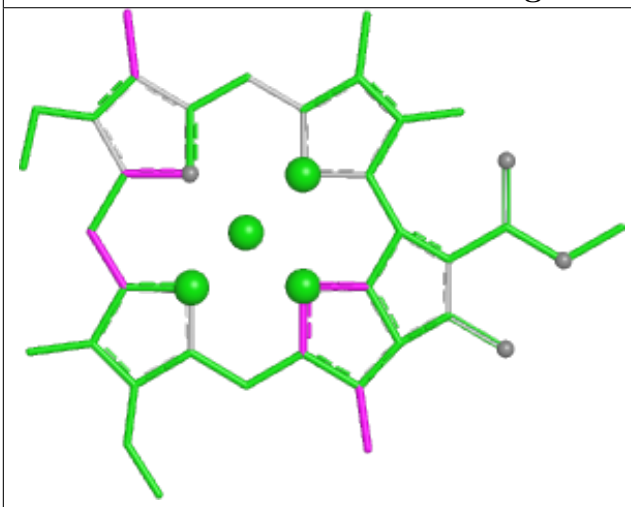
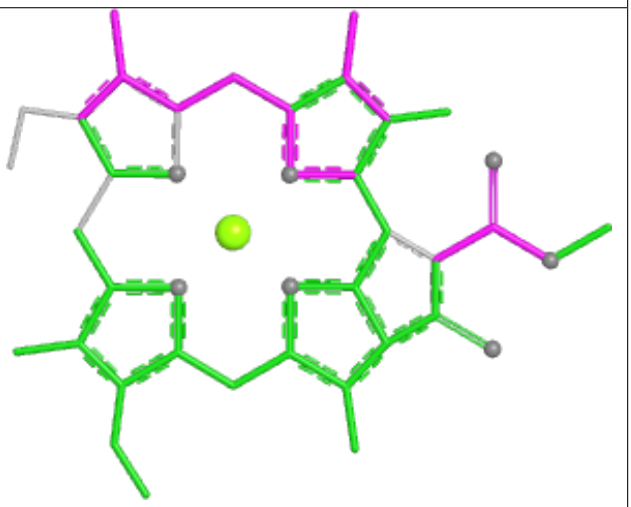
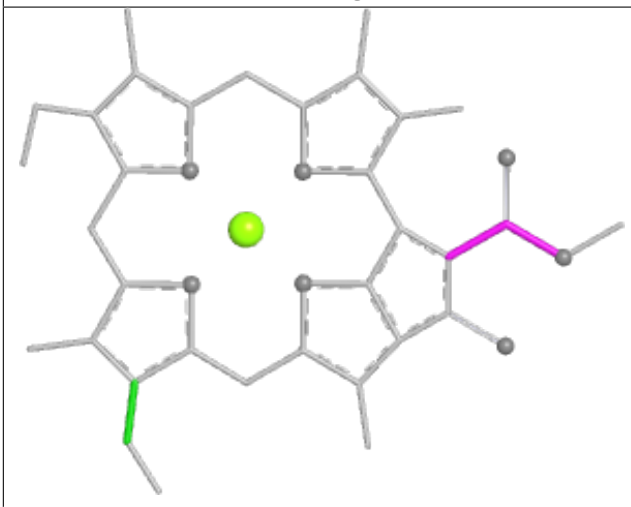
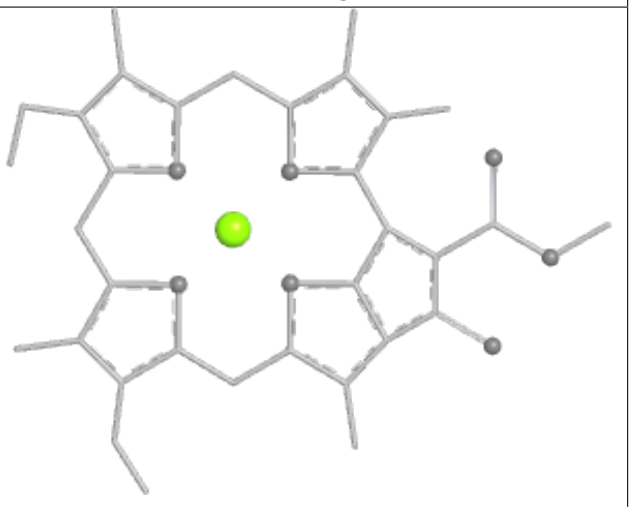
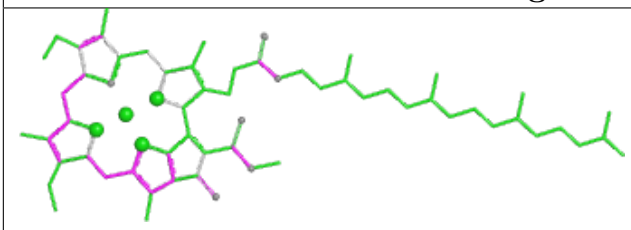
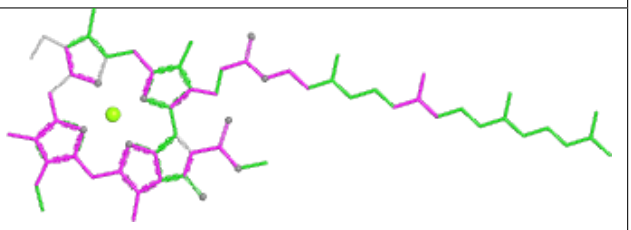
 Bond lengths	 Bond angles
 Torsions	 Rings

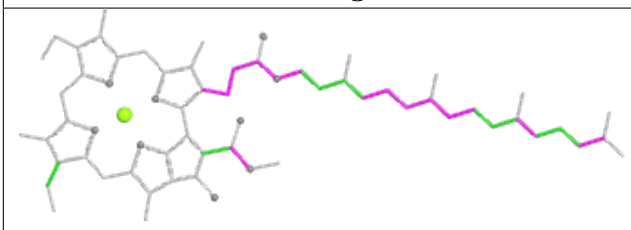
Ligand CL0 A 803



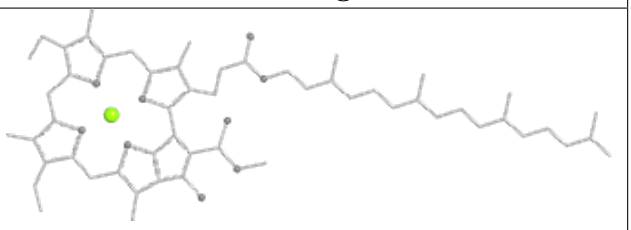
Bond lengths



Bond angles

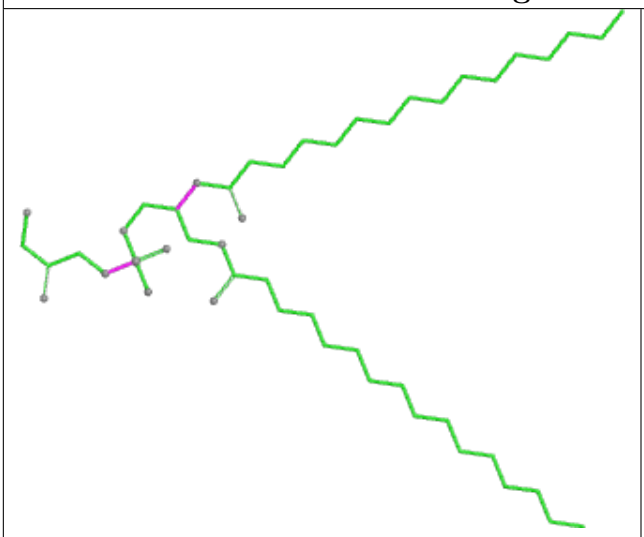


Torsions

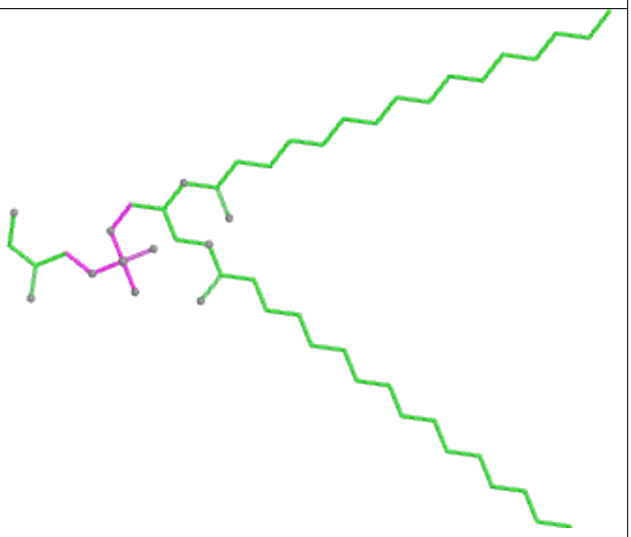


Rings

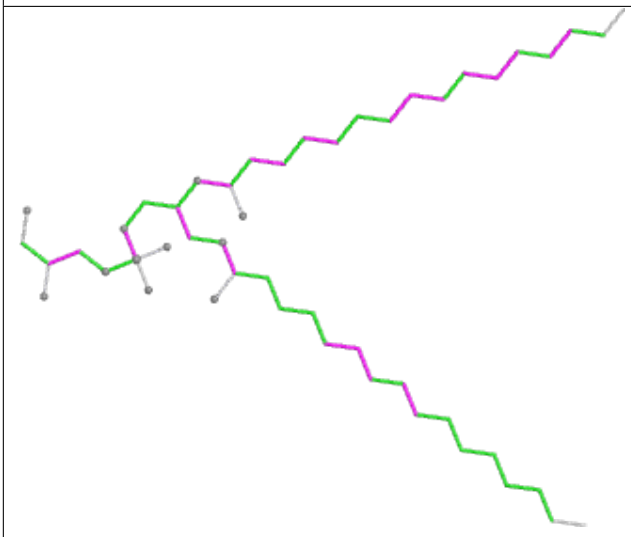
Ligand LHG A1 845



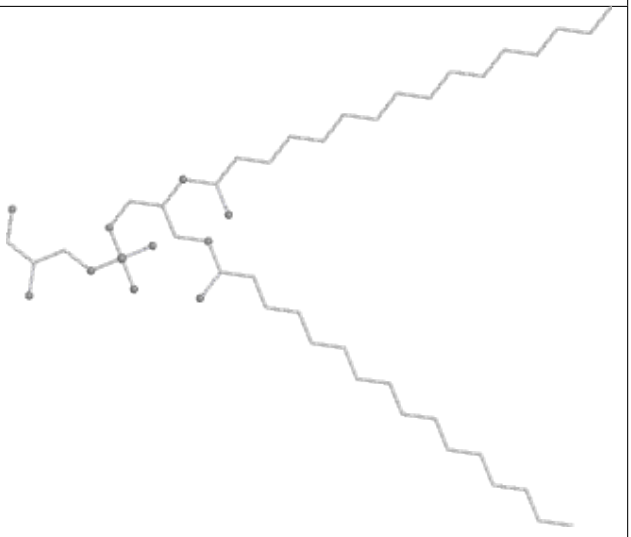
Bond lengths



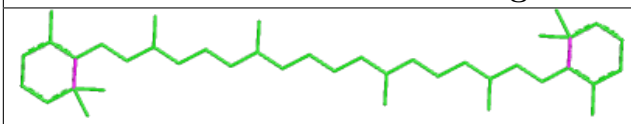
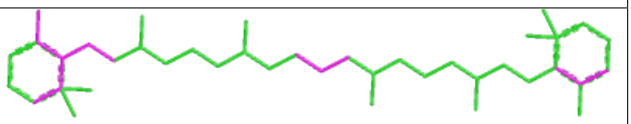
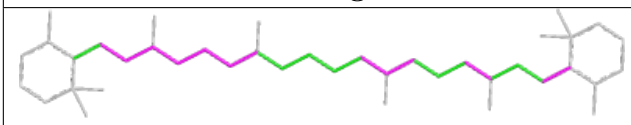
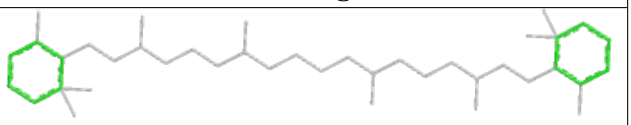
Bond angles

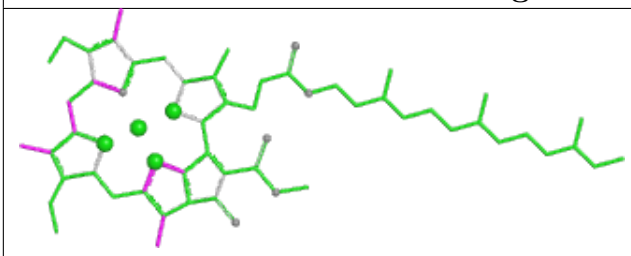
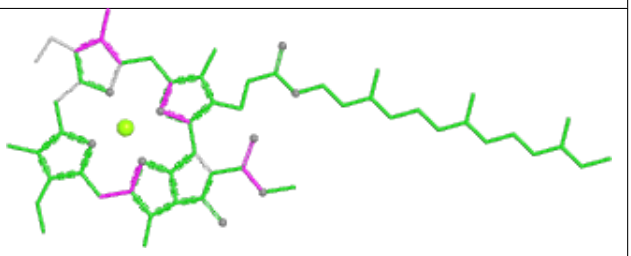
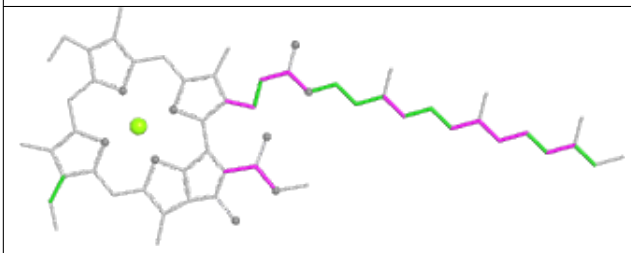
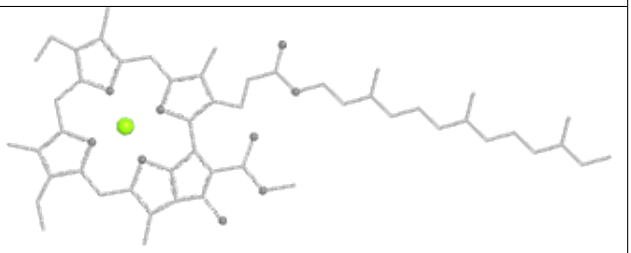


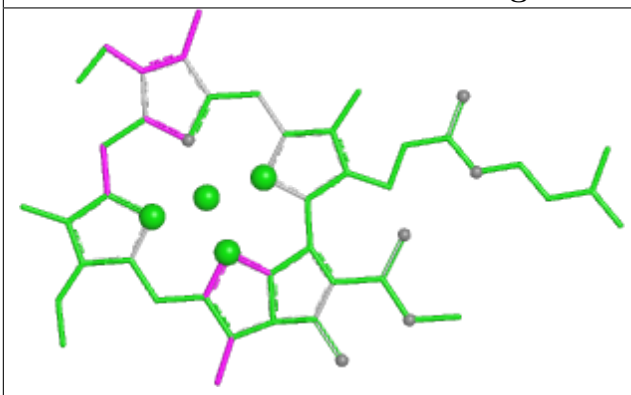
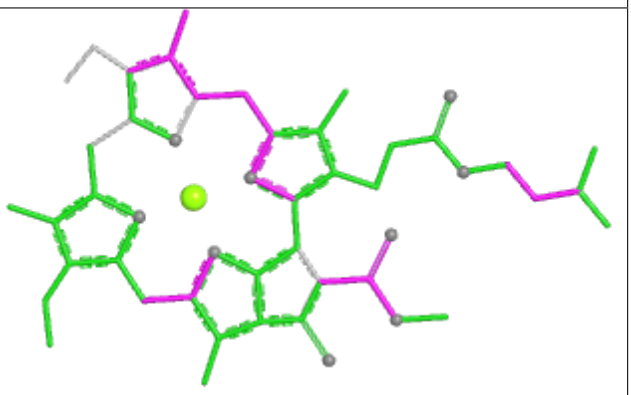
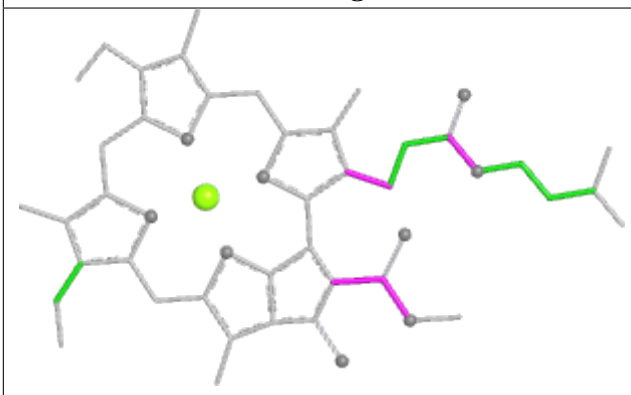
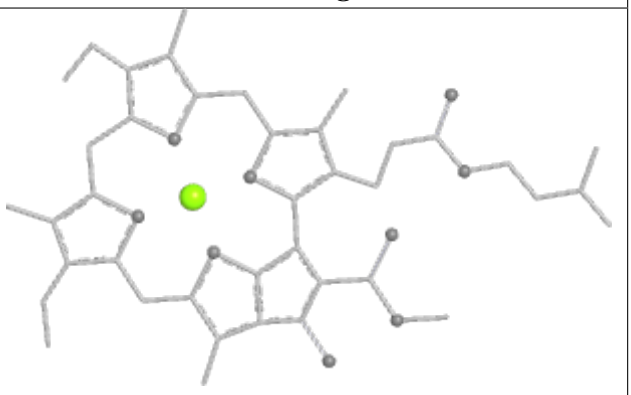
Torsions

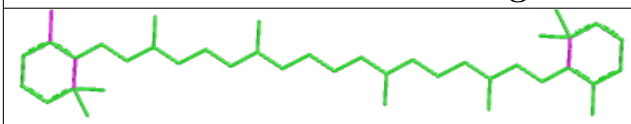
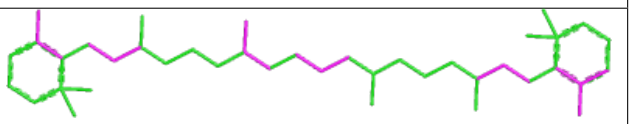
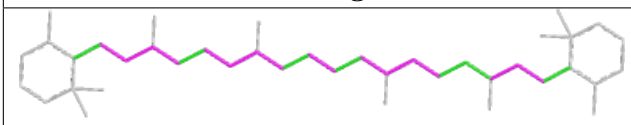
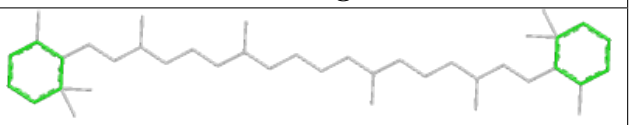


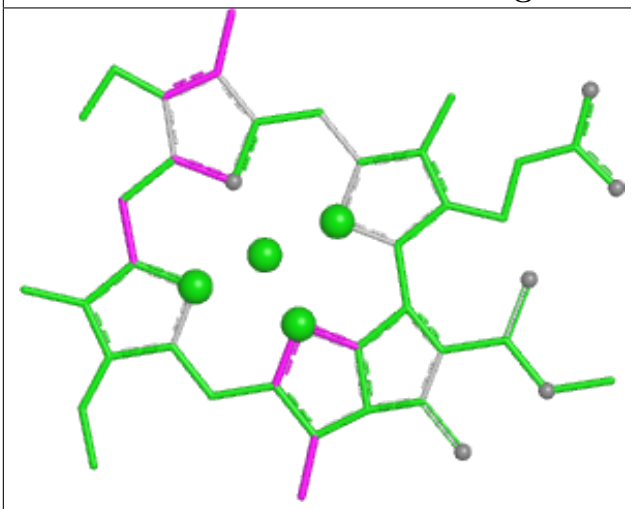
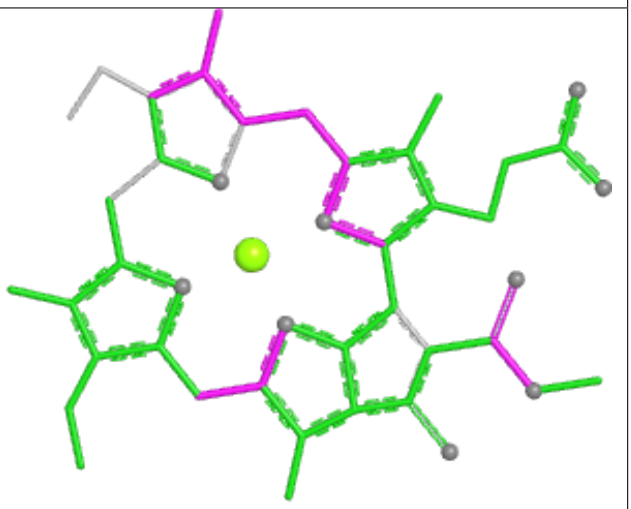
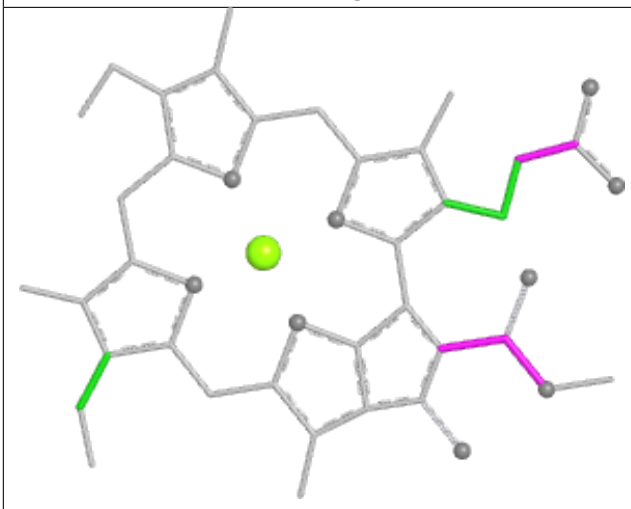
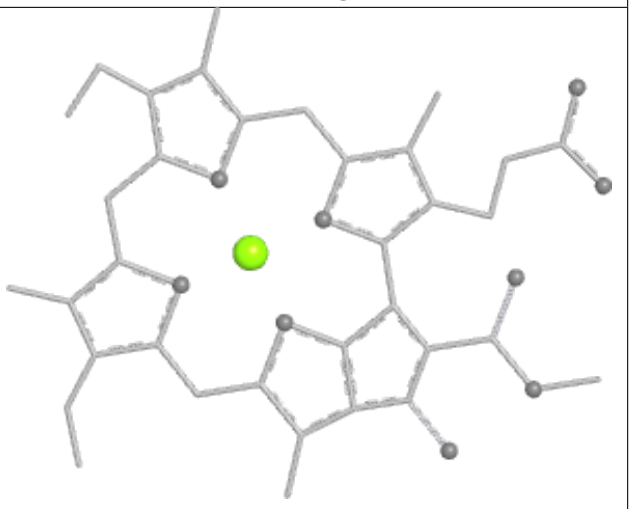
Rings

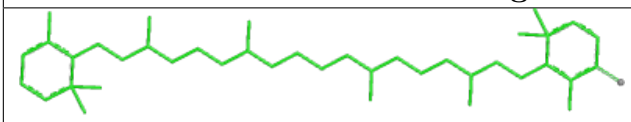
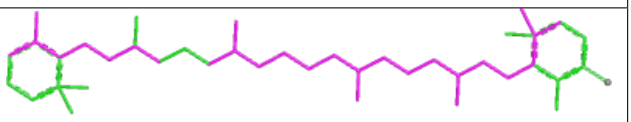
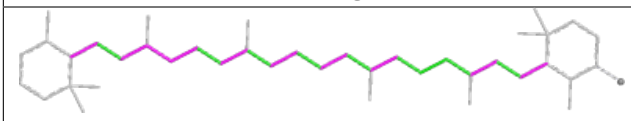
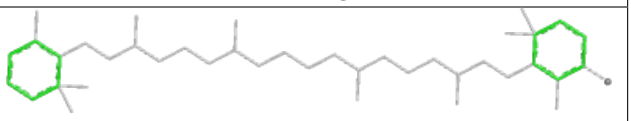
Ligand BCR BB 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

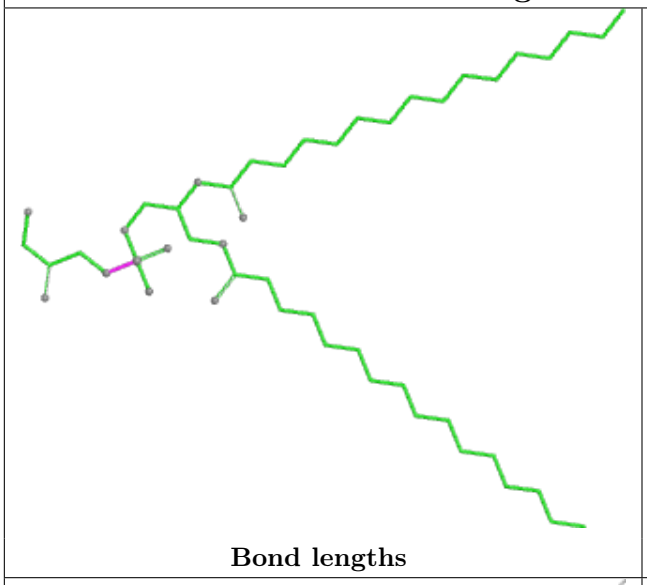
Ligand CLA AA 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR M1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

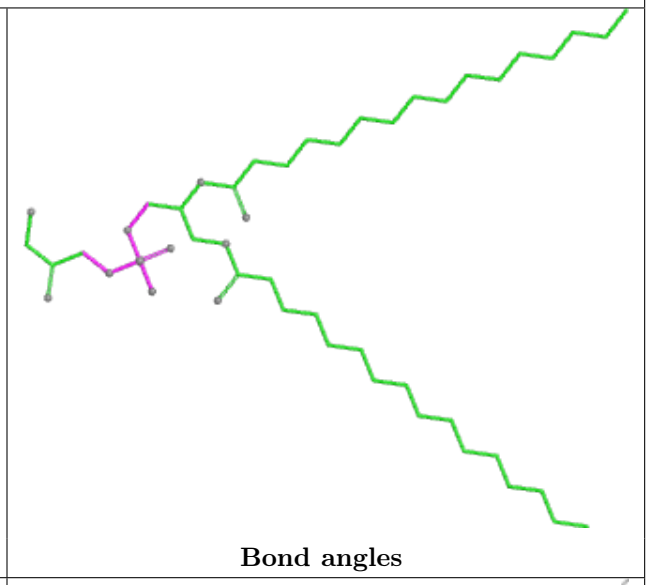
Ligand CLA A1 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ECH BB 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

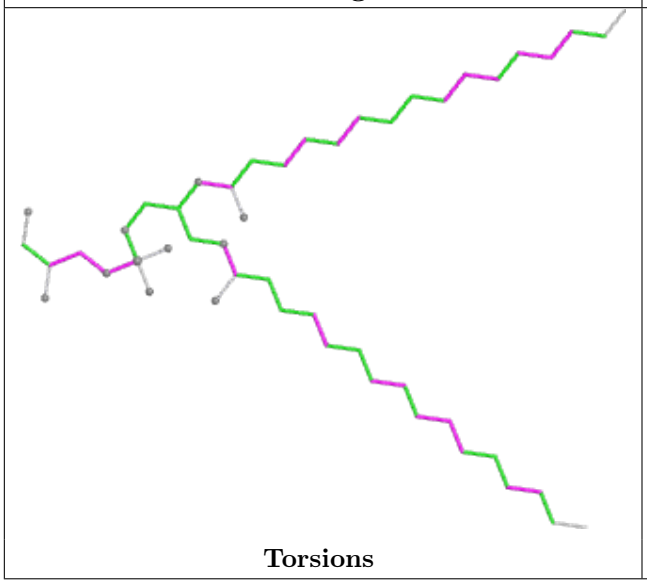
Ligand LHG X1 103



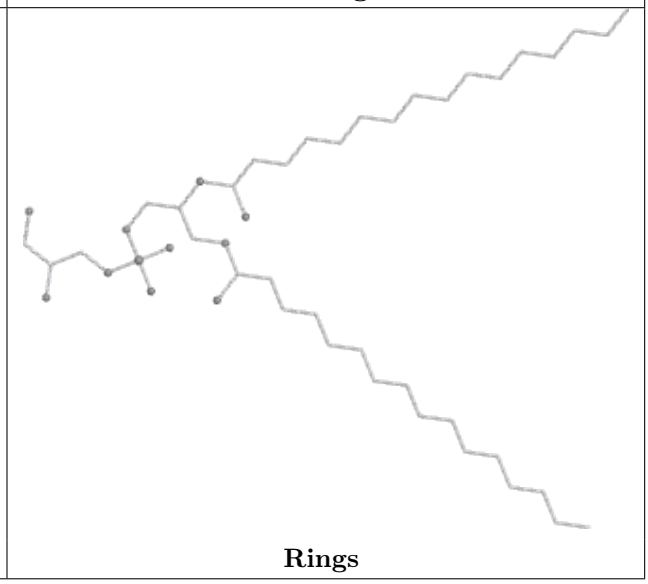
Bond lengths



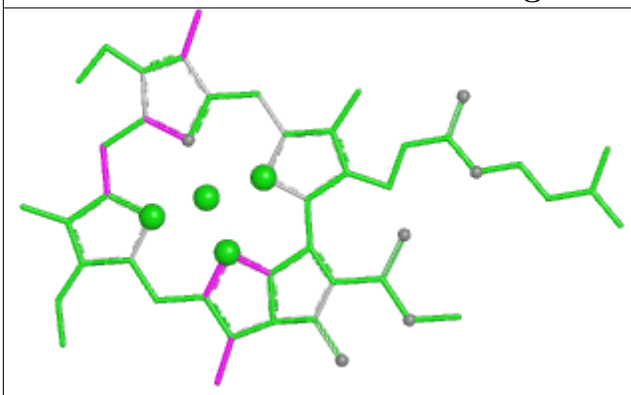
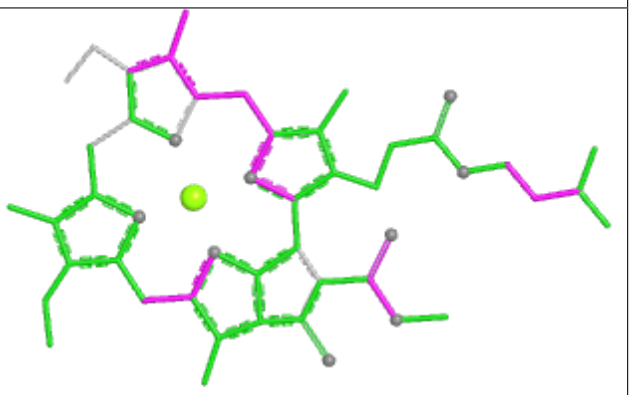
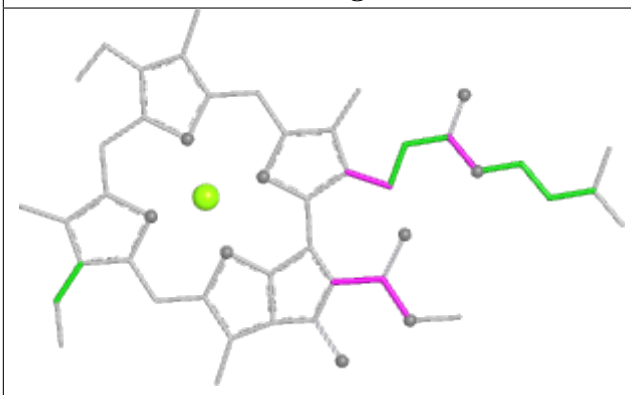
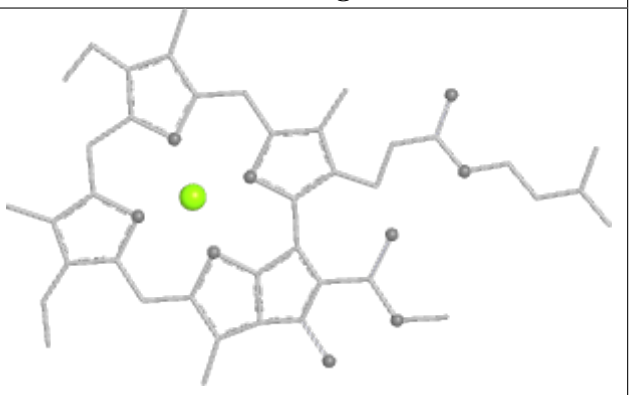
Bond angles

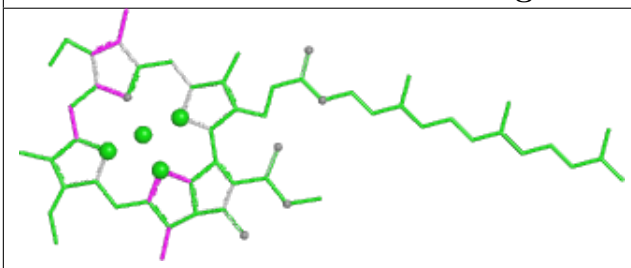
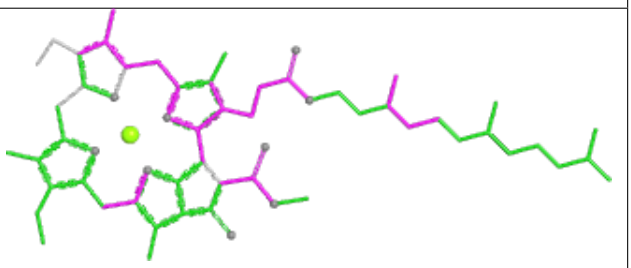
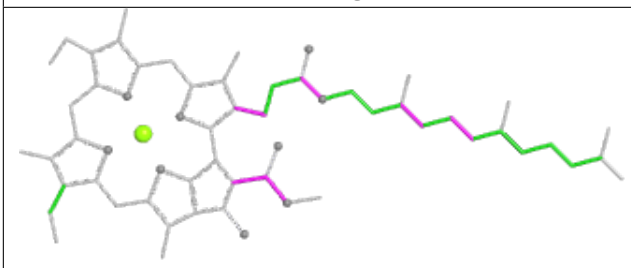
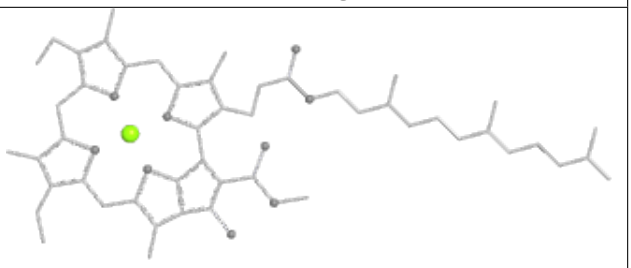


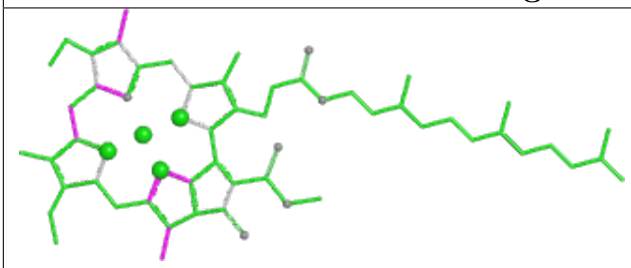
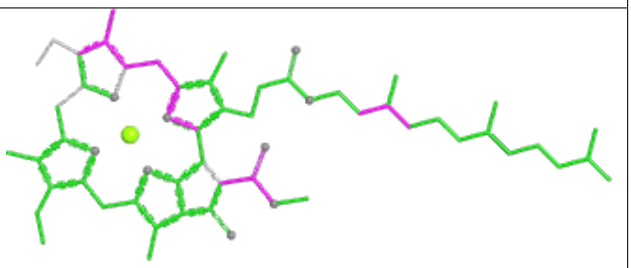
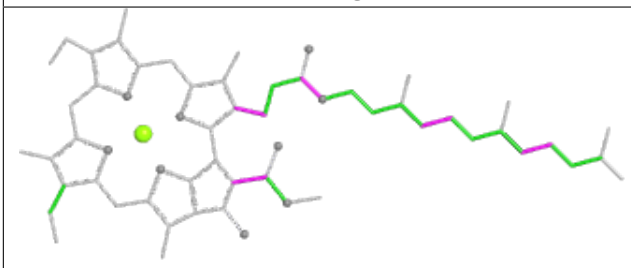
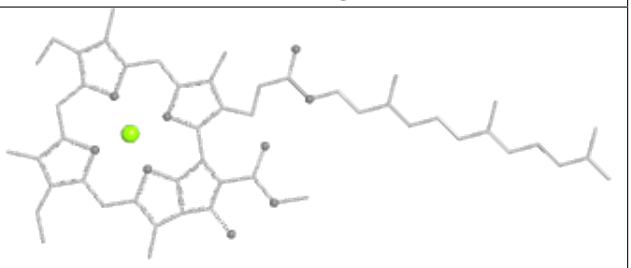
Torsions

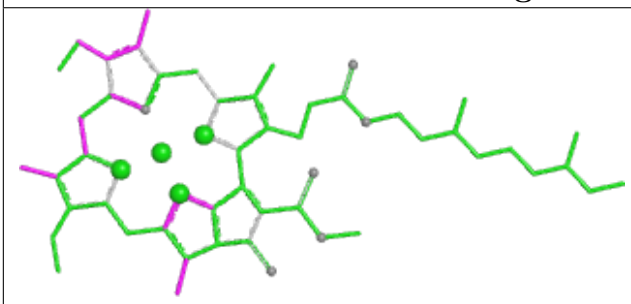
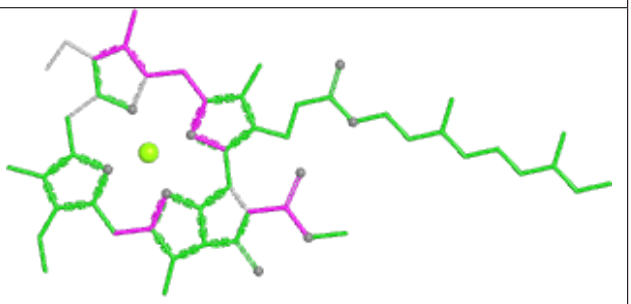
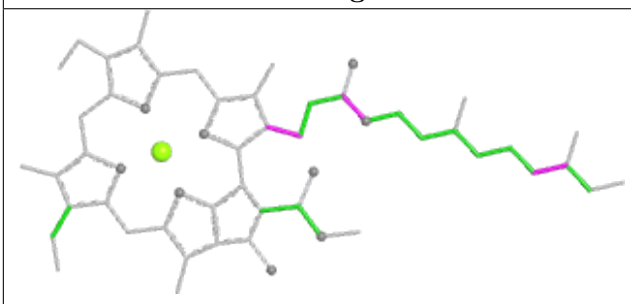
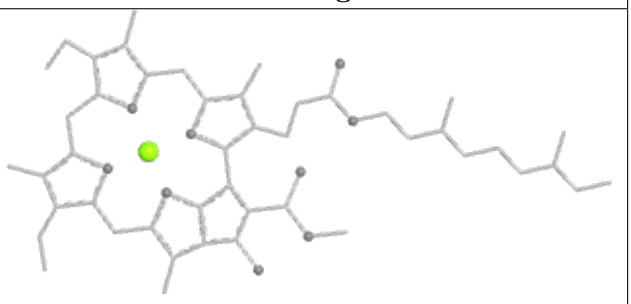


Rings

Ligand CLA A 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

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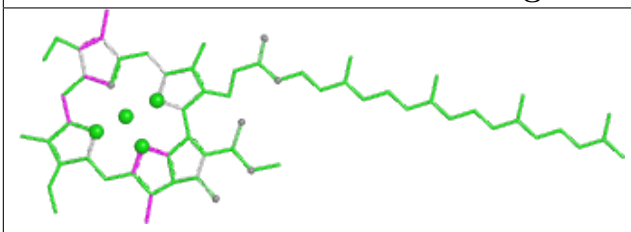
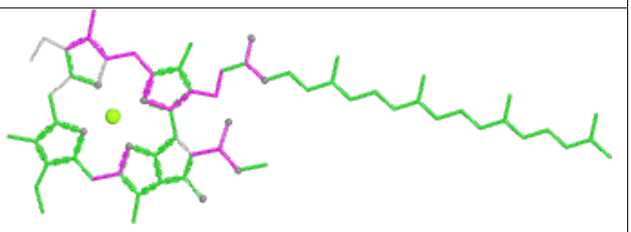
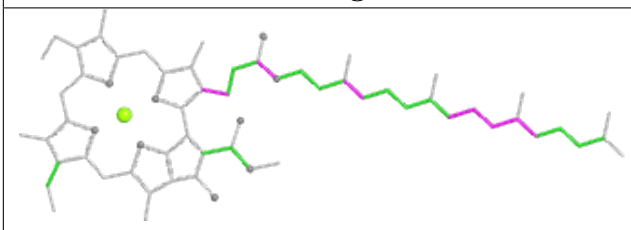
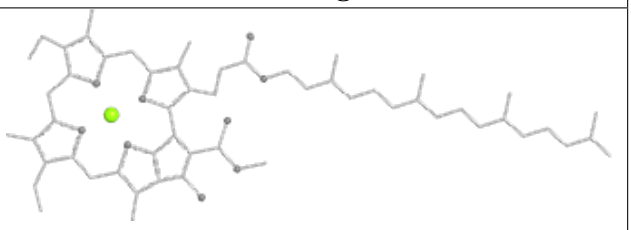
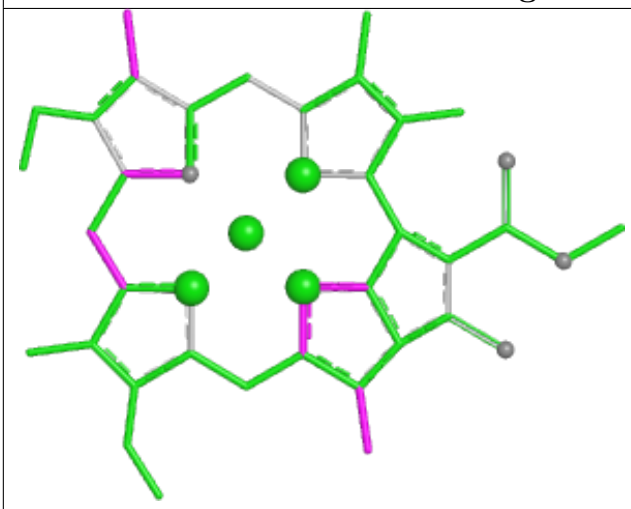
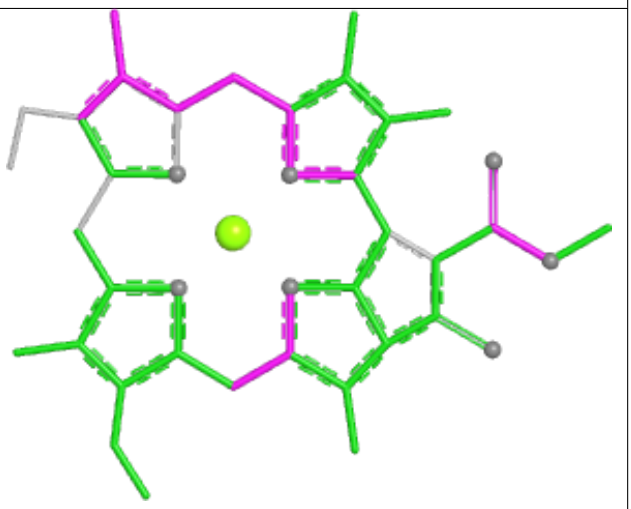
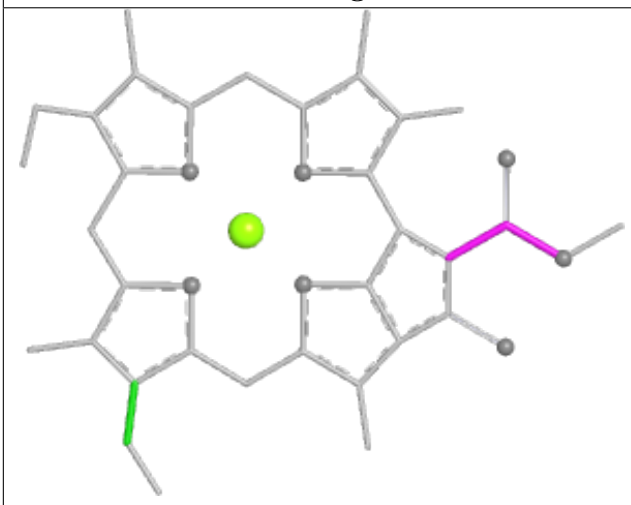
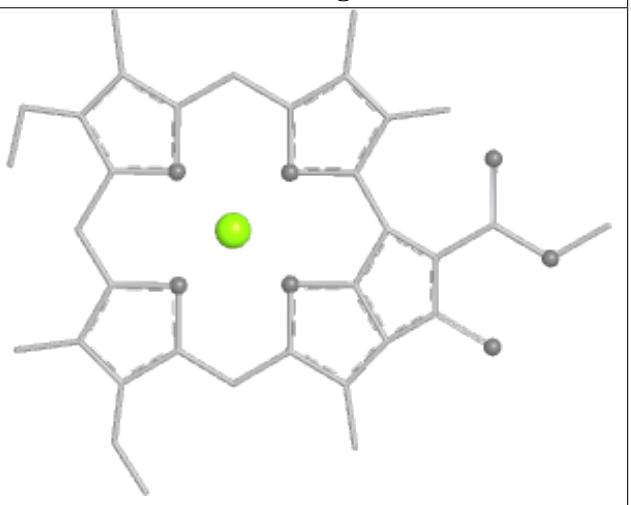
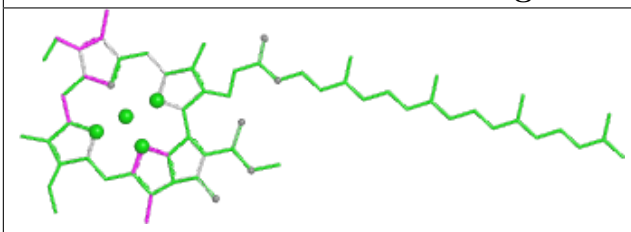
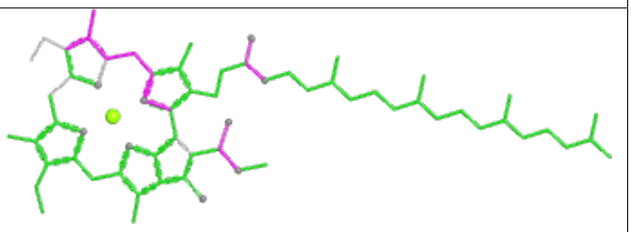
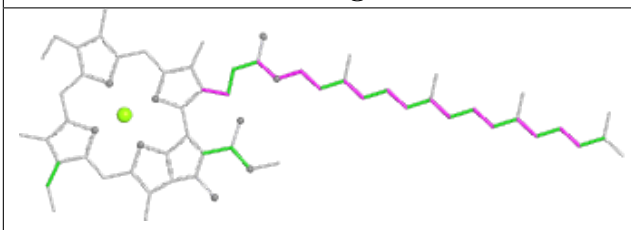
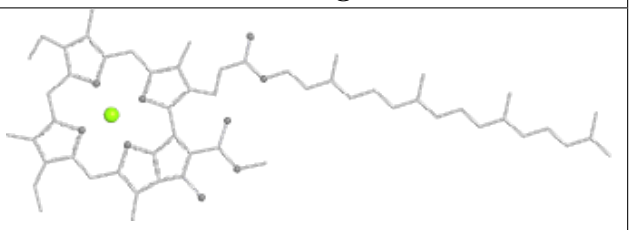
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

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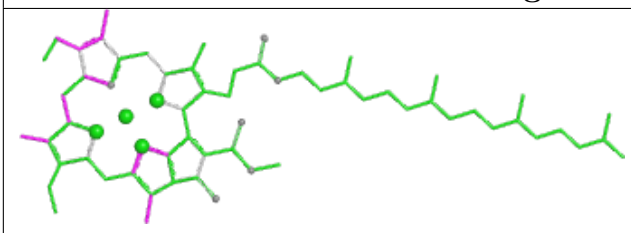
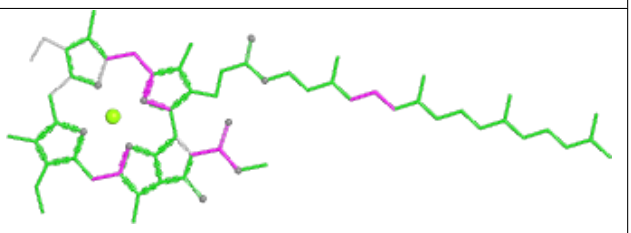
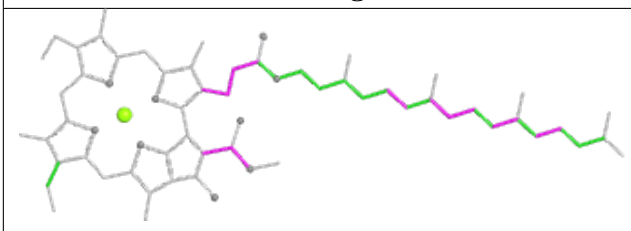
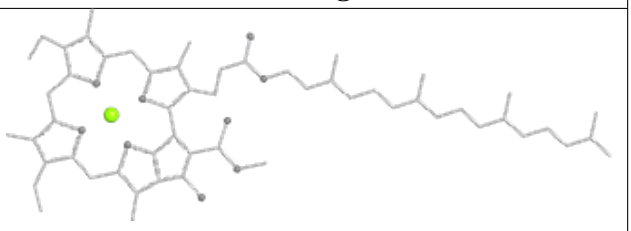
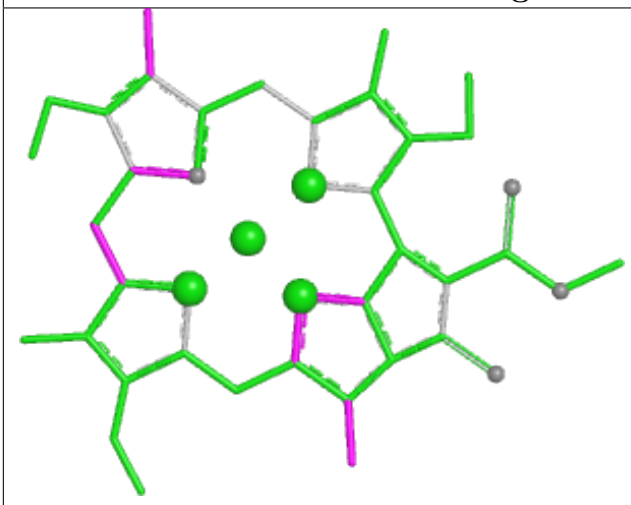
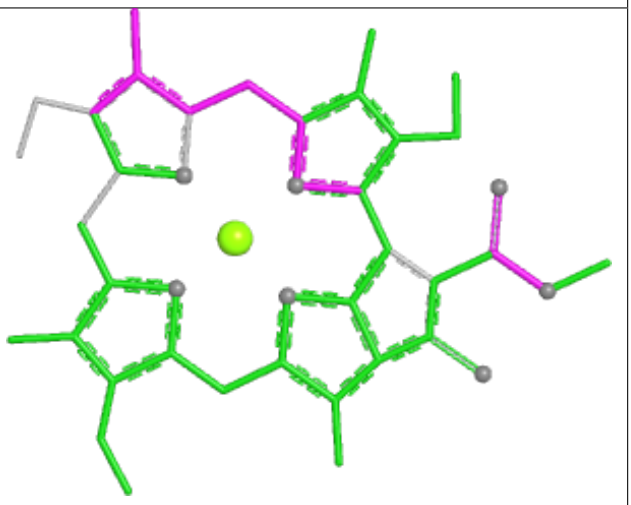
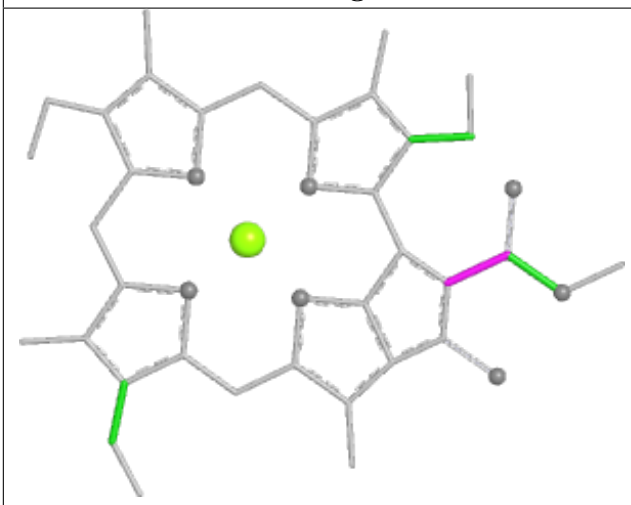
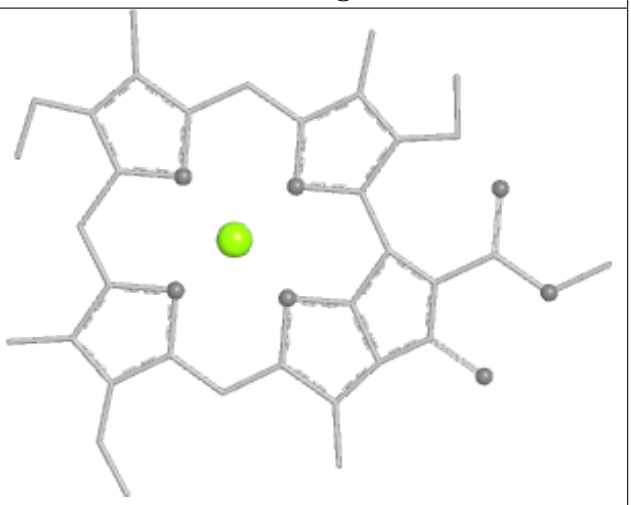
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

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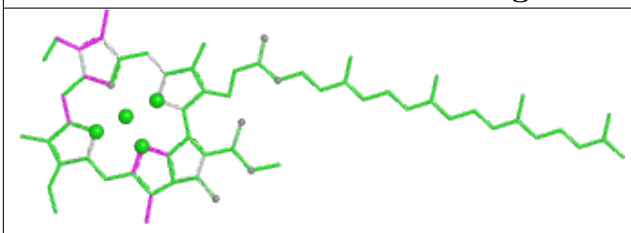
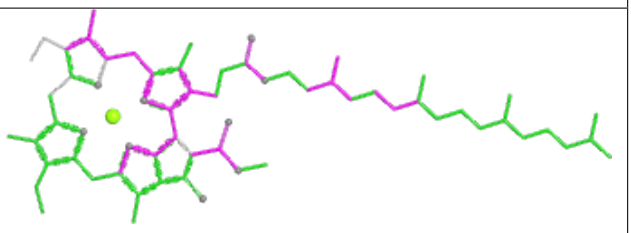
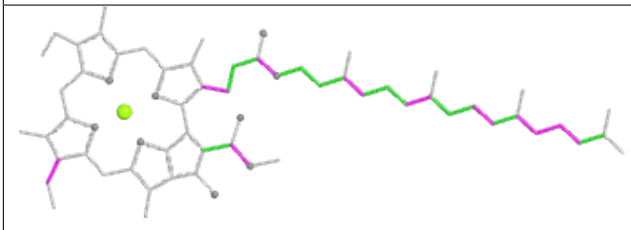
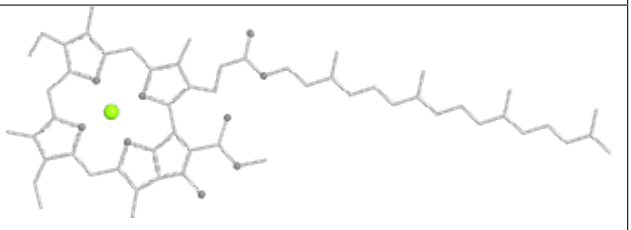
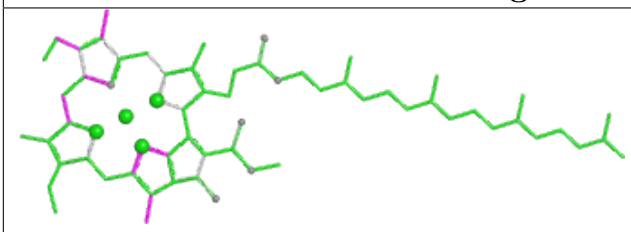
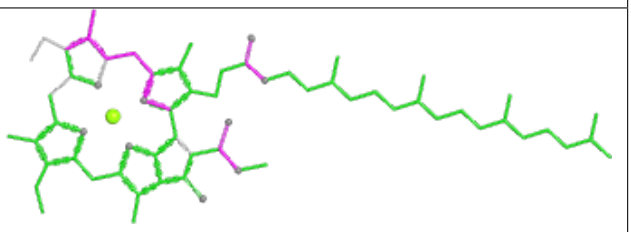
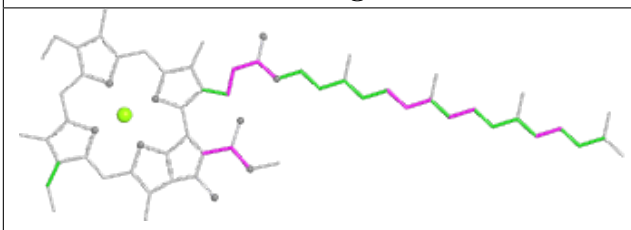
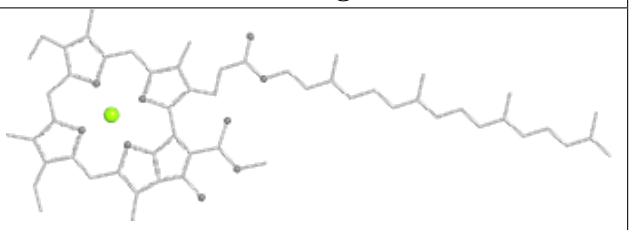
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

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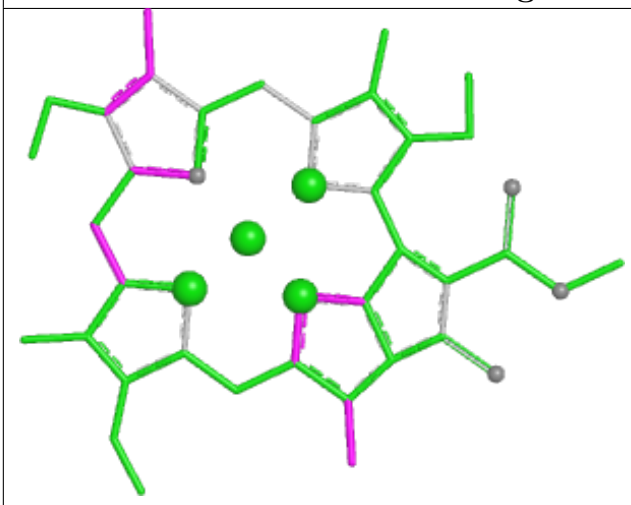
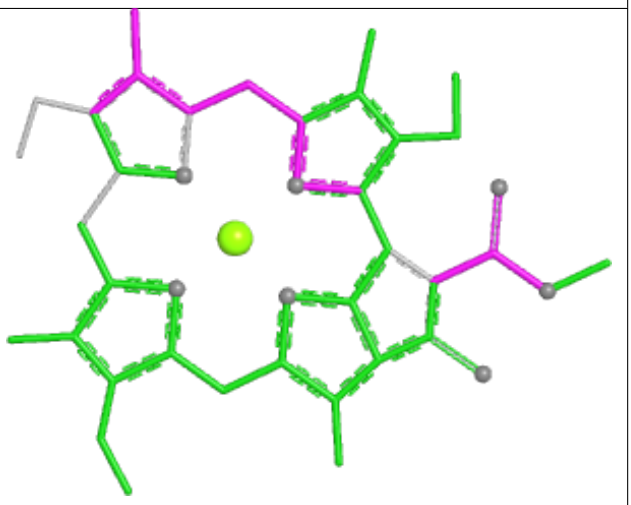
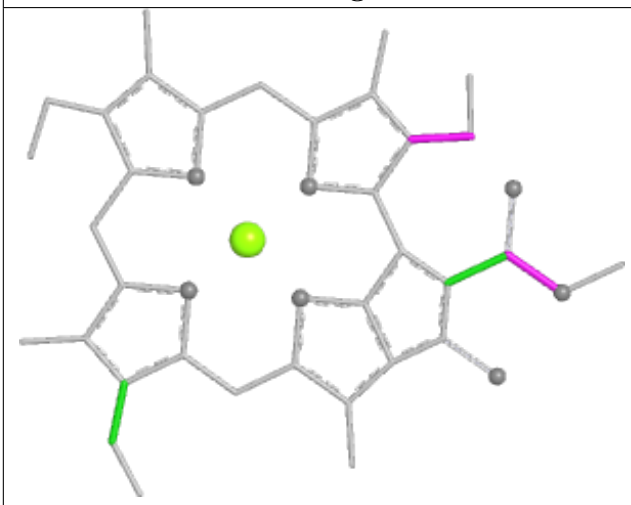
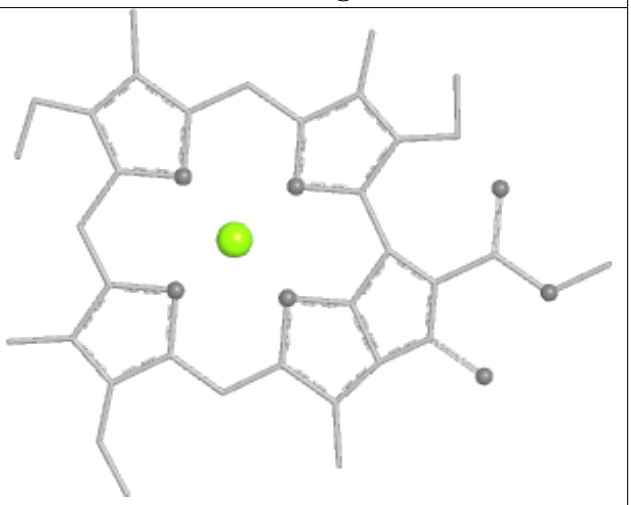
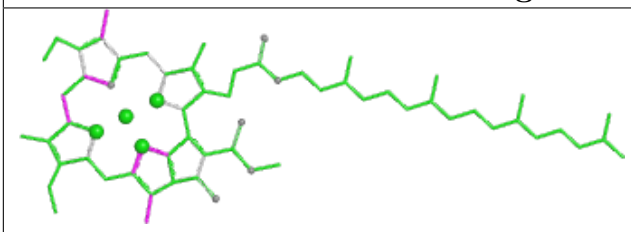
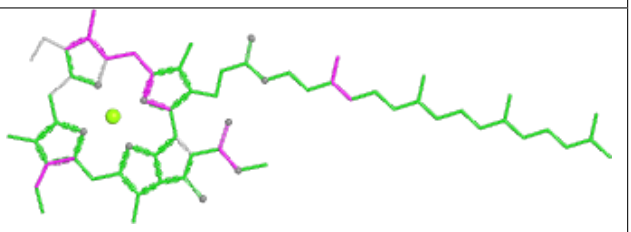
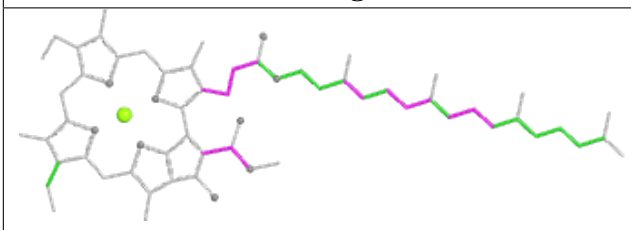
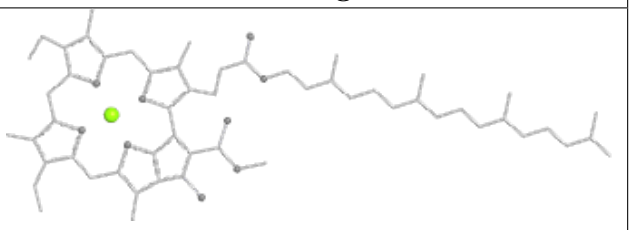
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

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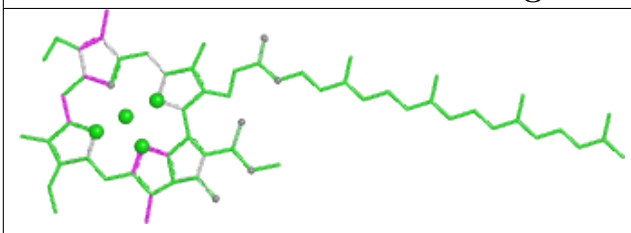
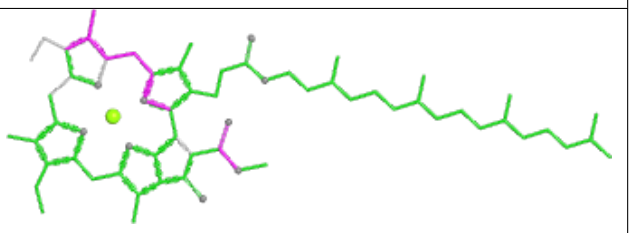
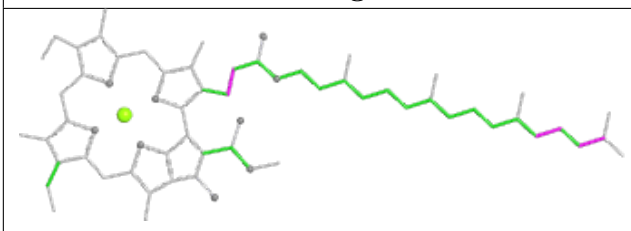
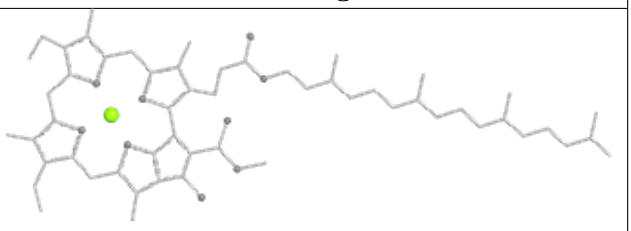
 Bond lengths	 Bond angles
 Torsions	 Rings

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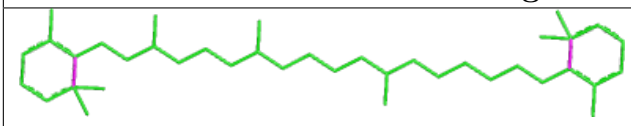
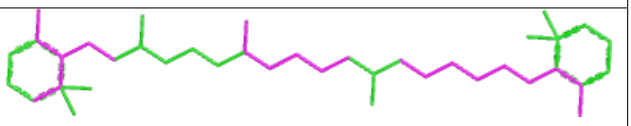
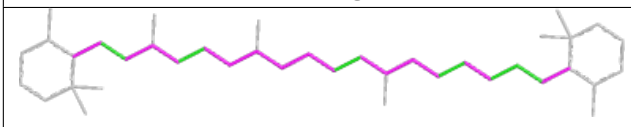
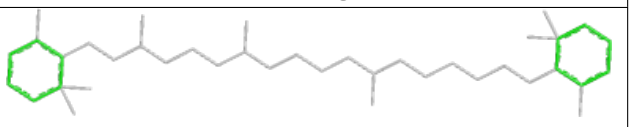
 Bond lengths	 Bond angles
 Torsions	 Rings

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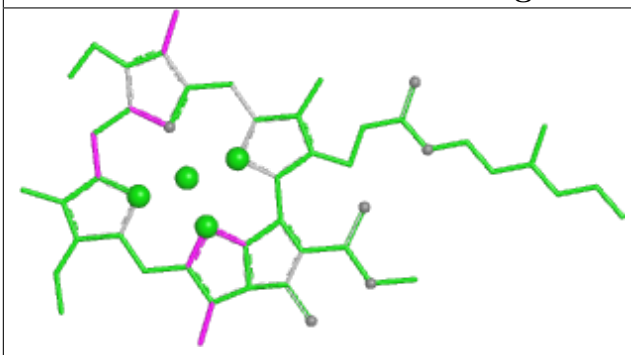
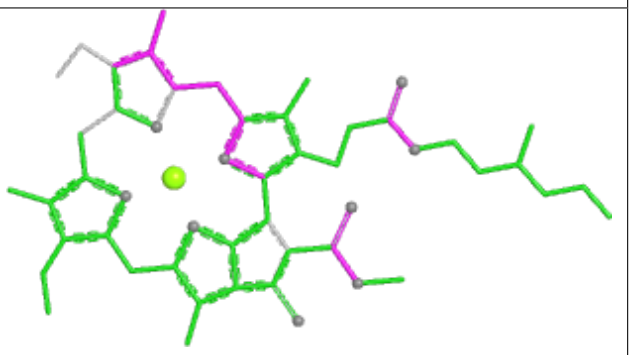
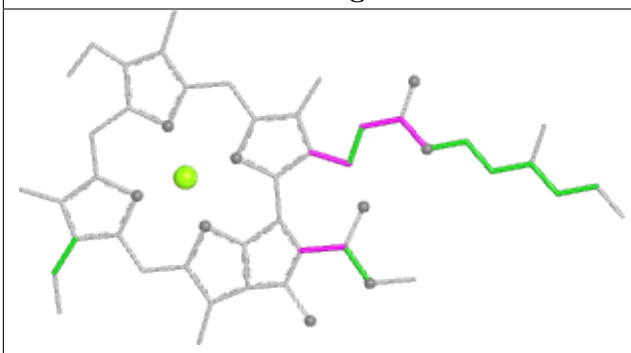
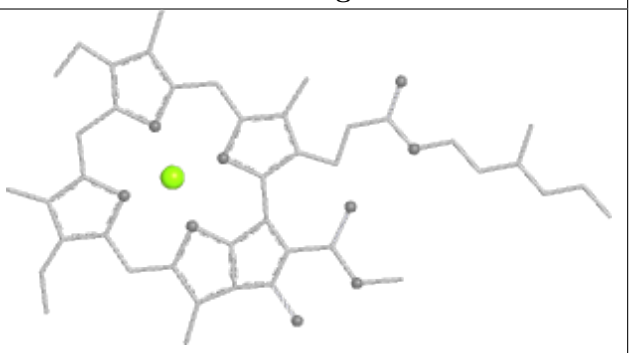
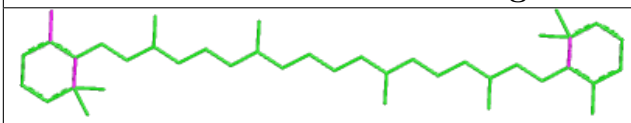
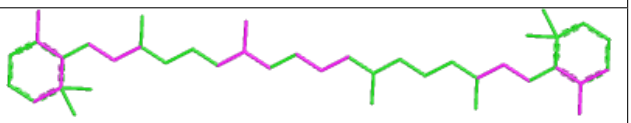
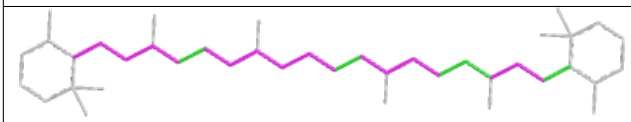
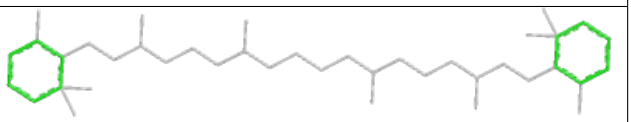
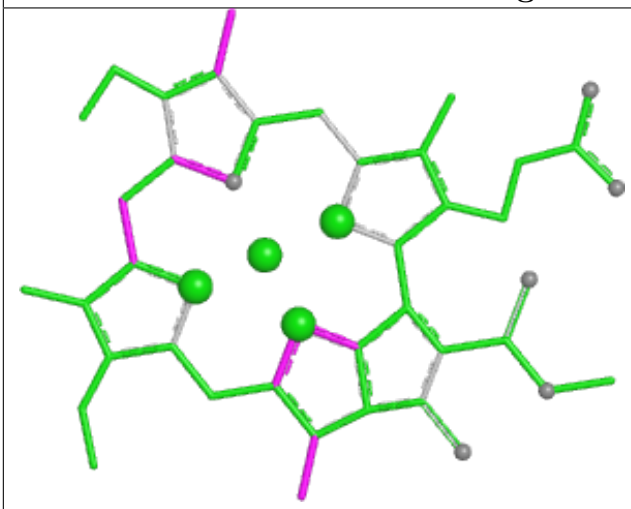
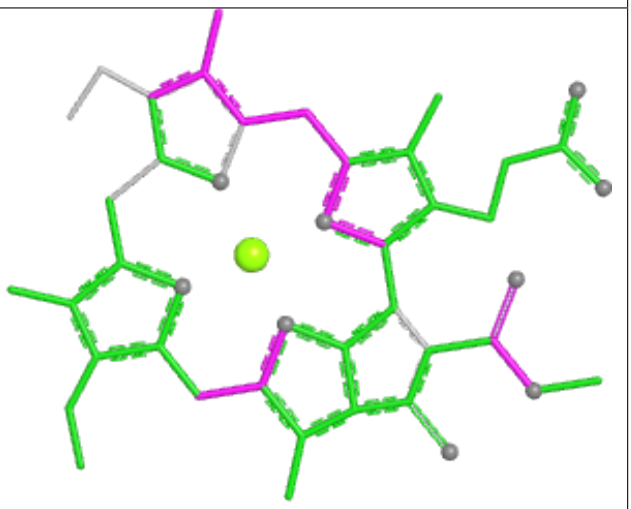
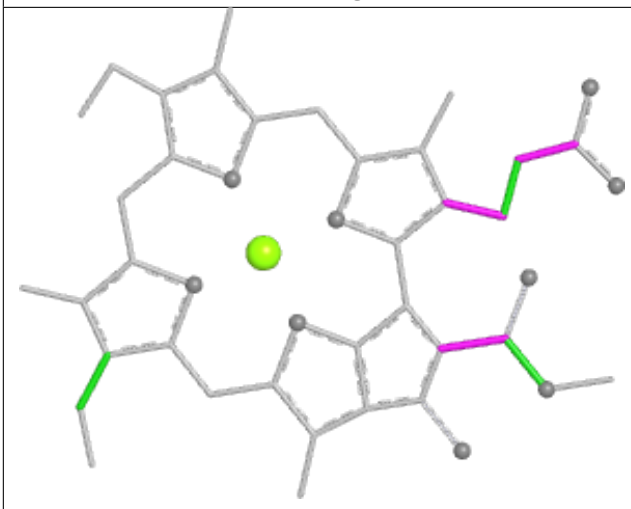
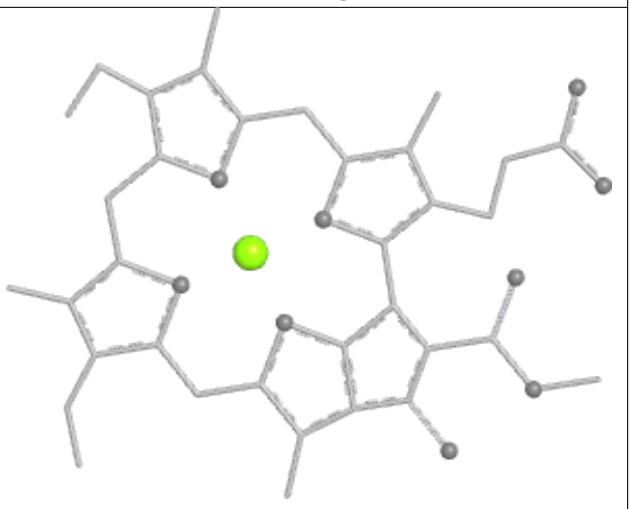
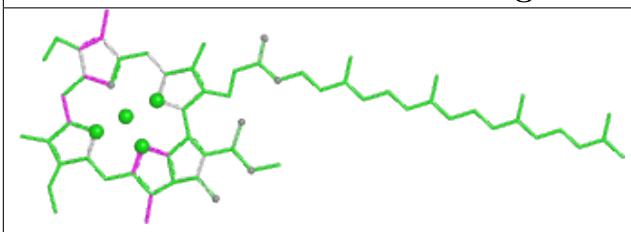
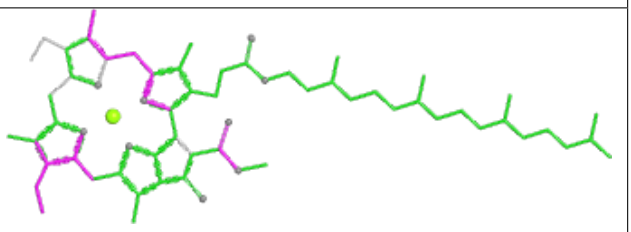
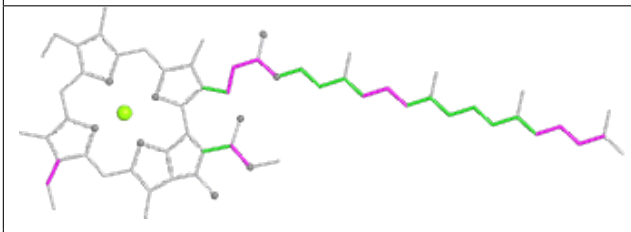
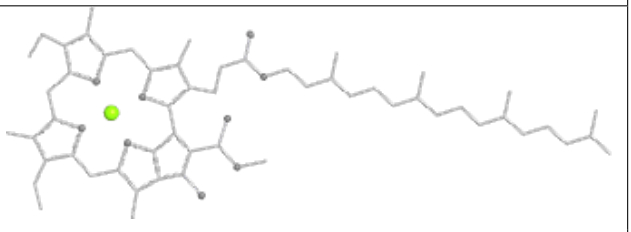
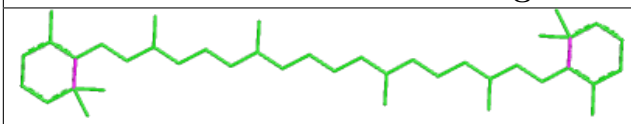
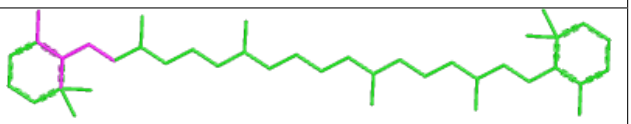
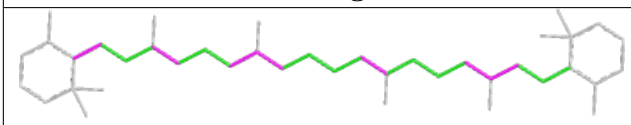
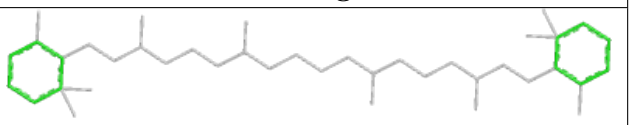
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR M2 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F1 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B2 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B1 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

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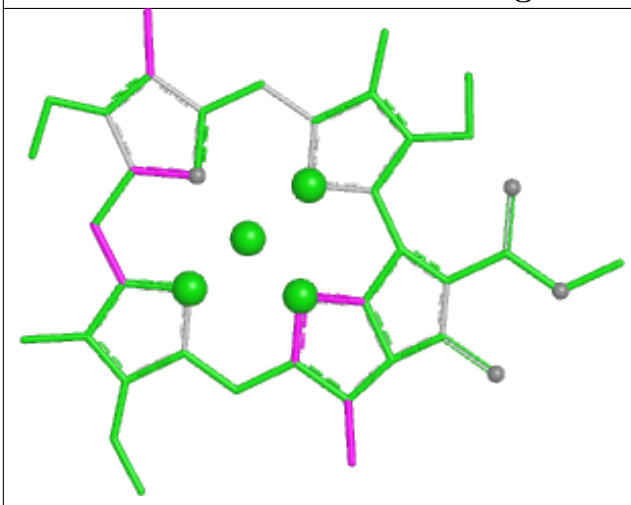
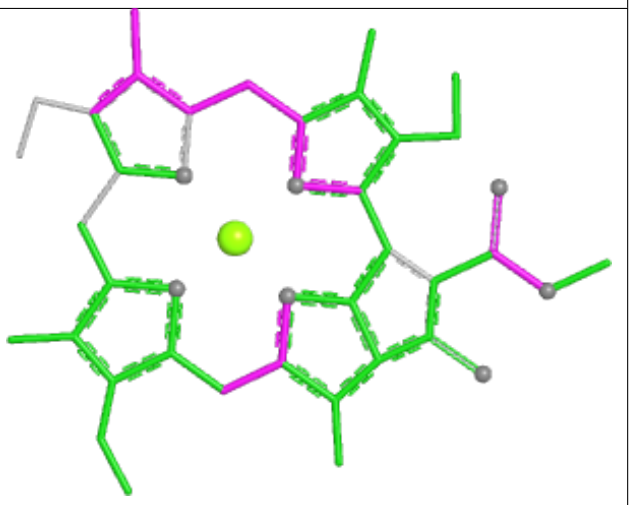
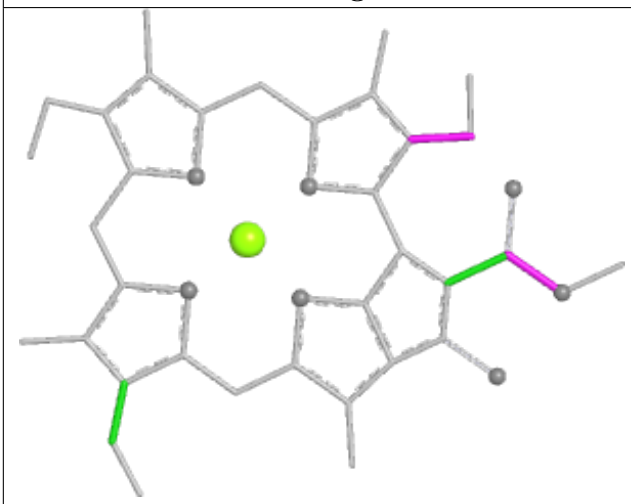
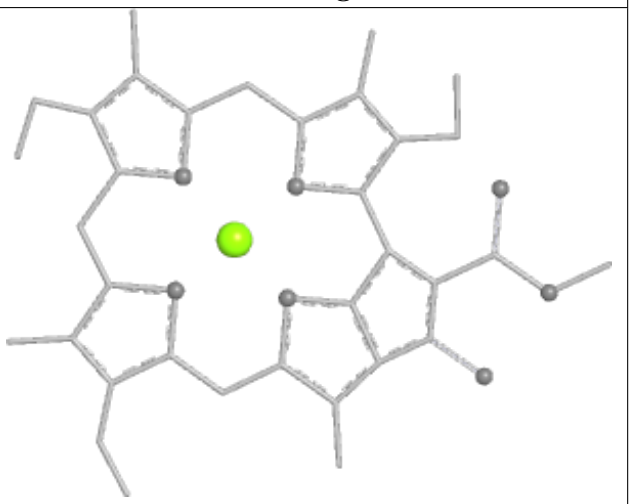
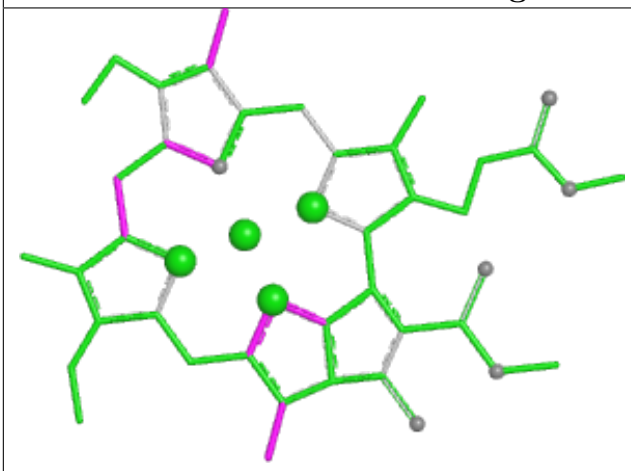
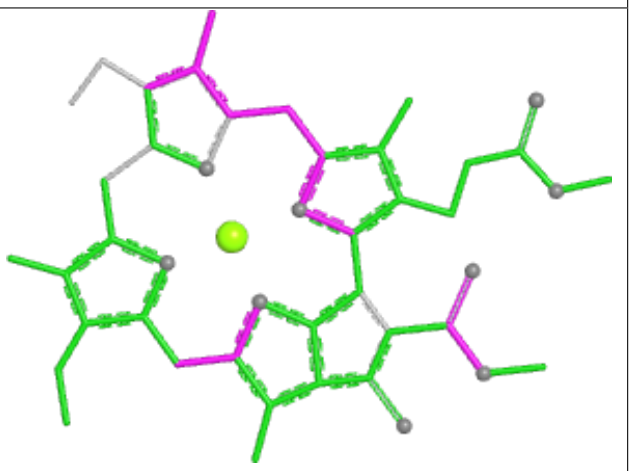
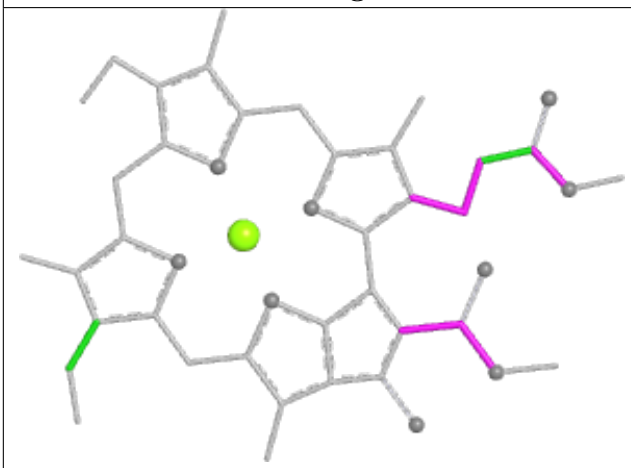
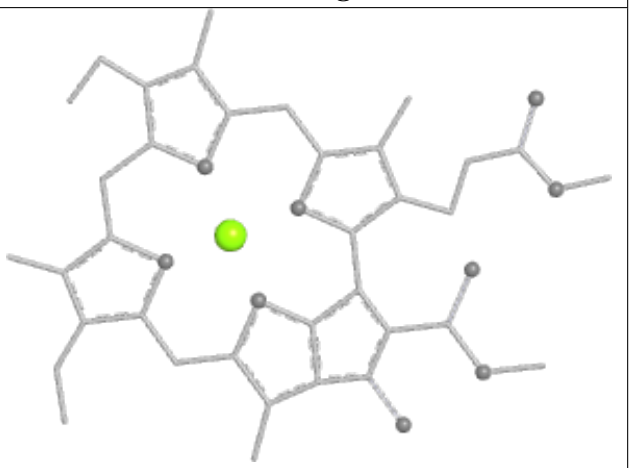
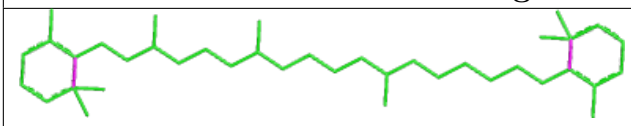
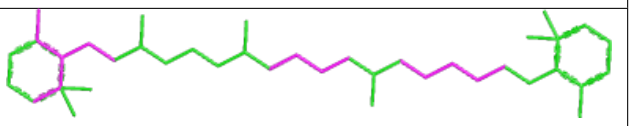
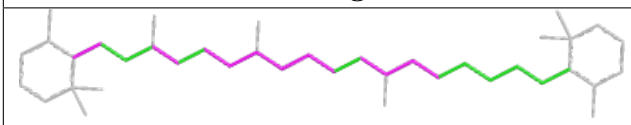
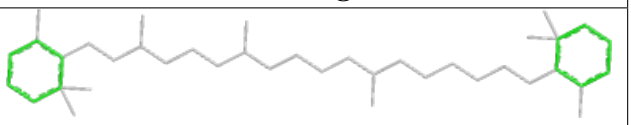
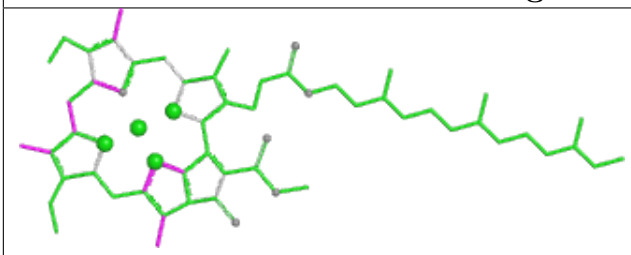
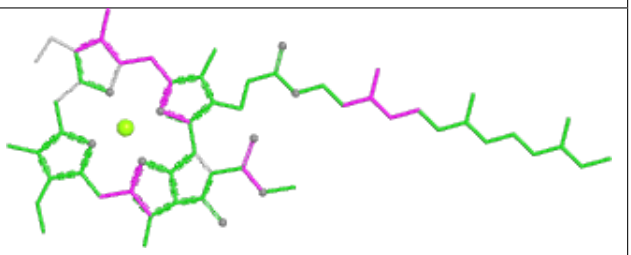
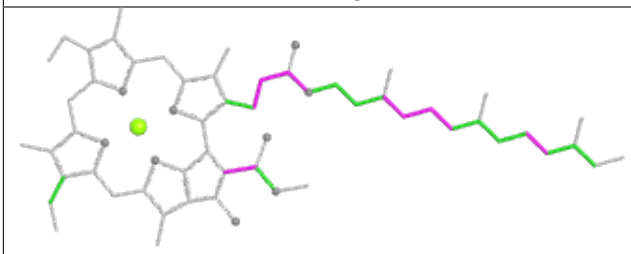
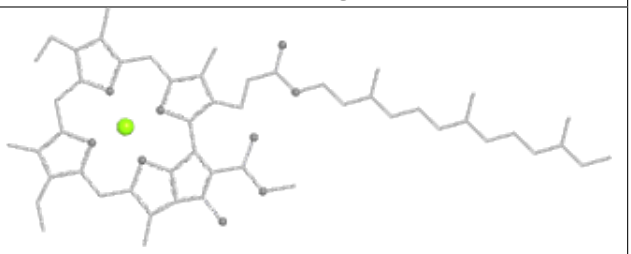
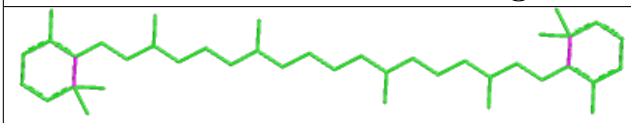
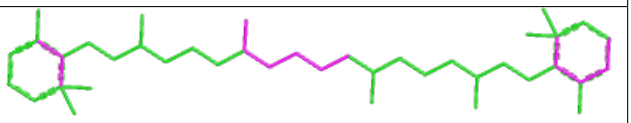
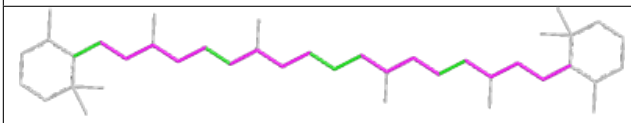
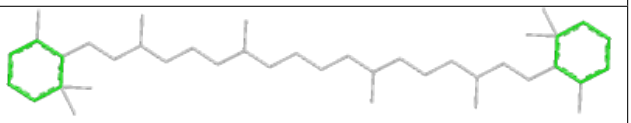
 Bond lengths	 Bond angles
 Torsions	 Rings

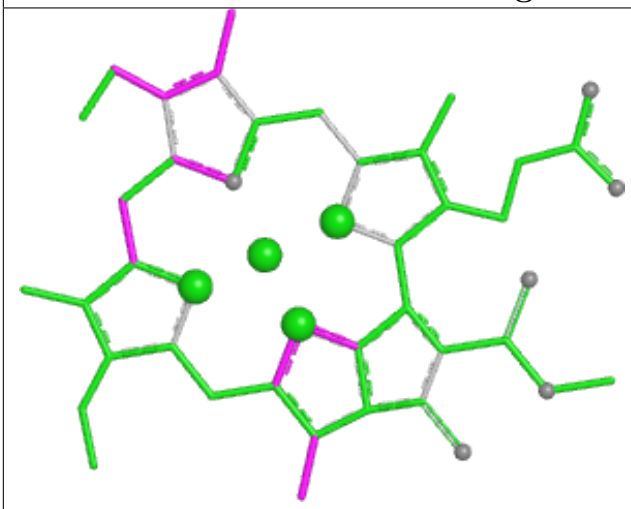
Ligand CLA KK 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A1 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

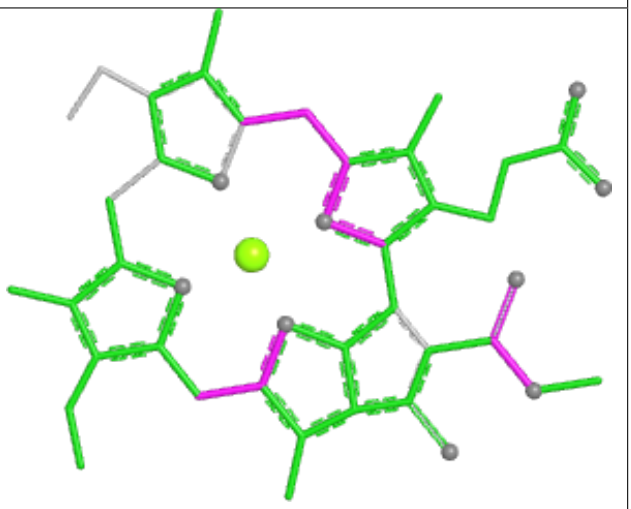
Ligand CLA L 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR BB 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

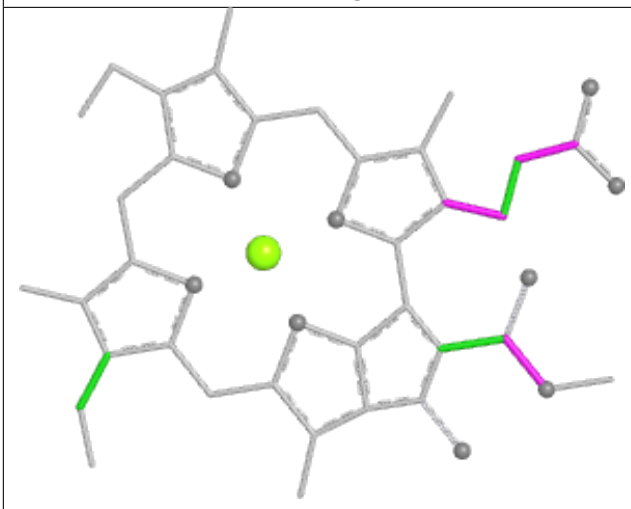
Ligand CLA B2 832



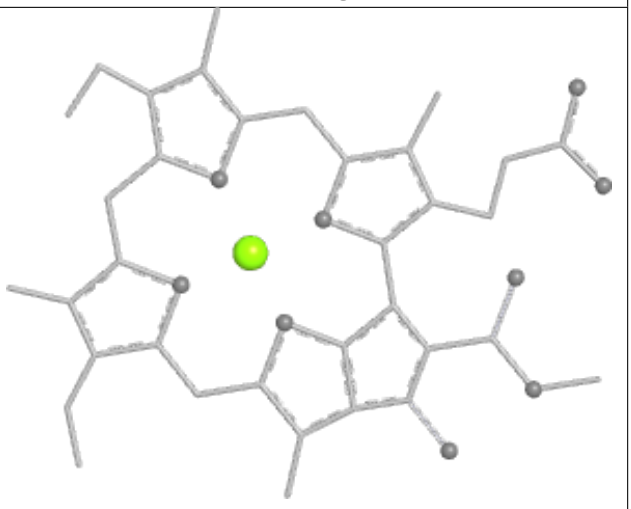
Bond lengths



Bond angles

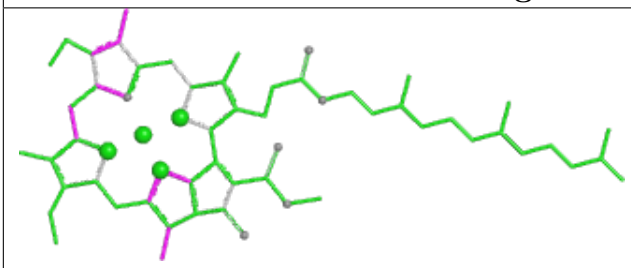


Torsions

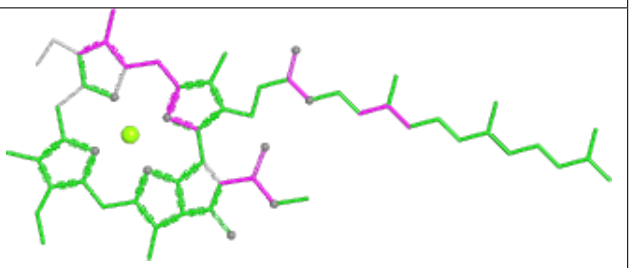


Rings

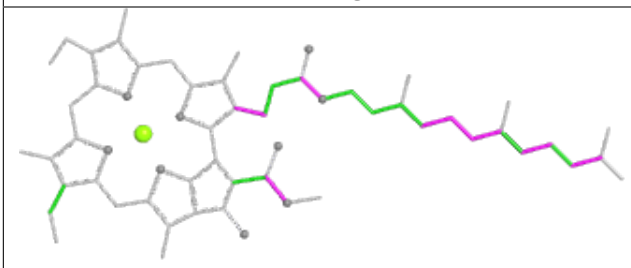
Ligand CLA A2 823



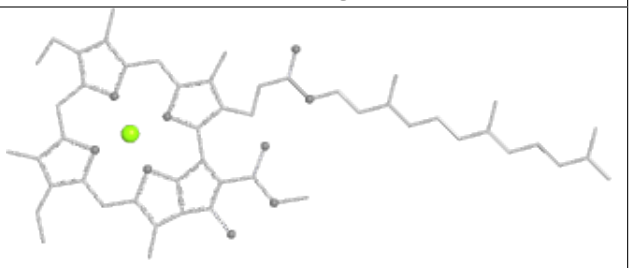
Bond lengths



Bond angles

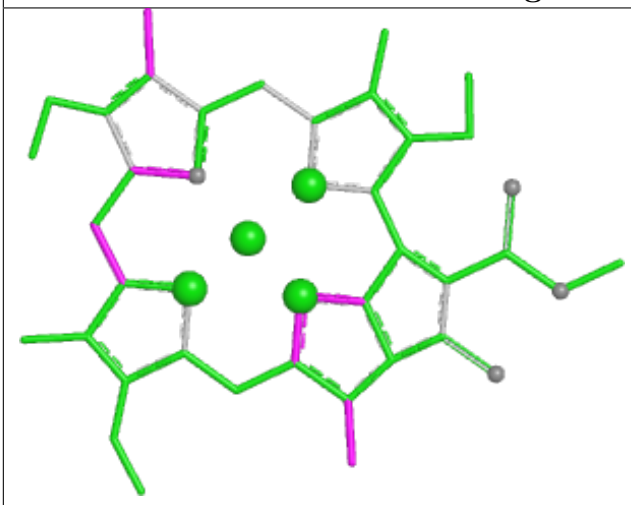


Torsions

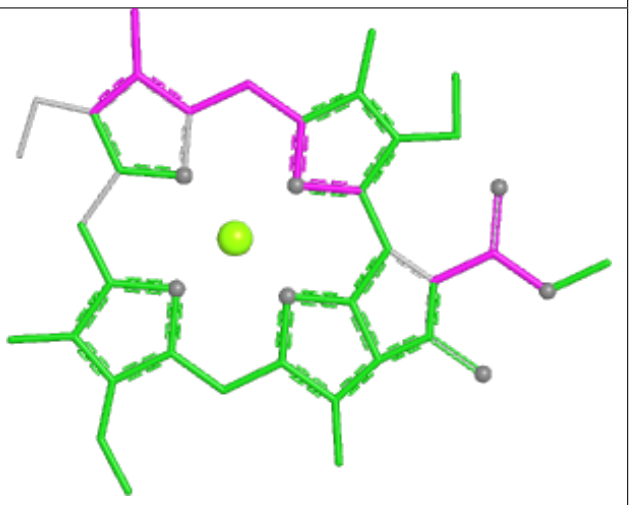


Rings

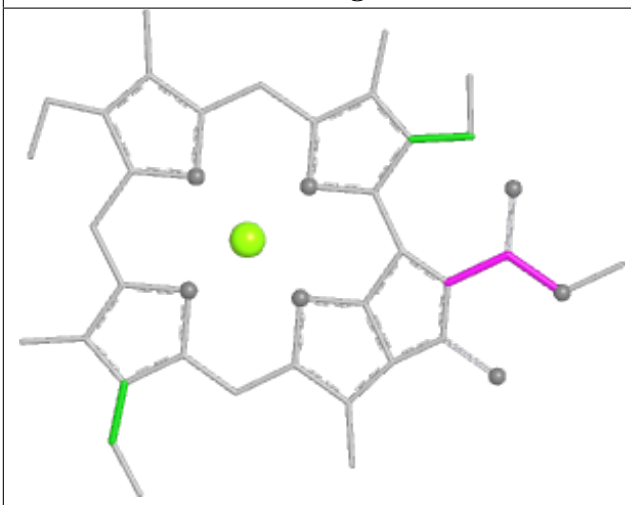
Ligand CLA B 817



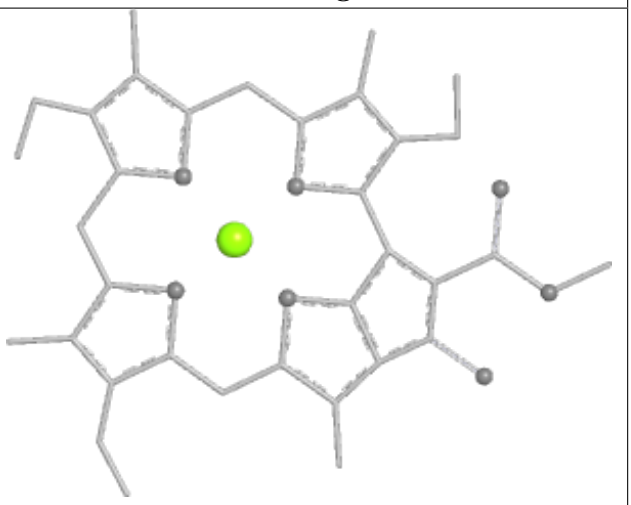
Bond lengths



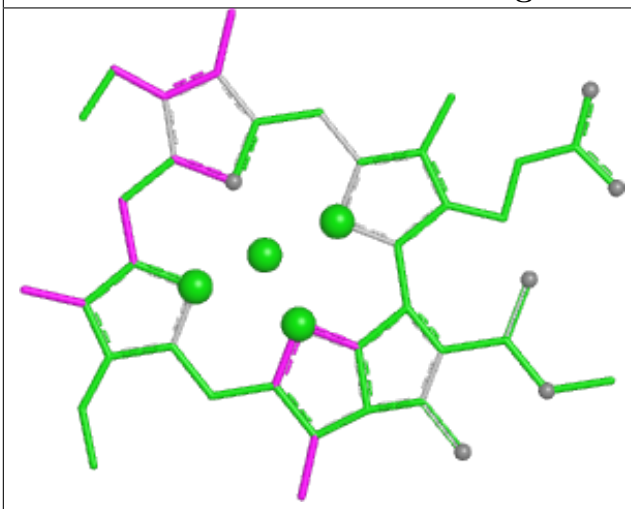
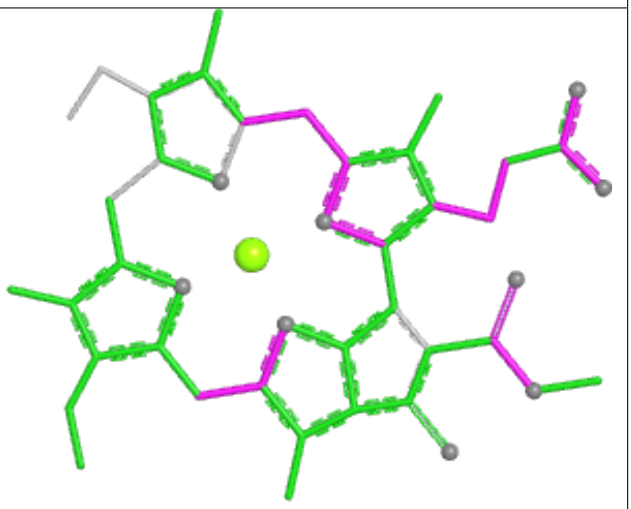
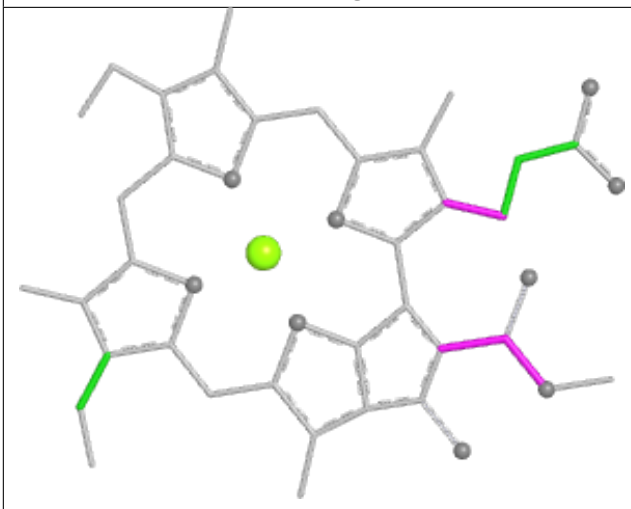
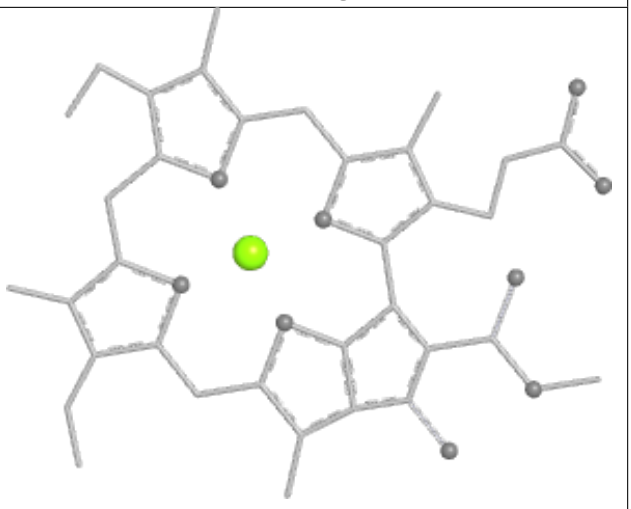
Bond angles

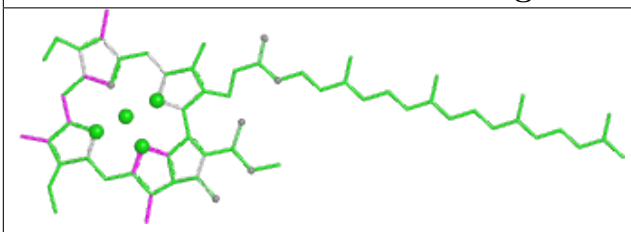
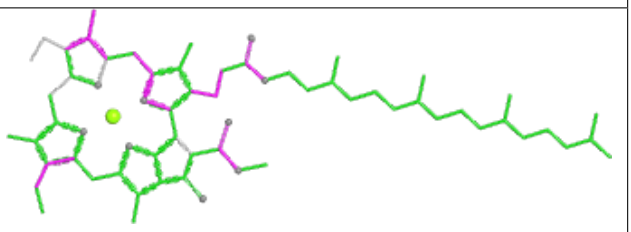
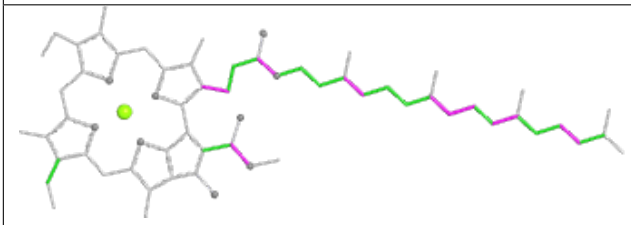
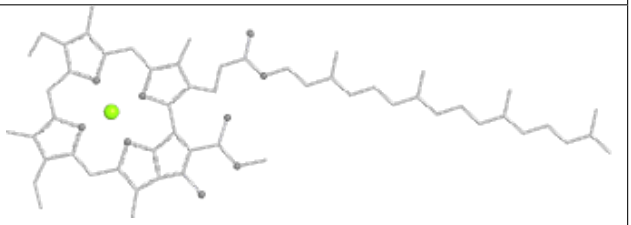


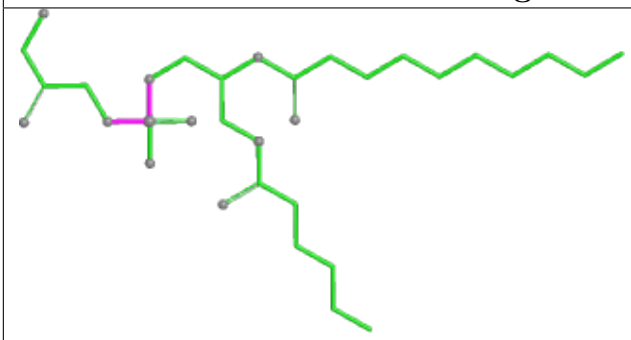
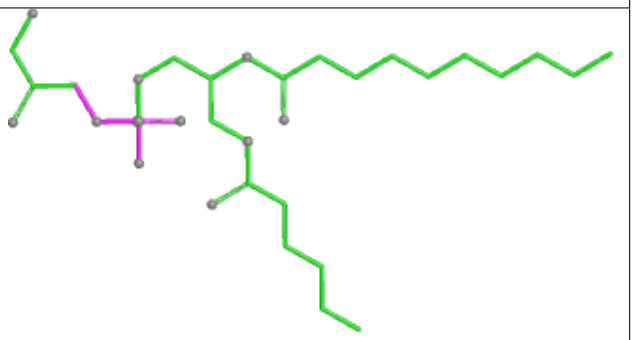
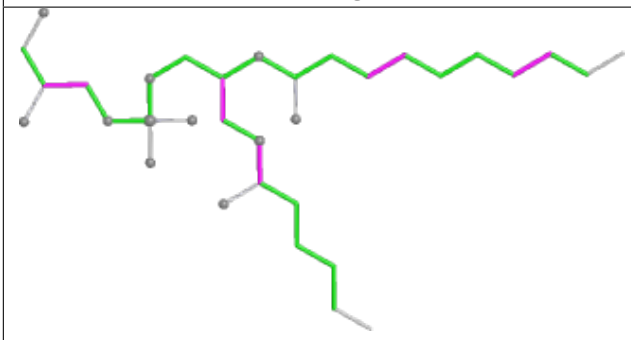
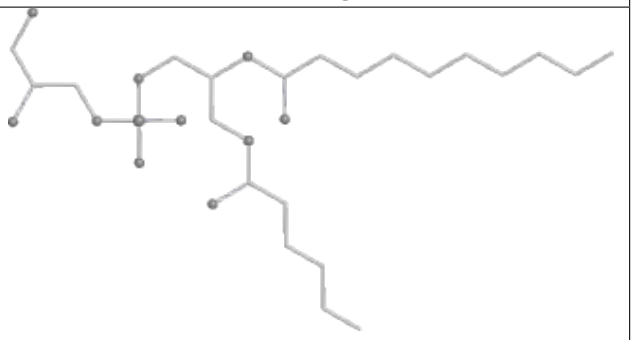
Torsions

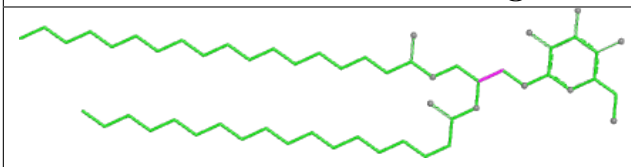
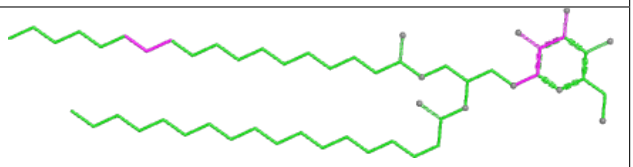
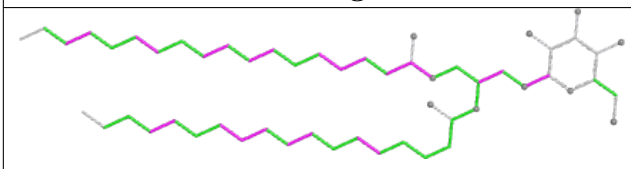
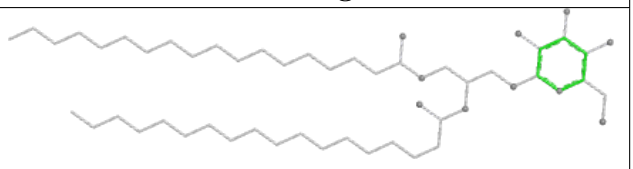


Rings

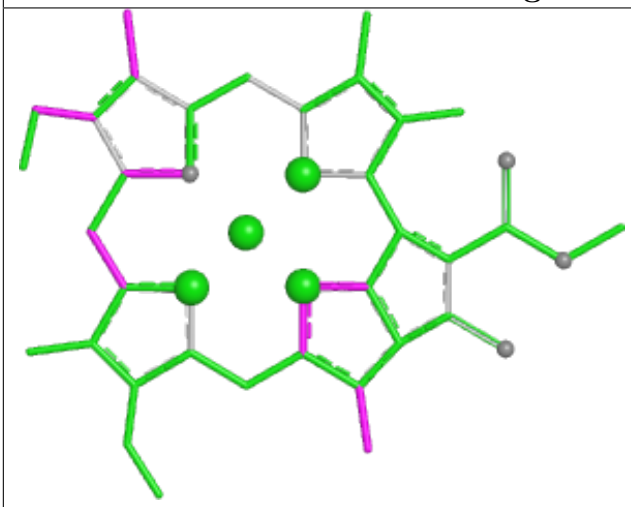
Ligand CLA B1 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

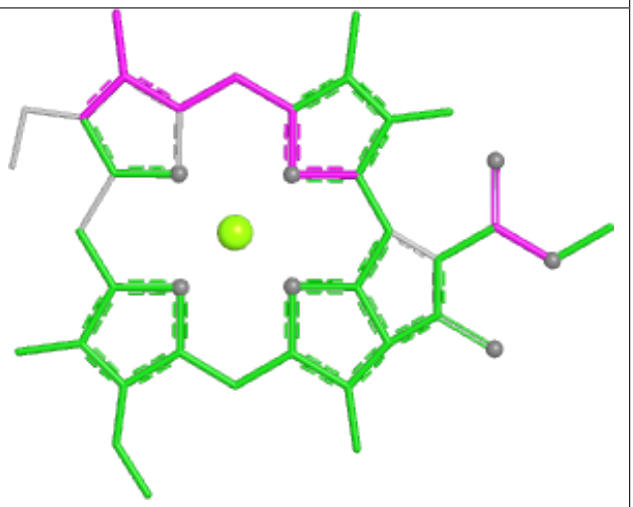
Ligand LHG B2 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG BB 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

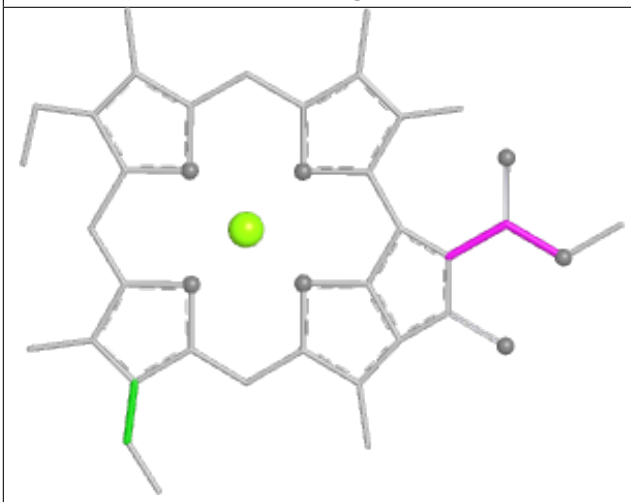
Ligand CLA A 844



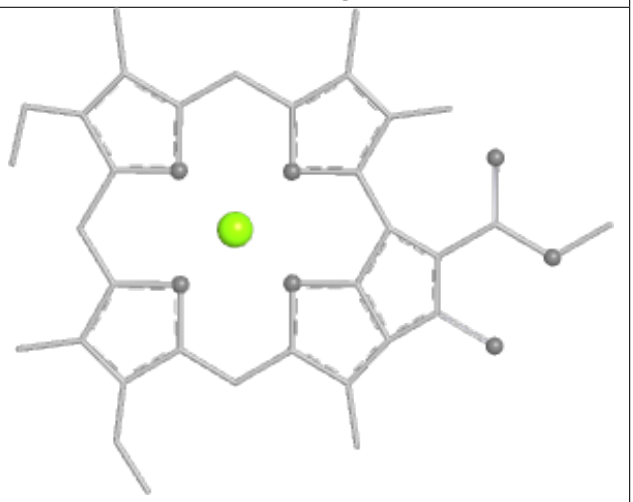
Bond lengths



Bond angles

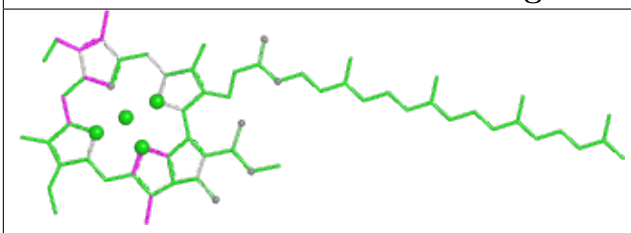


Torsions

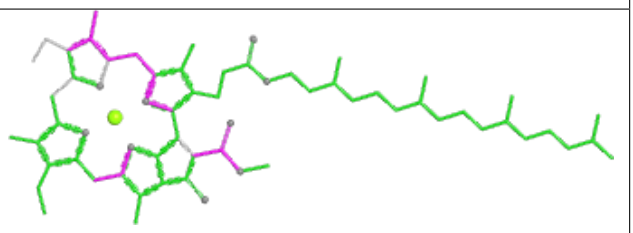


Rings

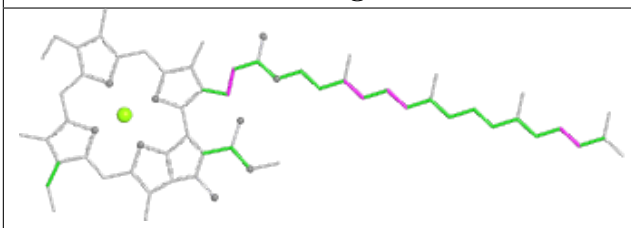
Ligand CLA B 858



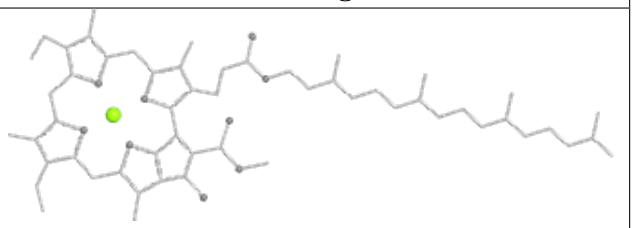
Bond lengths



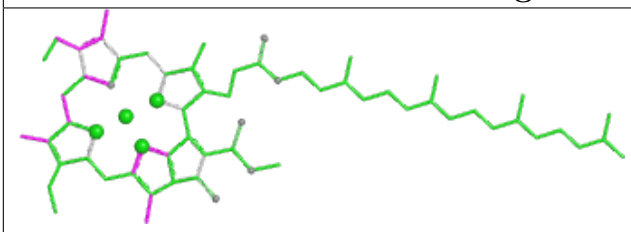
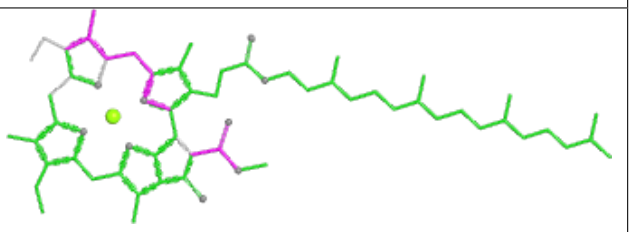
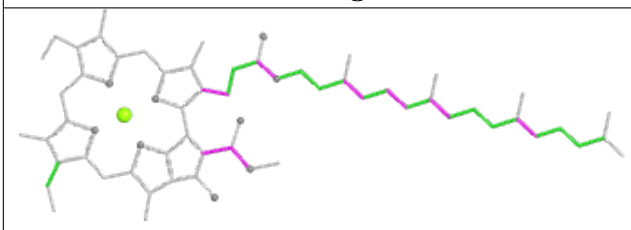
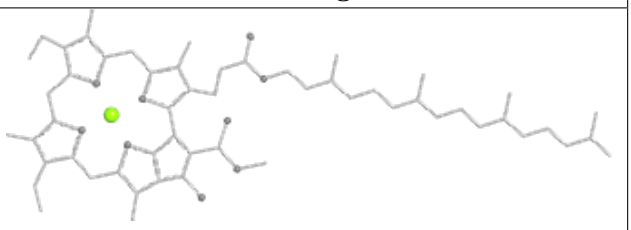
Bond angles

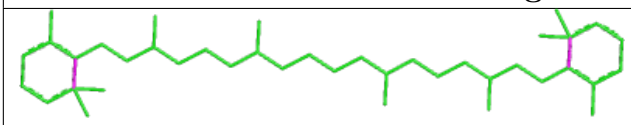
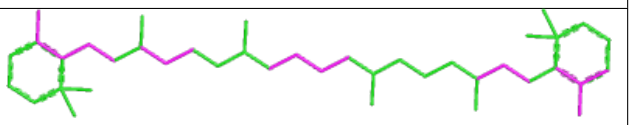
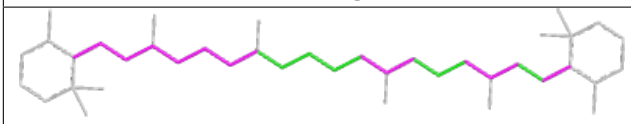
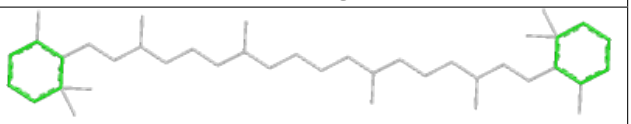


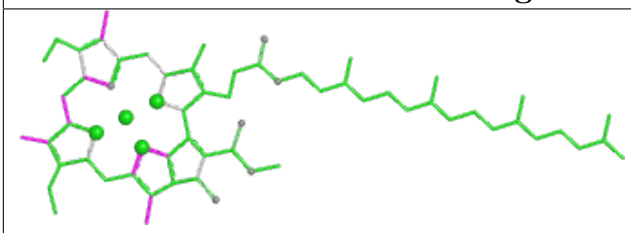
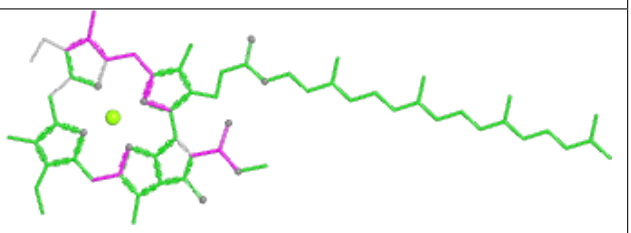
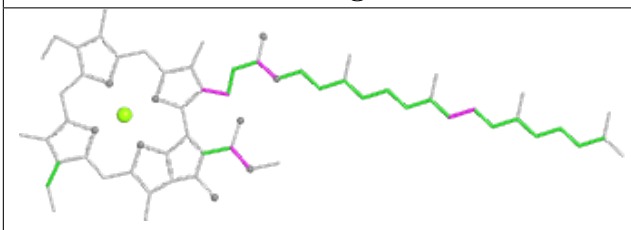
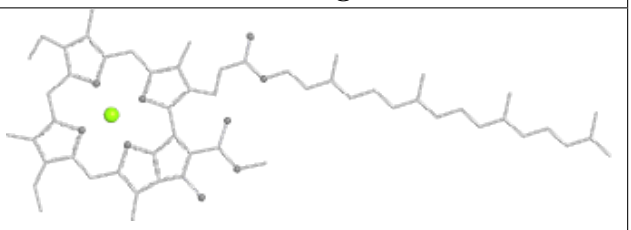
Torsions



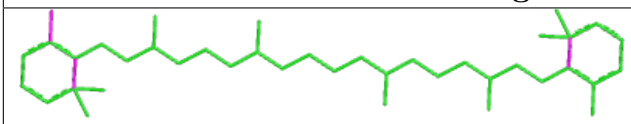
Rings

Ligand CLA A2 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

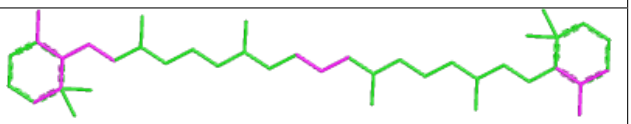
Ligand BCR L 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

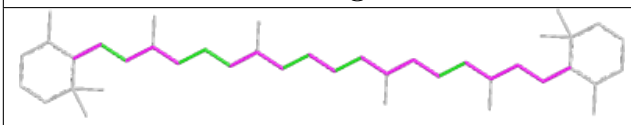
Ligand BCR K1 104



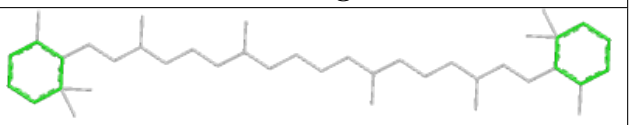
Bond lengths



Bond angles

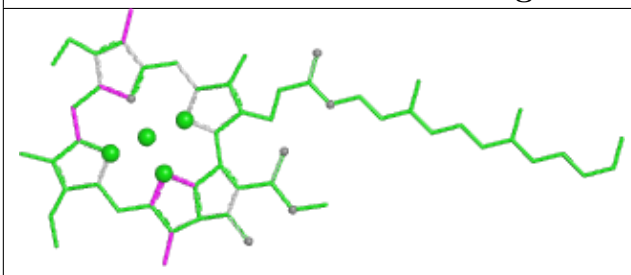


Torsions

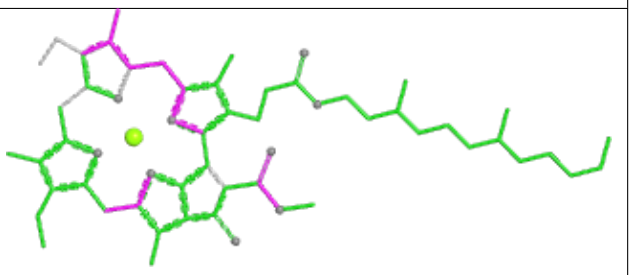


Rings

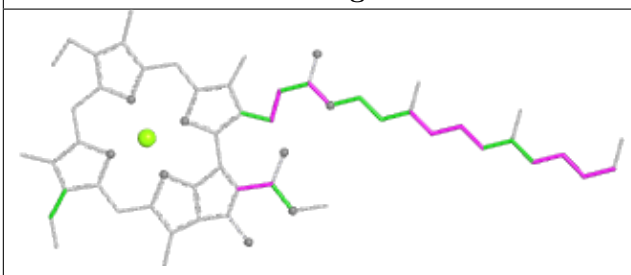
Ligand CLA B1 814



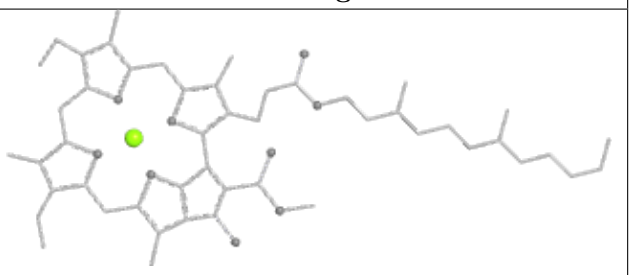
Bond lengths



Bond angles

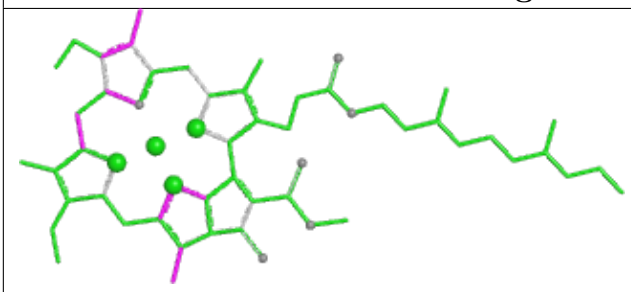


Torsions

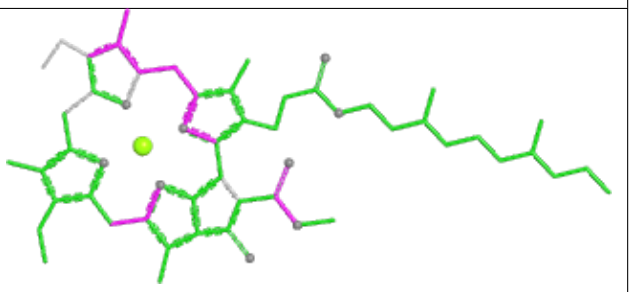


Rings

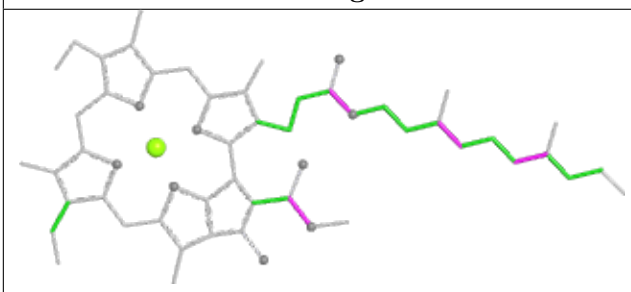
Ligand CLA B2 816



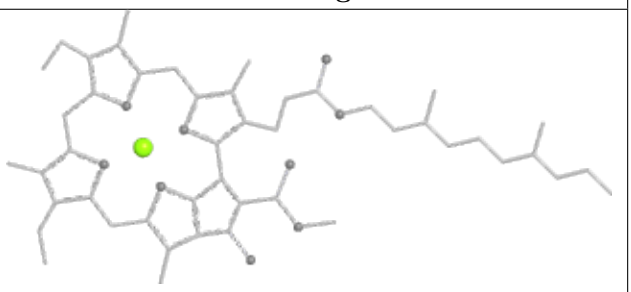
Bond lengths



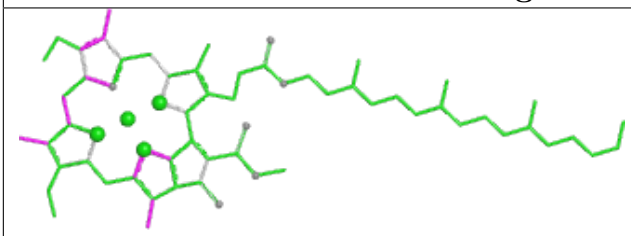
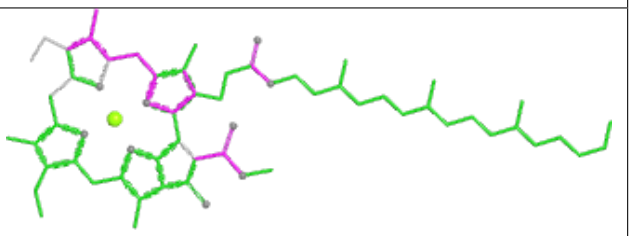
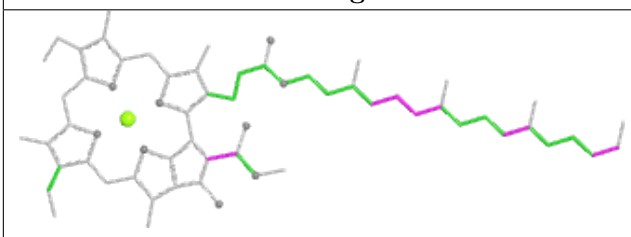
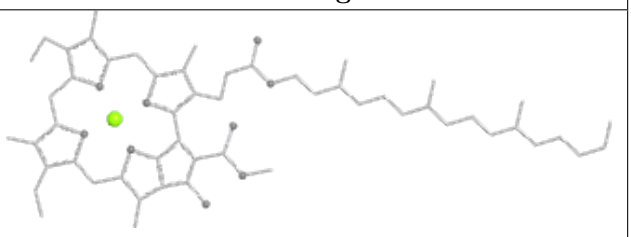
Bond angles

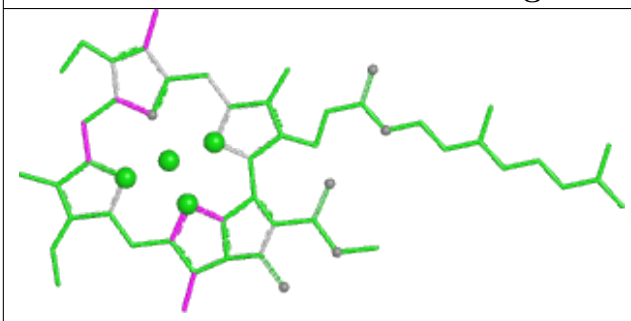
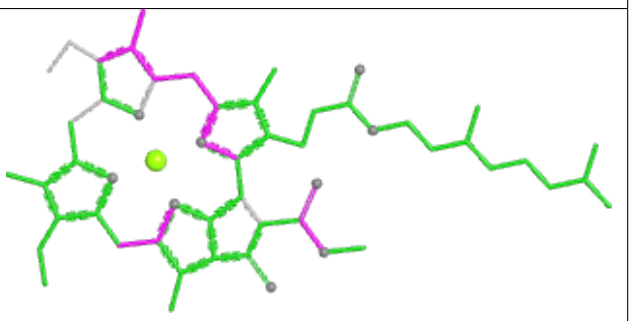
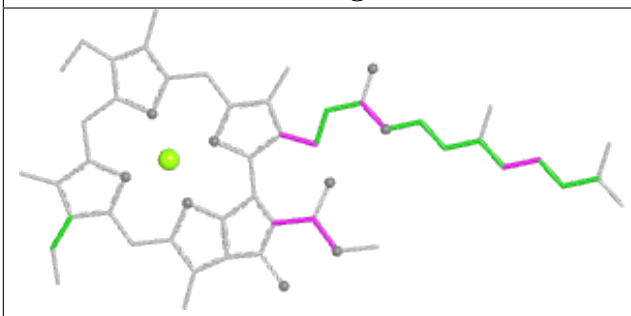
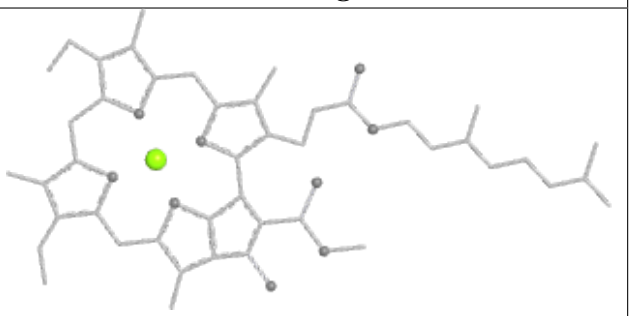


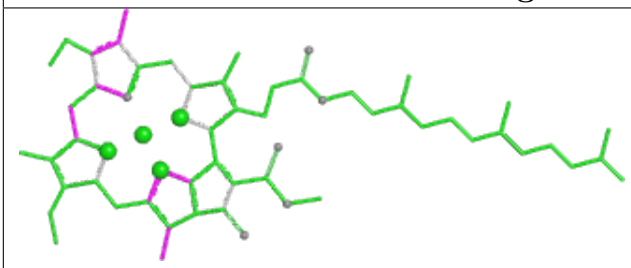
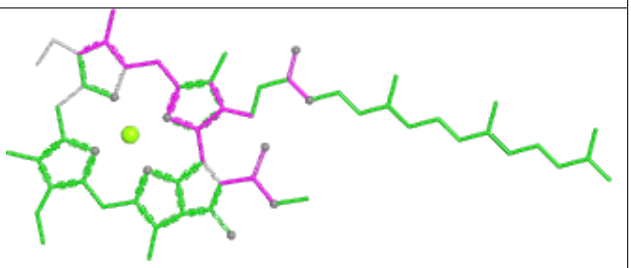
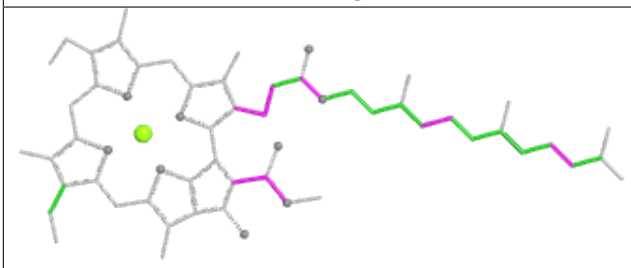
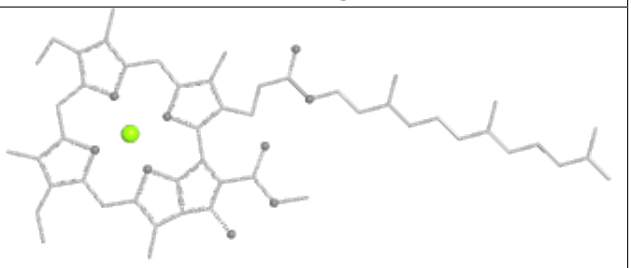
Torsions



Rings

Ligand CLA B2 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F1 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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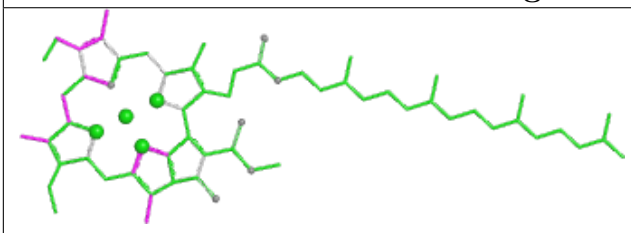
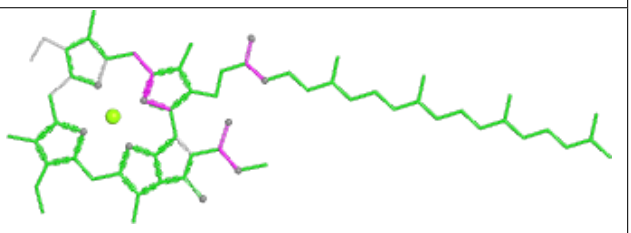
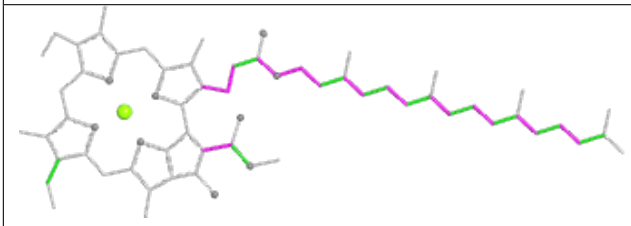
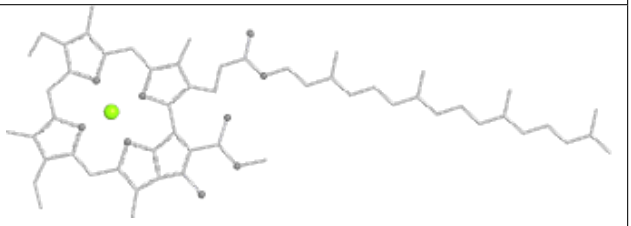
 Bond lengths	 Bond angles
 Torsions	 Rings

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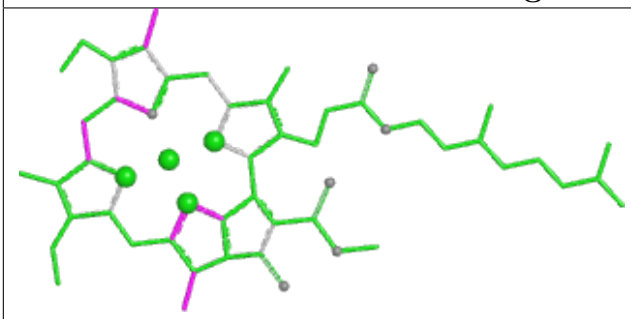
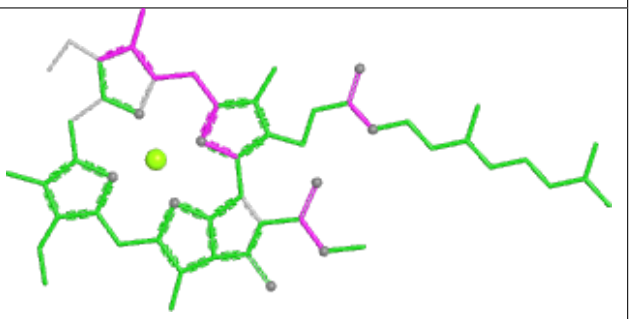
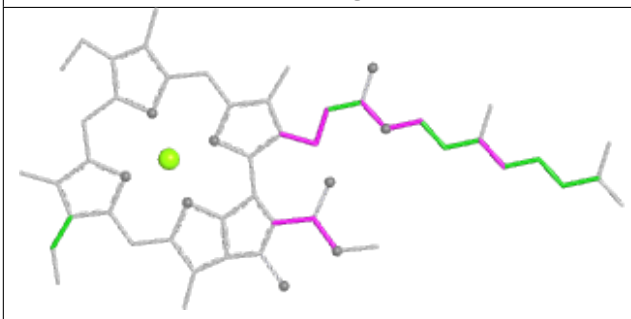
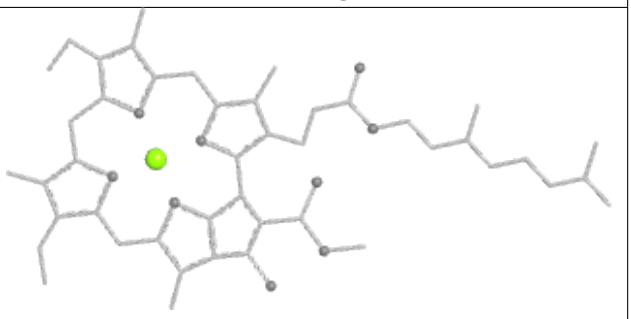
	
Bond lengths	Bond angles
	
Torsions	Rings

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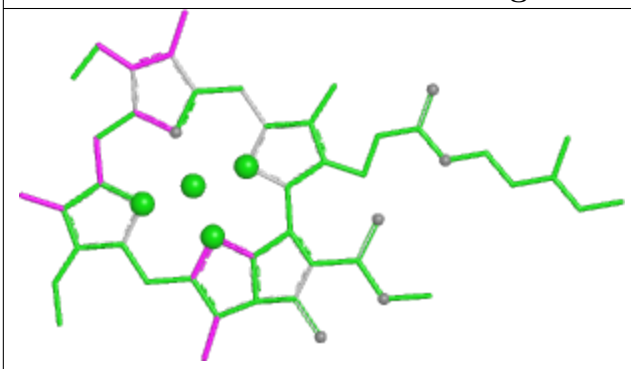
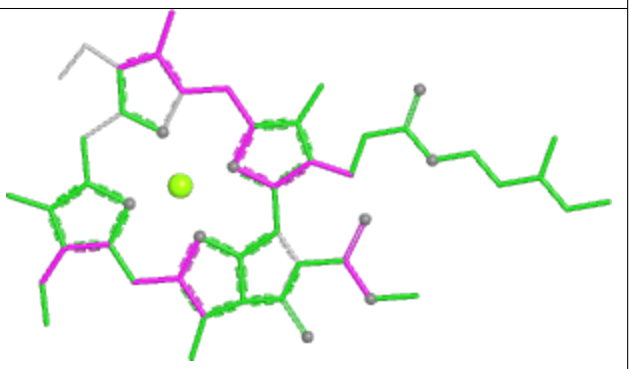
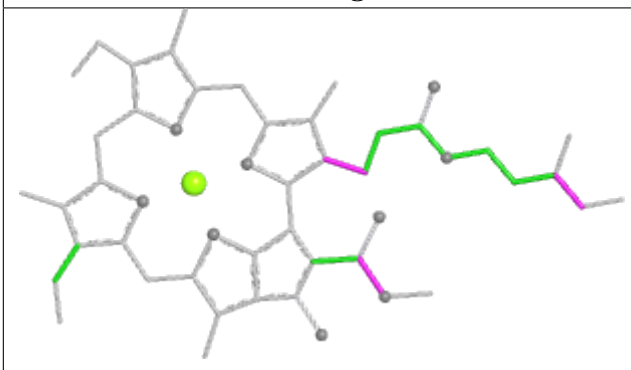
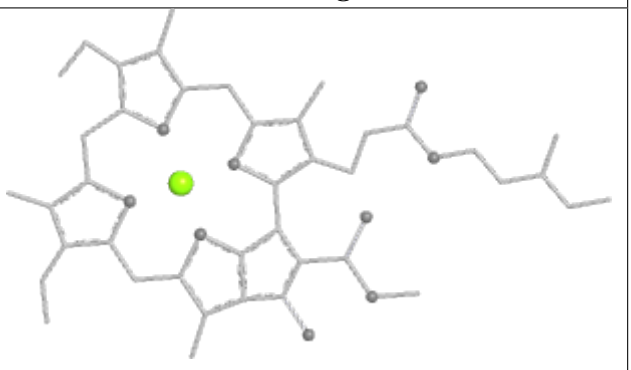
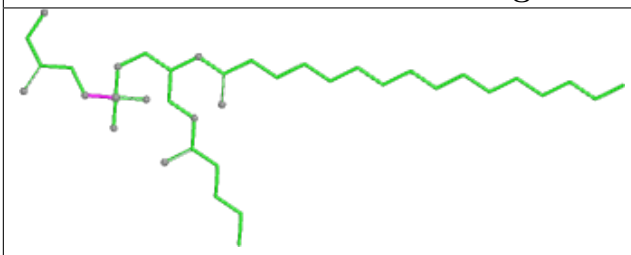
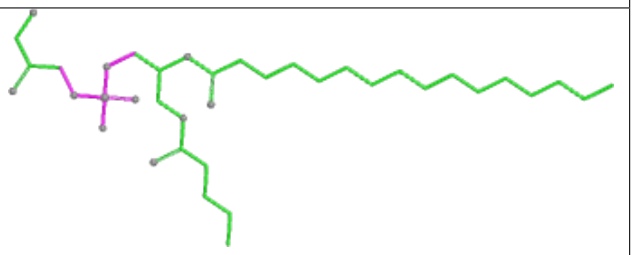
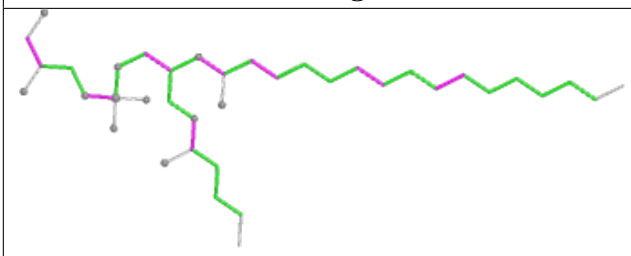
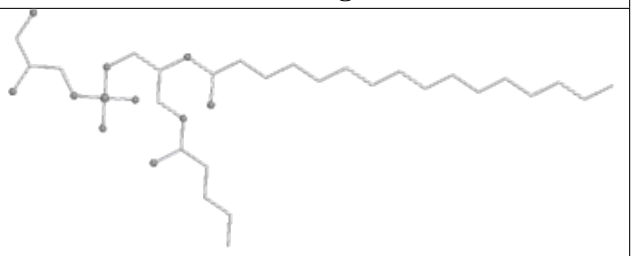
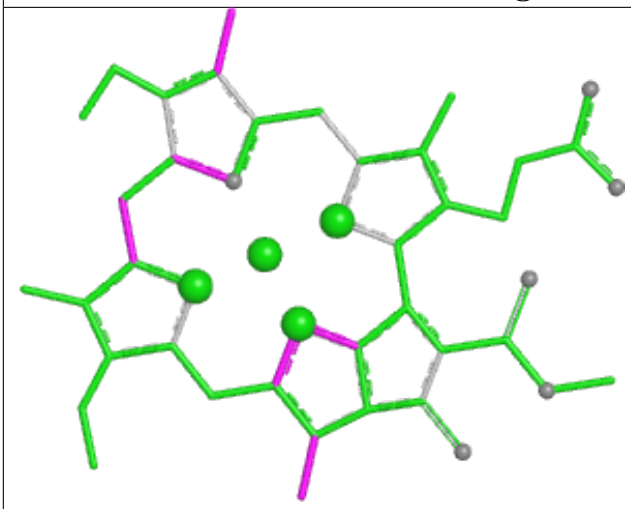
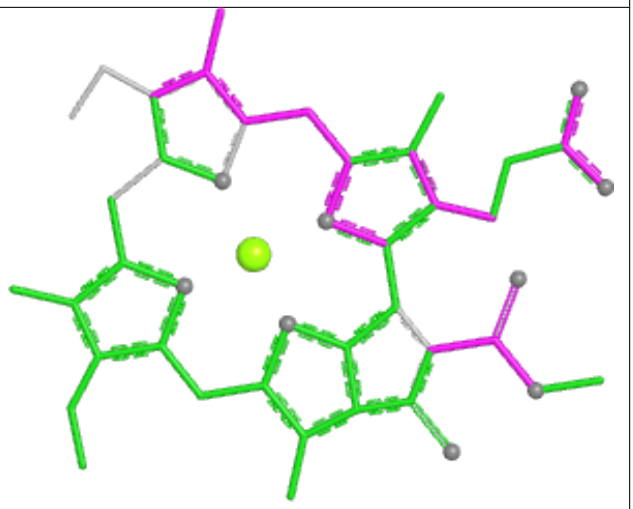
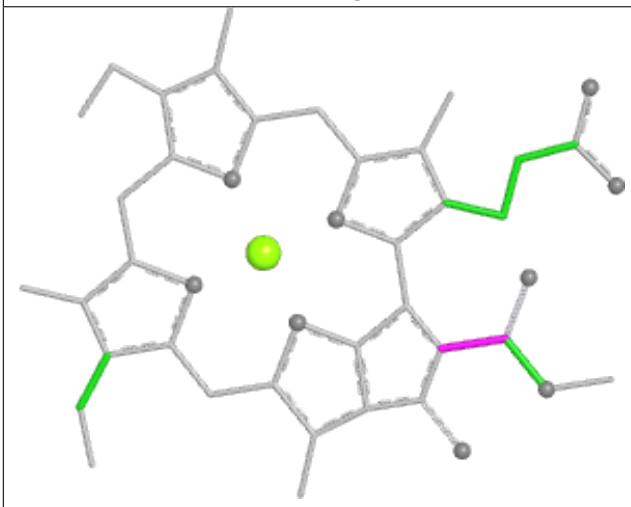
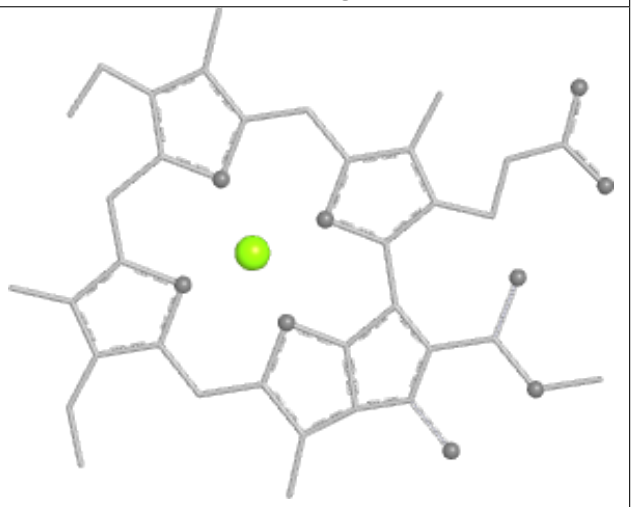
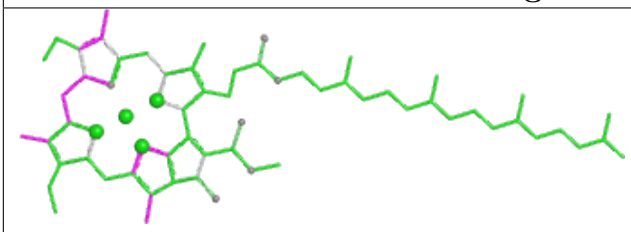
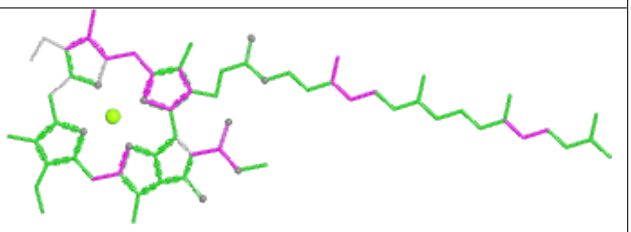
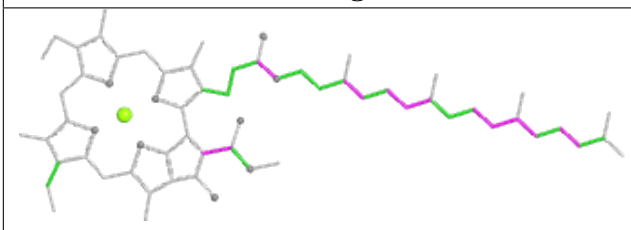
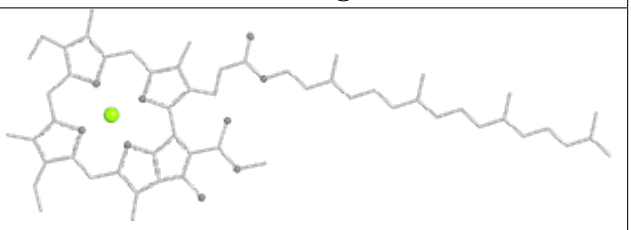
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG A1 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

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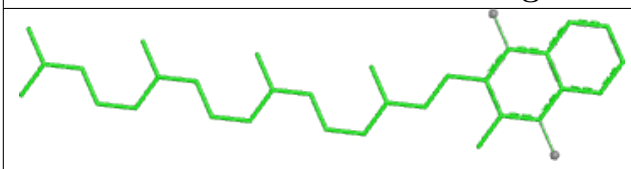
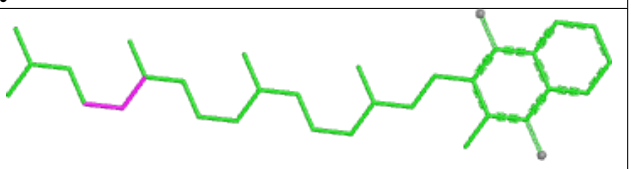
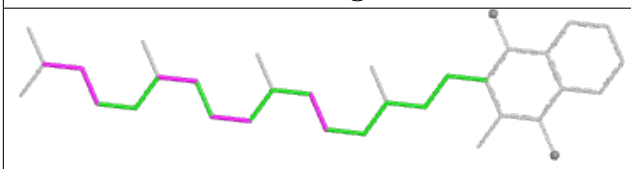
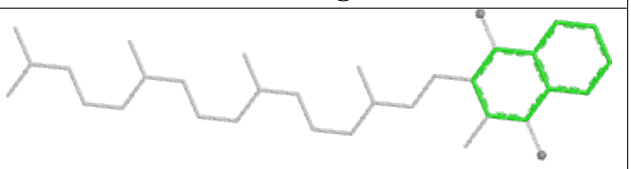
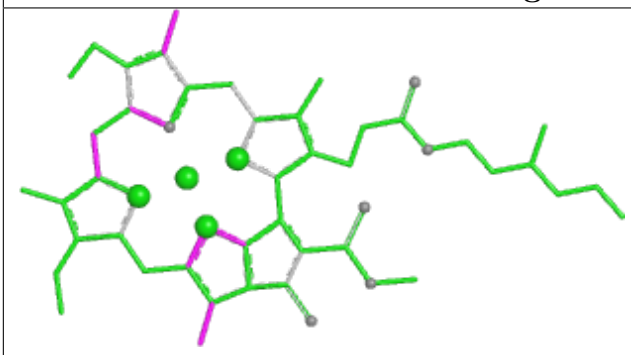
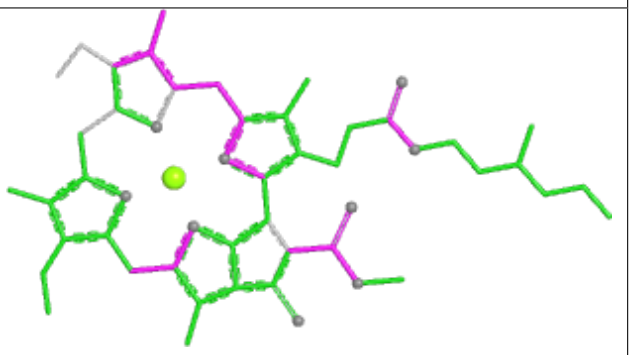
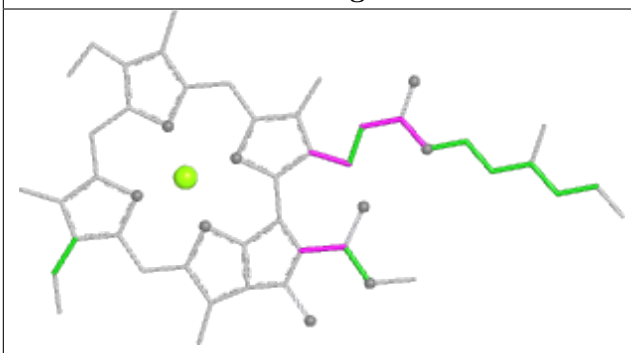
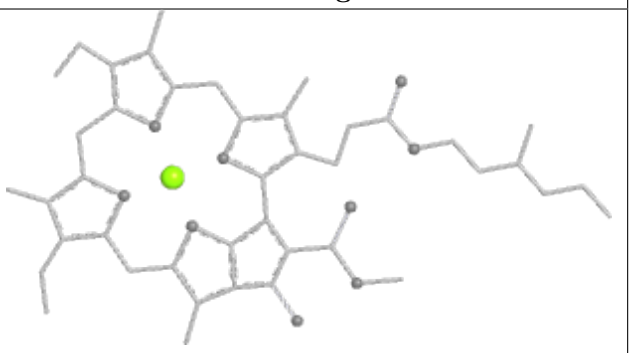
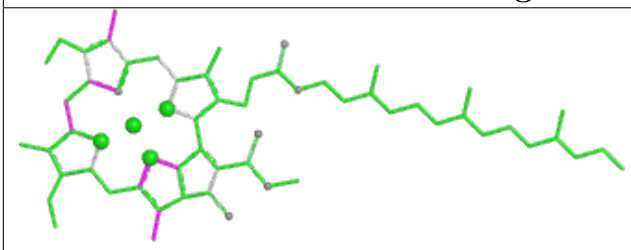
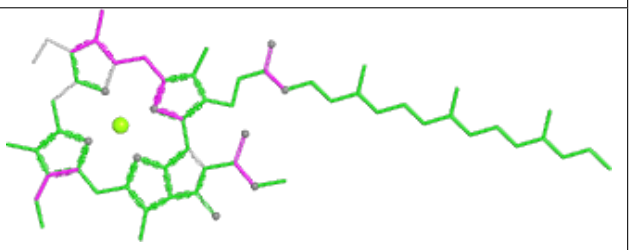
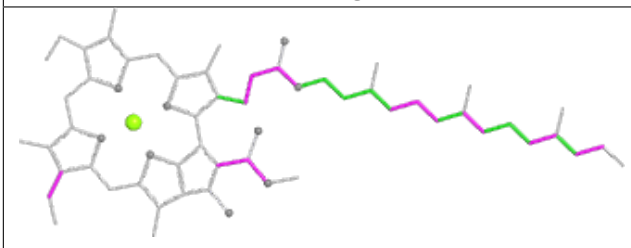
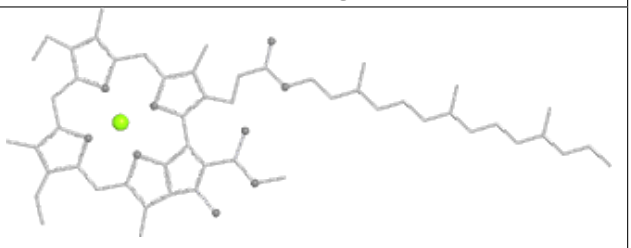
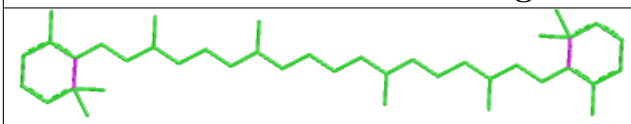
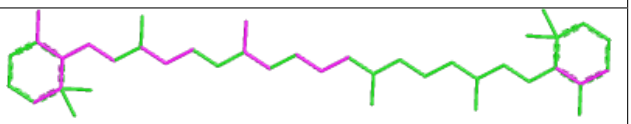
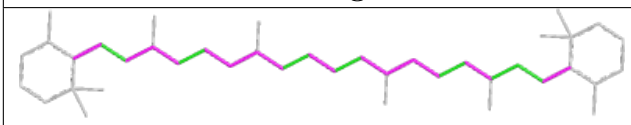
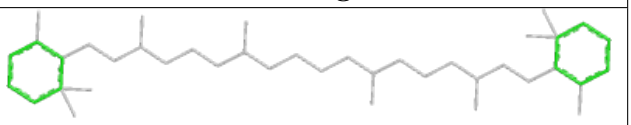
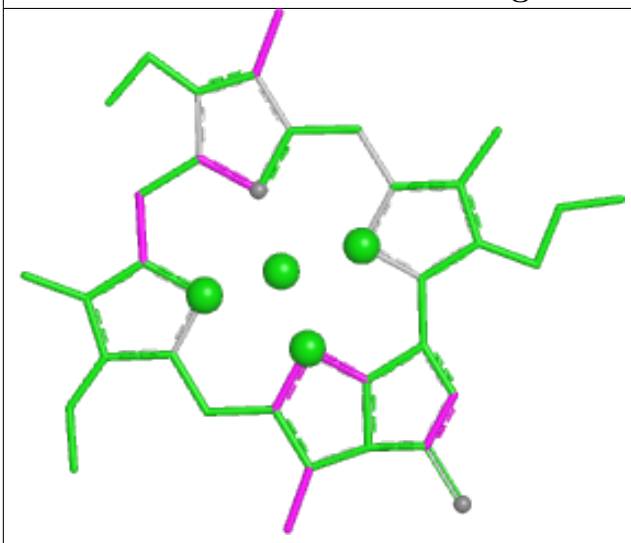
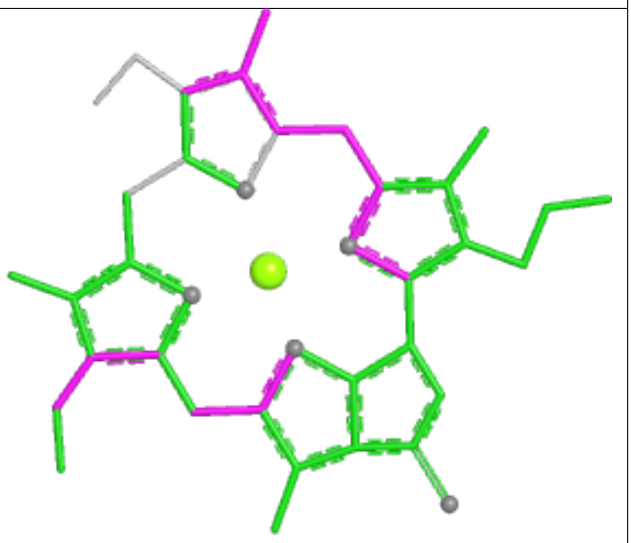
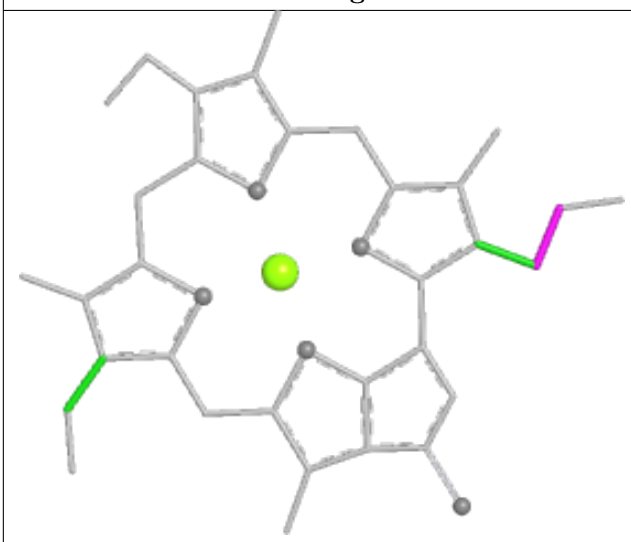
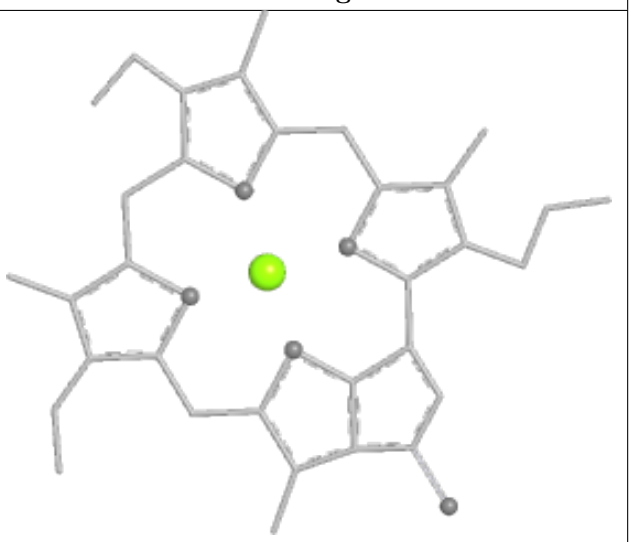
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F1 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

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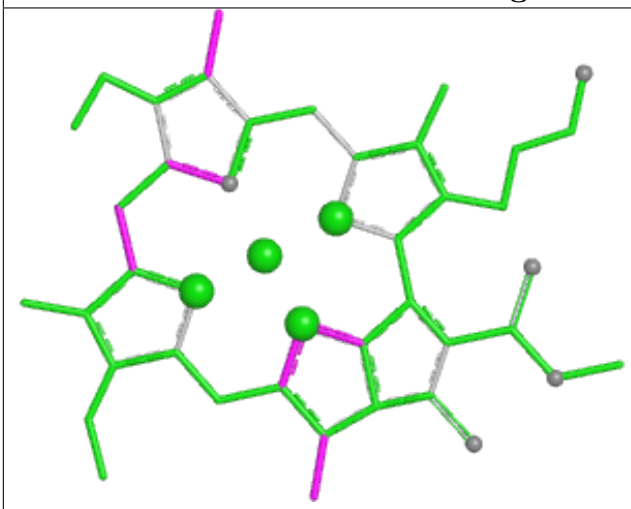
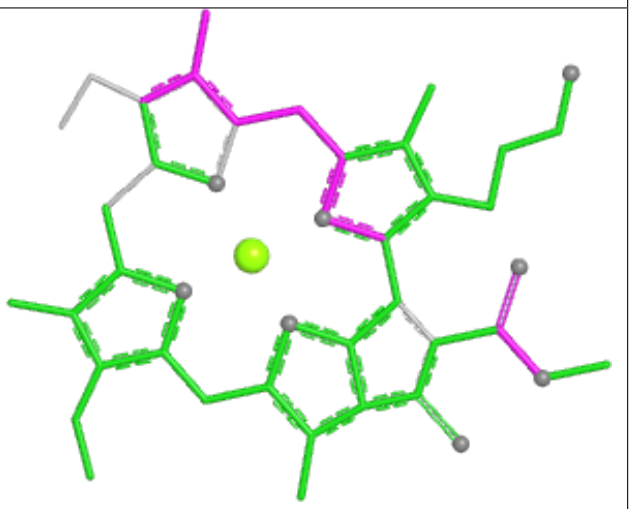
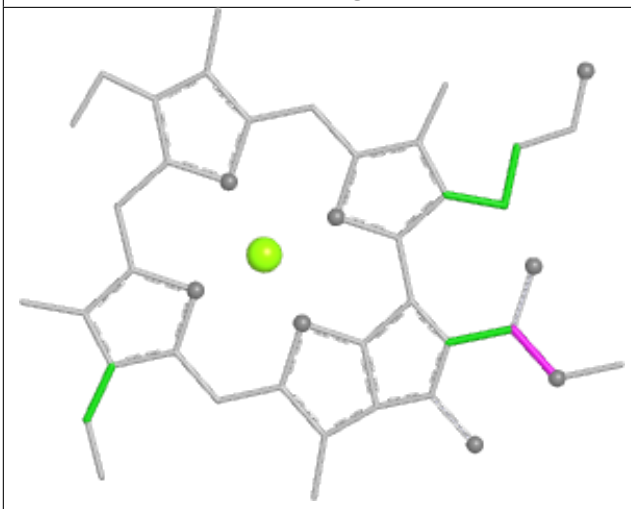
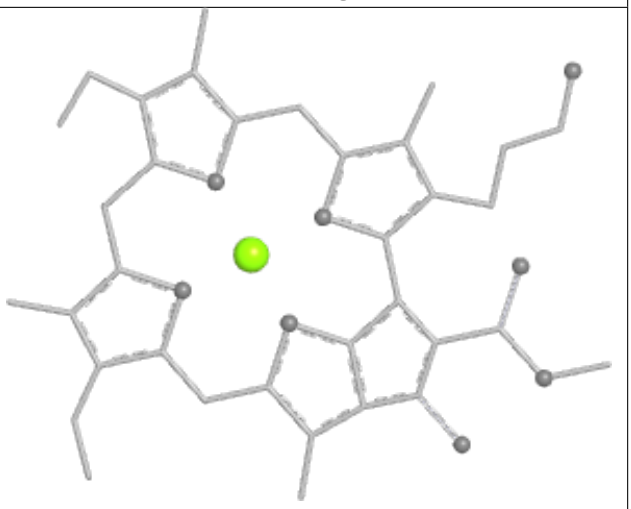
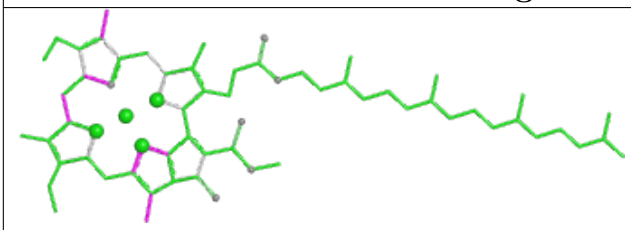
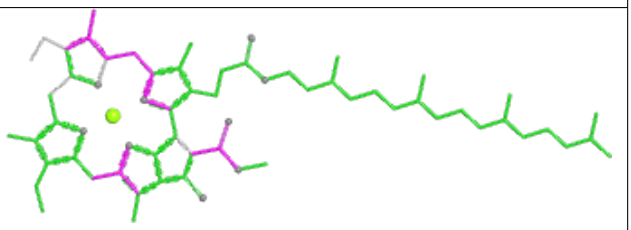
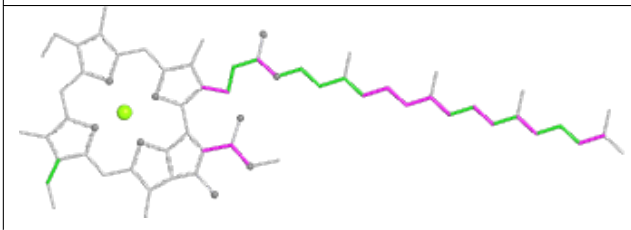
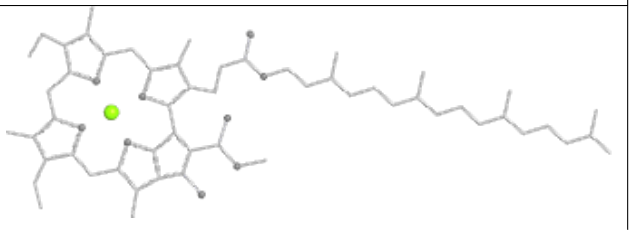
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

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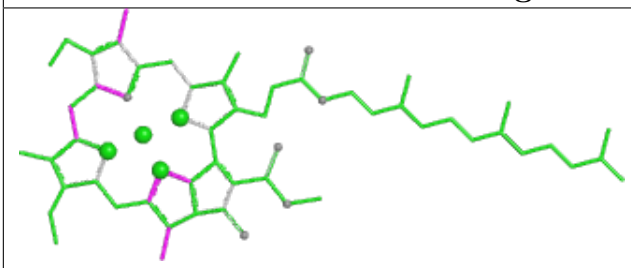
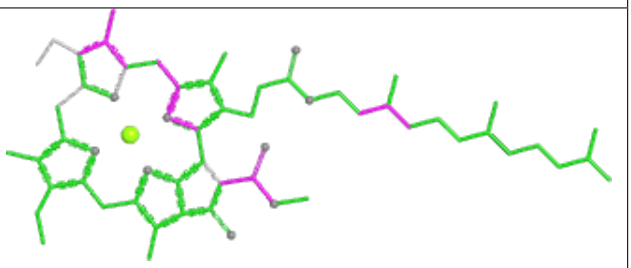
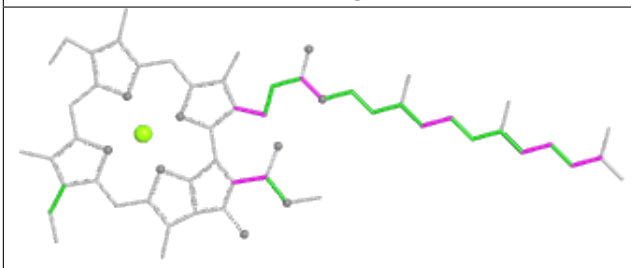
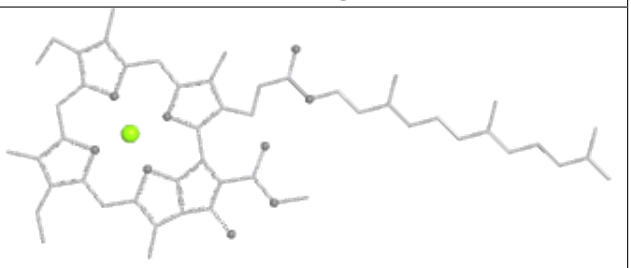
	
Bond lengths	Bond angles
	
Torsions	Rings

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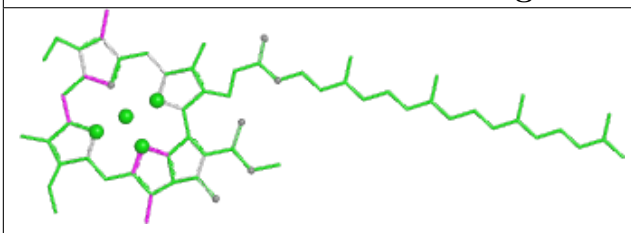
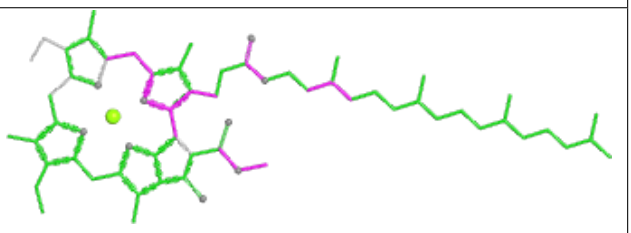
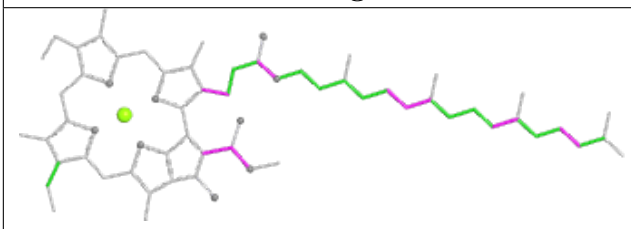
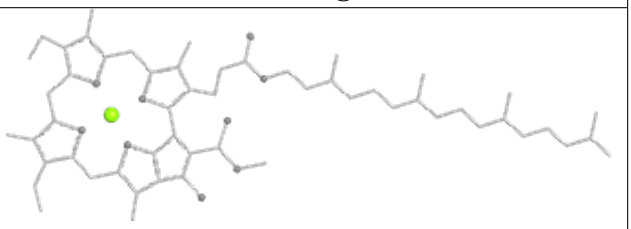
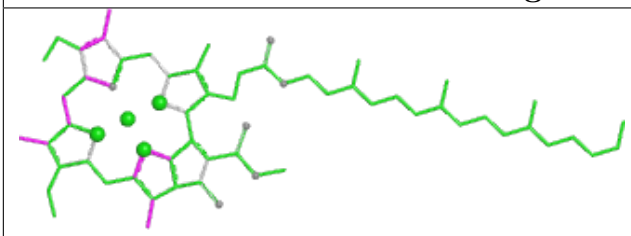
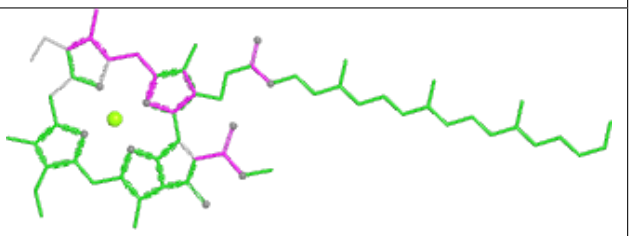
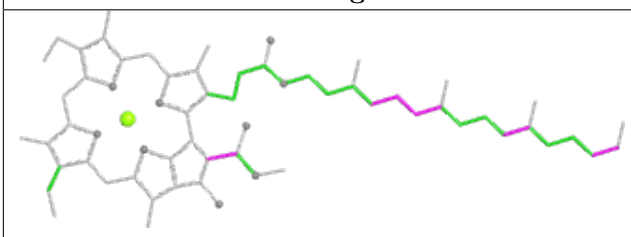
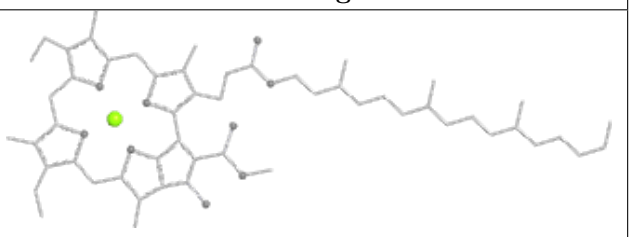
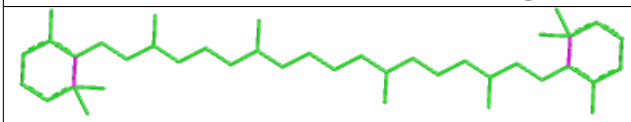
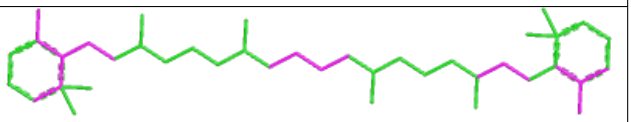
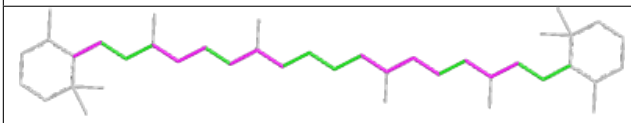
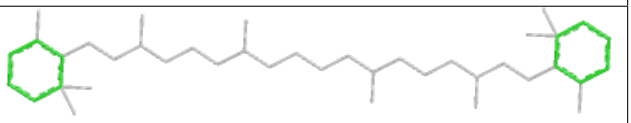
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR I1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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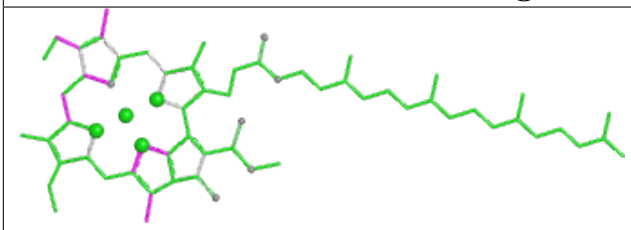
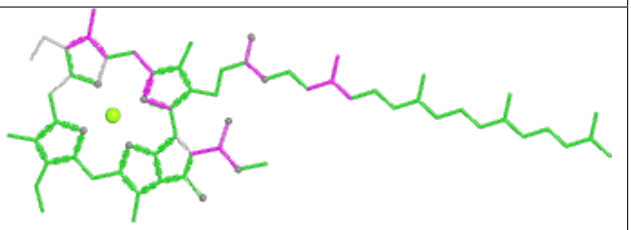
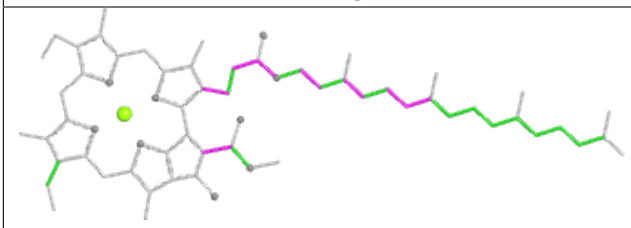
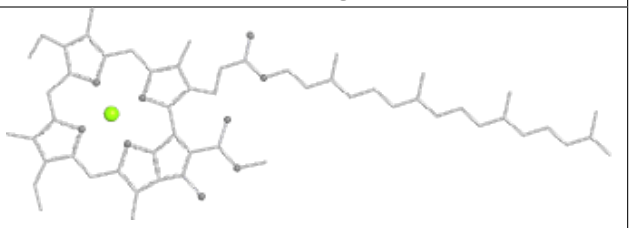
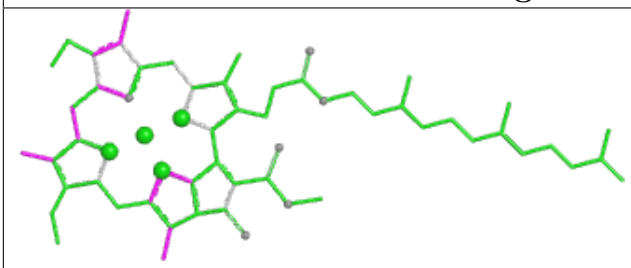
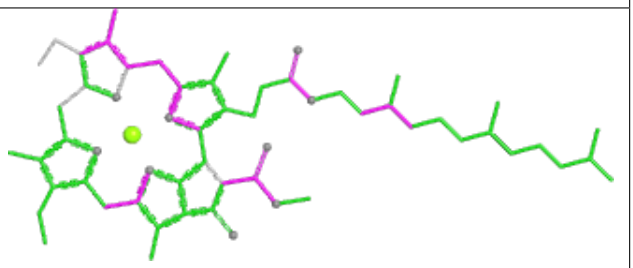
 Bond lengths	 Bond angles
 Torsions	 Rings

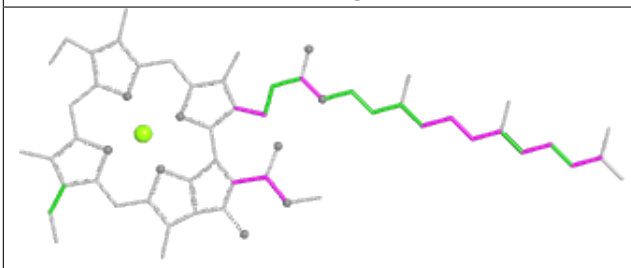
Ligand CLA A1 822



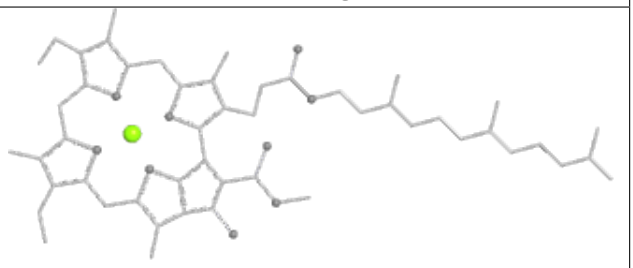
Bond lengths



Bond angles

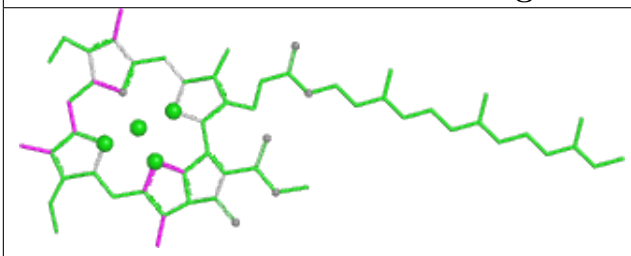


Torsions



Rings

Ligand CLA LL 201



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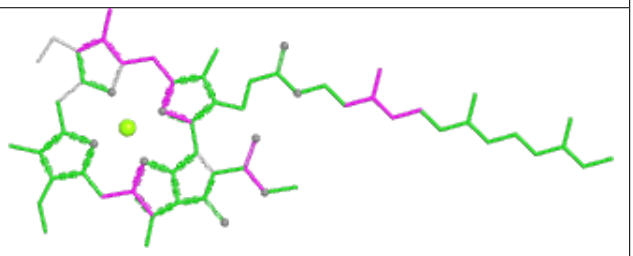

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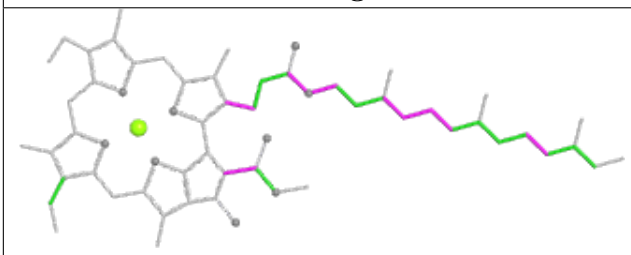

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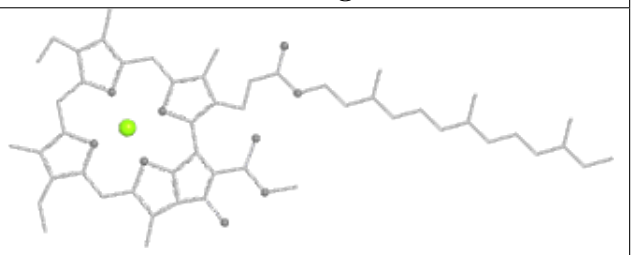
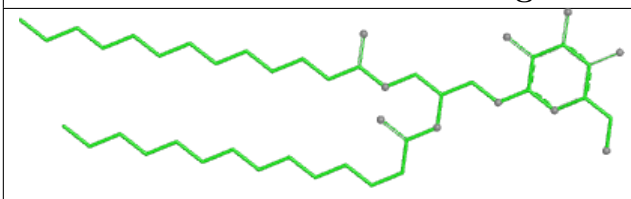


Rings

Ligand LMG M 102



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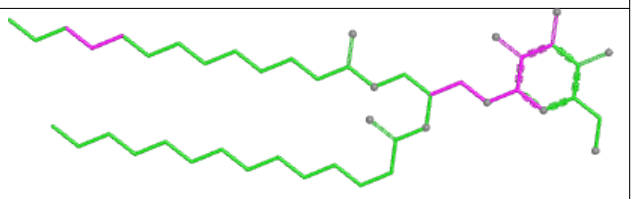
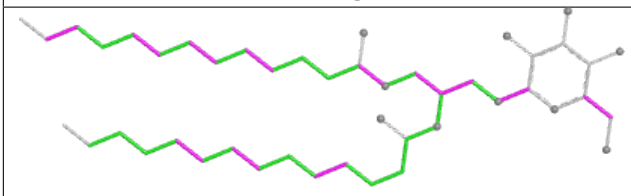


Bond angles



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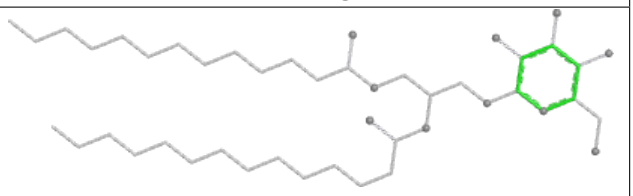
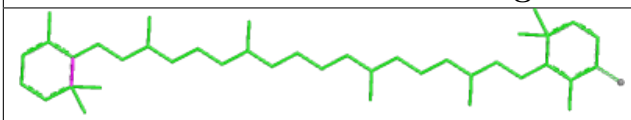


Rings

Ligand ECH B1 840



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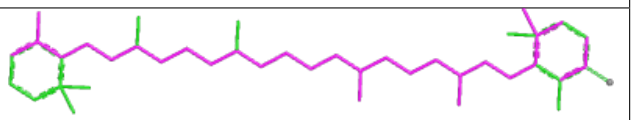

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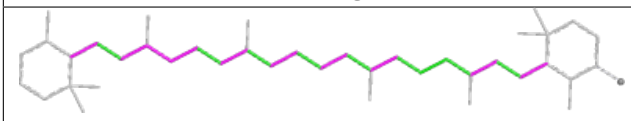

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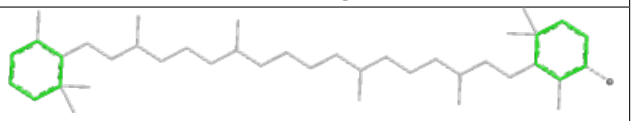
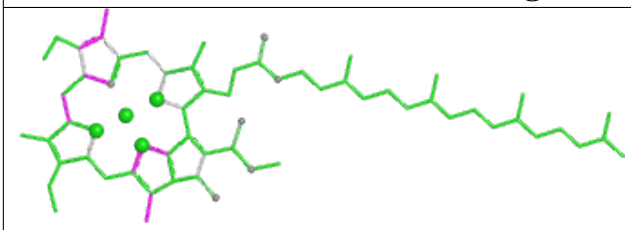


Rings

Ligand CLA A 807



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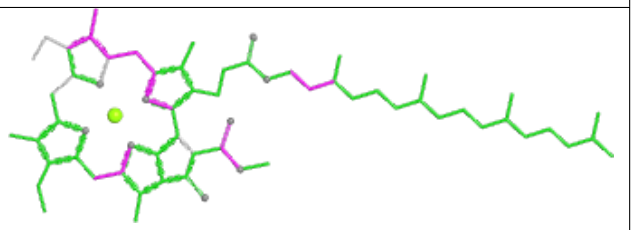
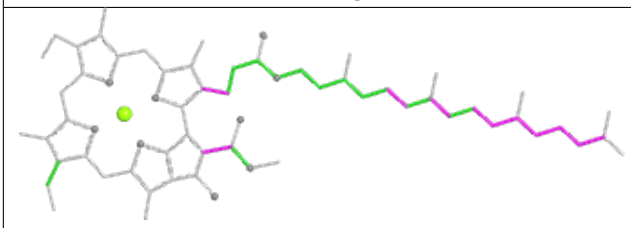
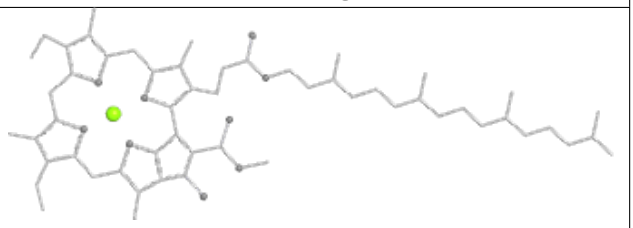


Bond angles

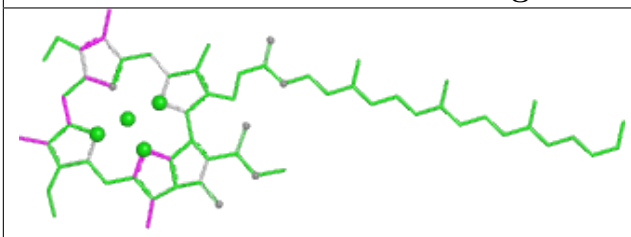


Torsions



Rings

Ligand CLA BB 805



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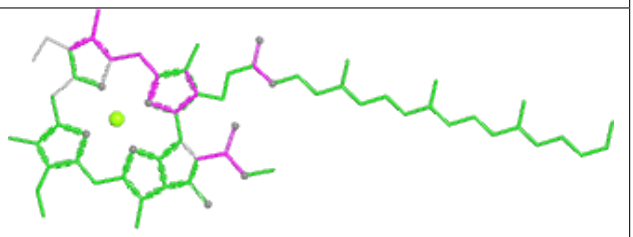
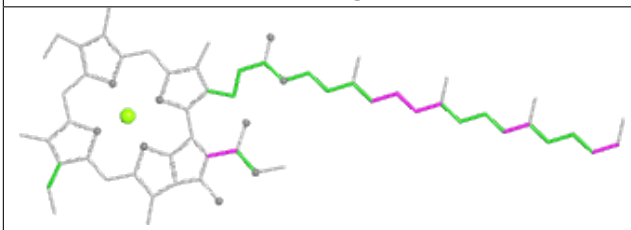
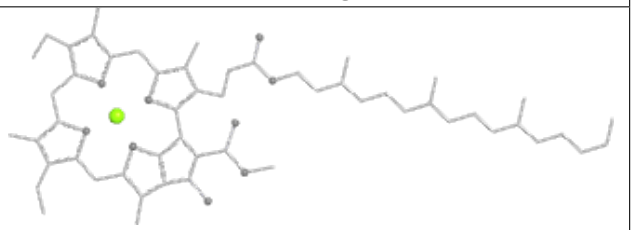


Bond angles

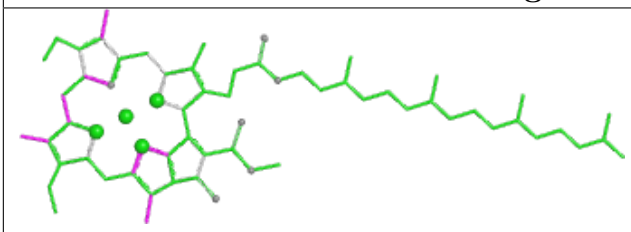


Torsions

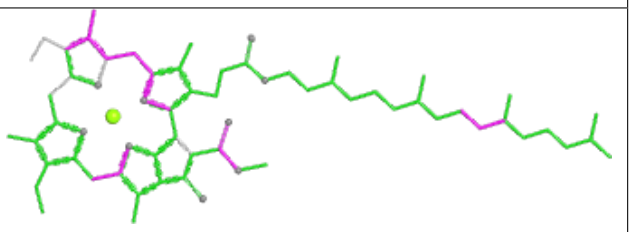


Rings

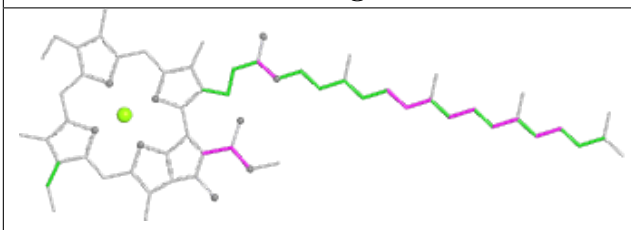
Ligand CLA B 803



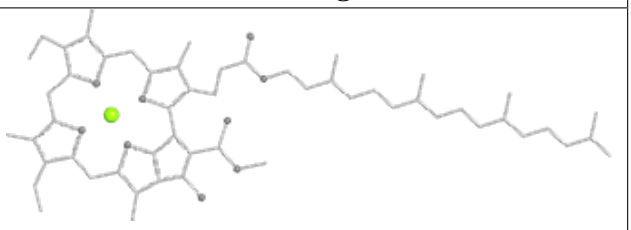
Bond lengths



Bond angles

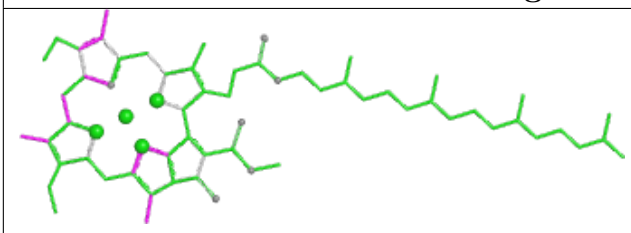


Torsions

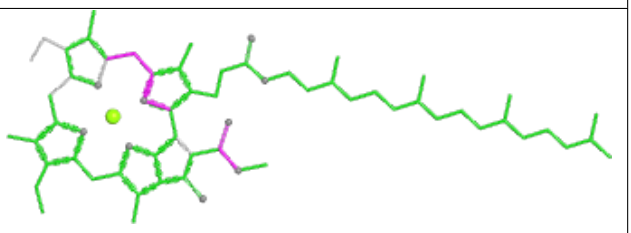


Rings

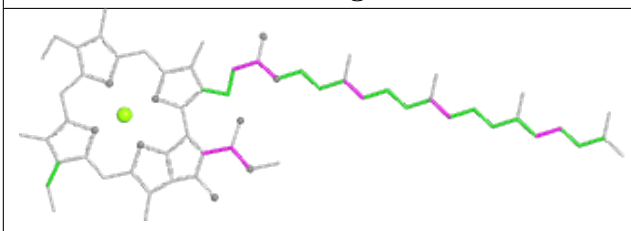
Ligand CLA B 854



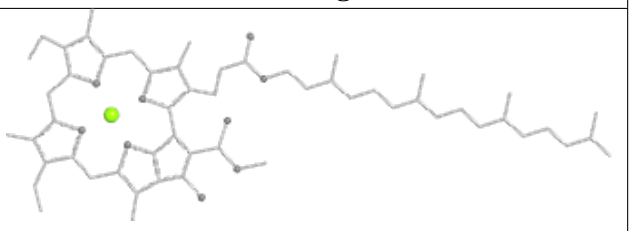
Bond lengths



Bond angles

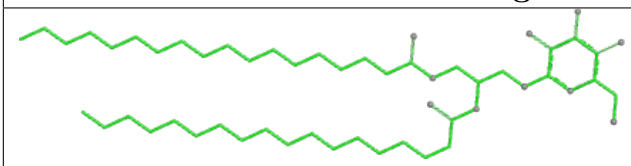


Torsions

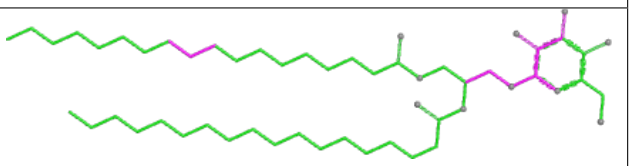


Rings

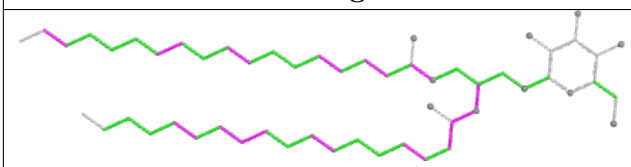
Ligand LMG L1 210



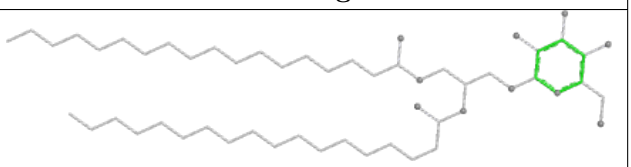
Bond lengths



Bond angles

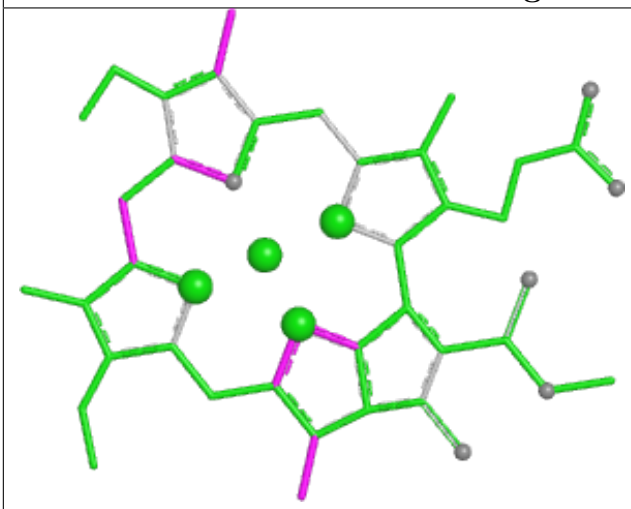


Torsions

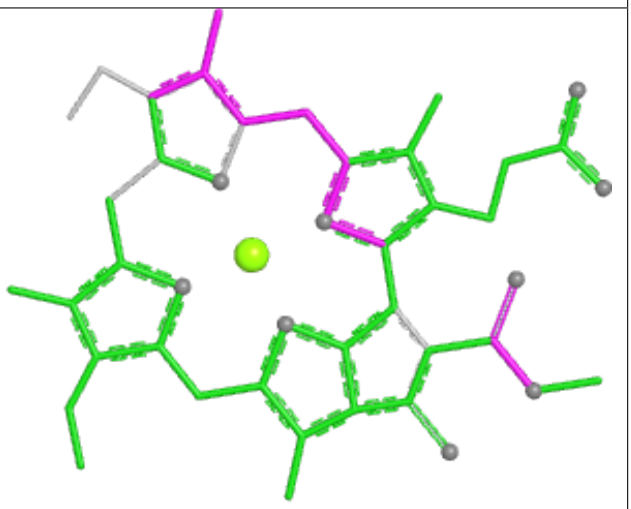


Rings

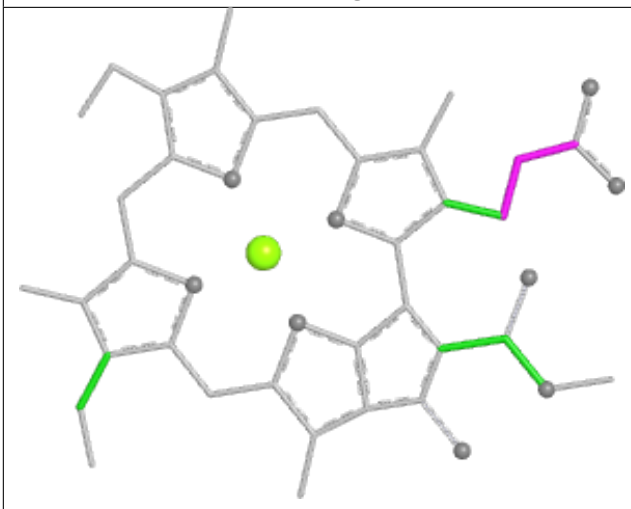
Ligand CLA X 101



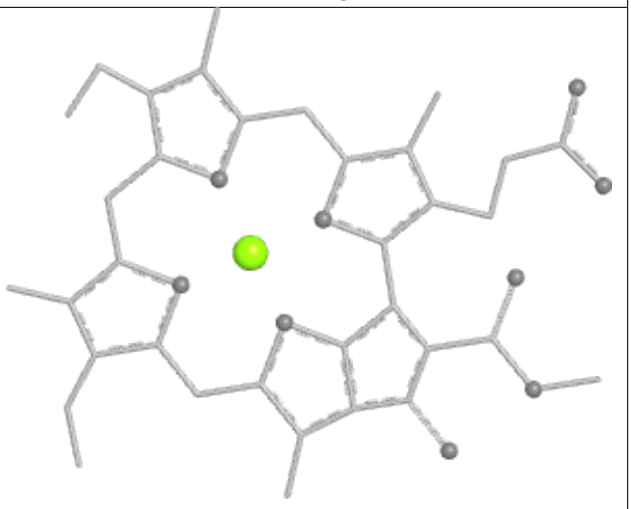
Bond lengths



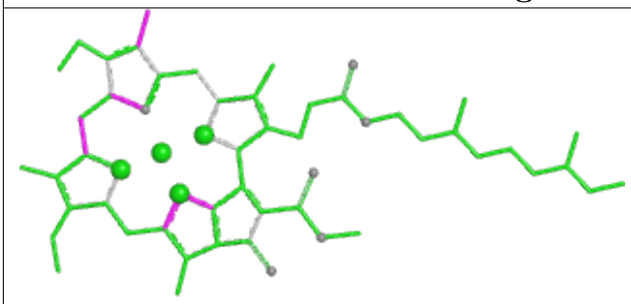
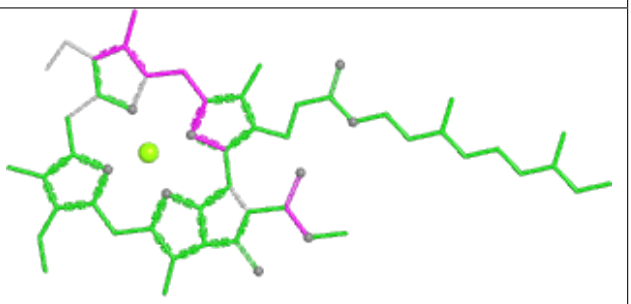
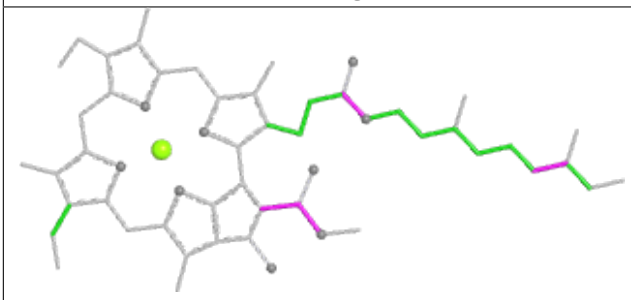
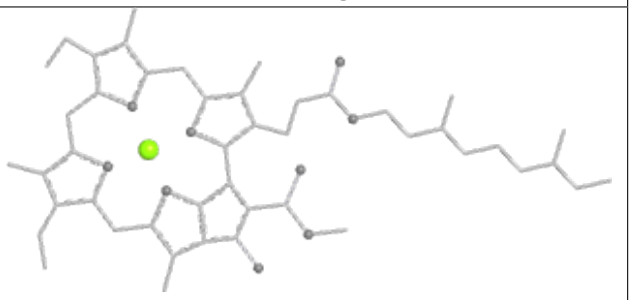
Bond angles

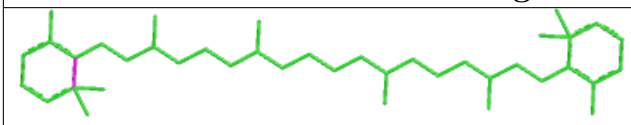
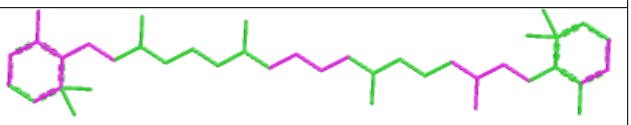
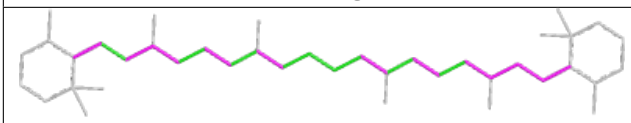
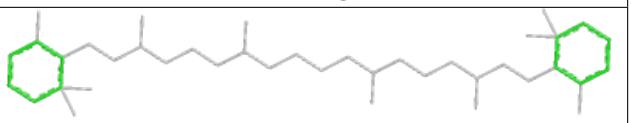


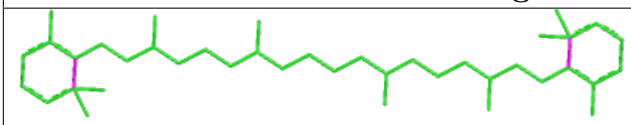
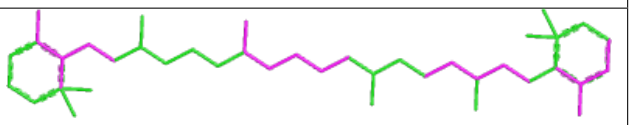
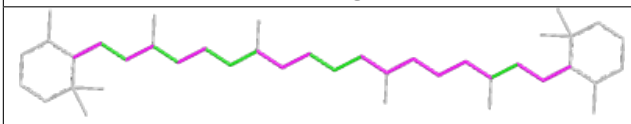
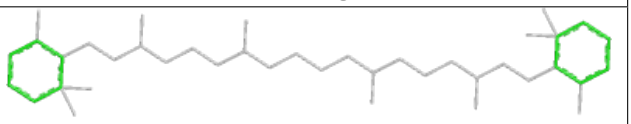
Torsions

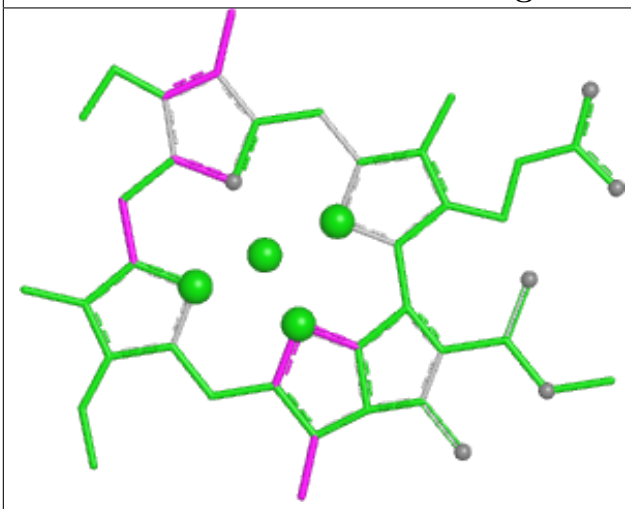
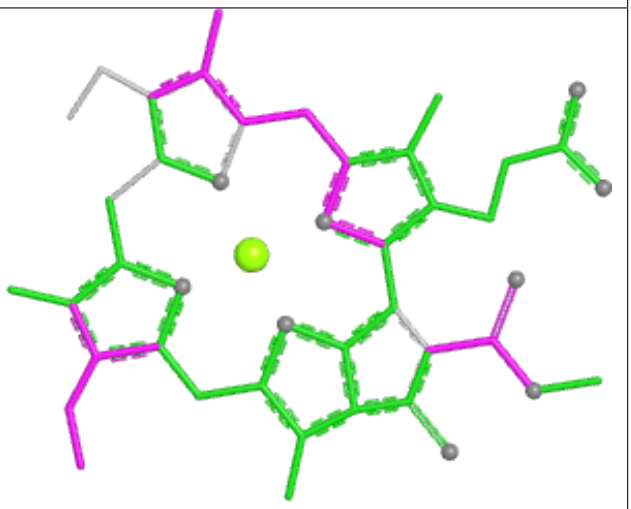
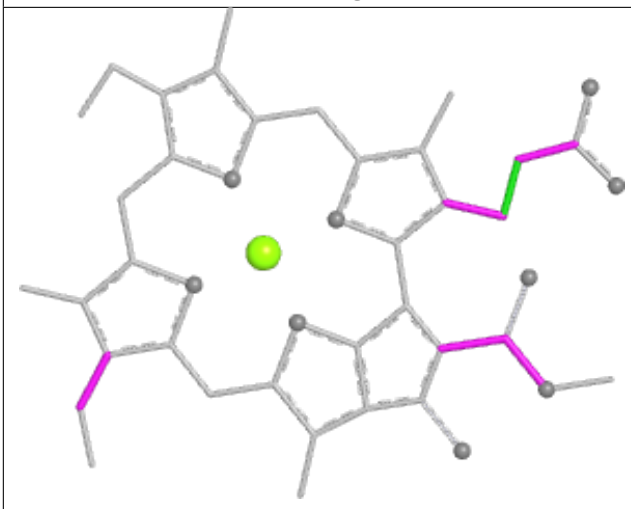
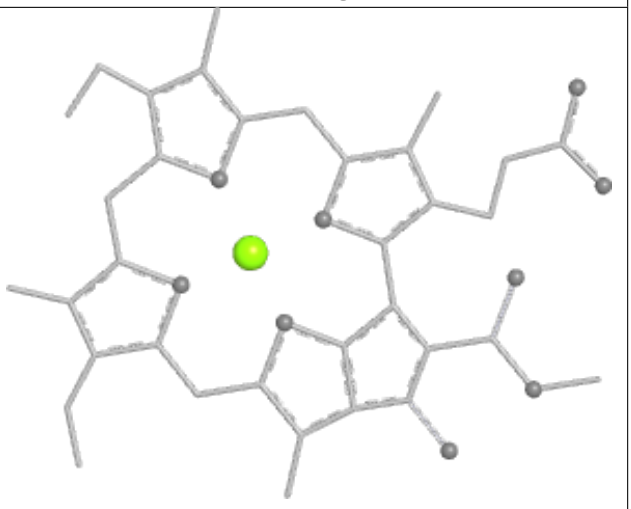


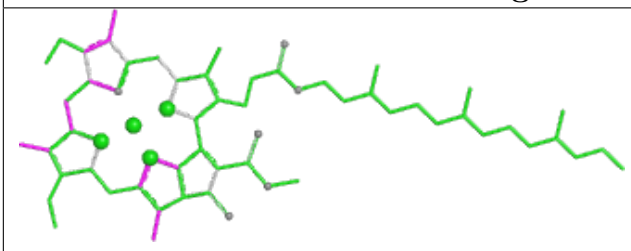
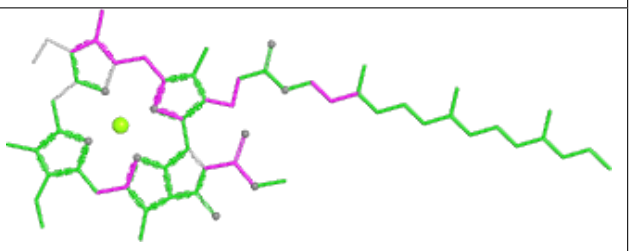
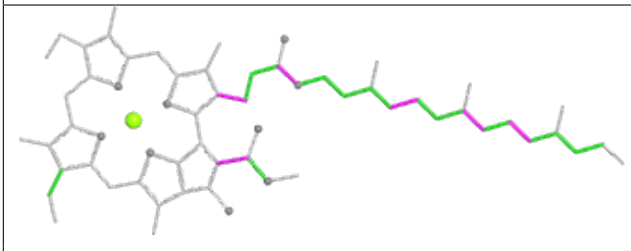
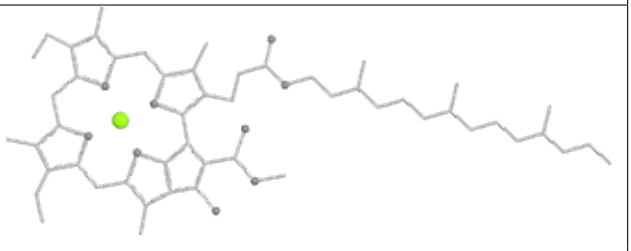
Rings

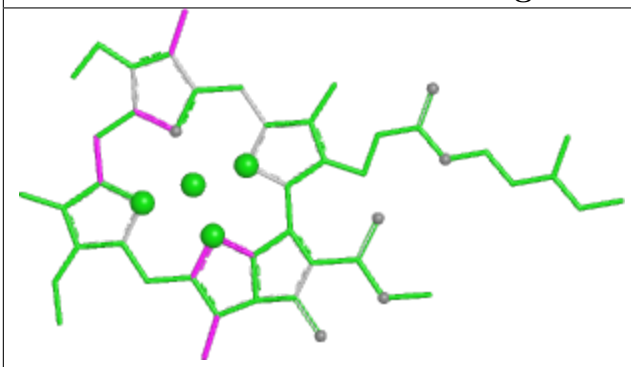
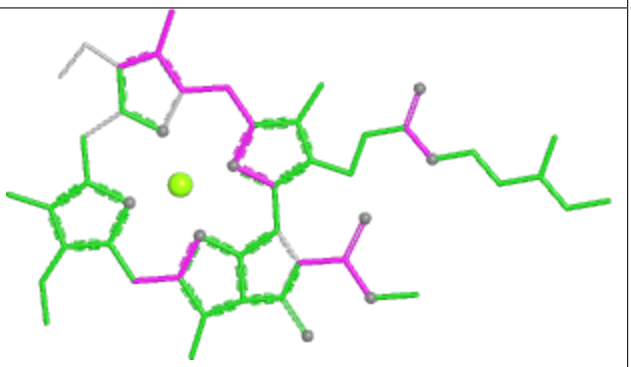
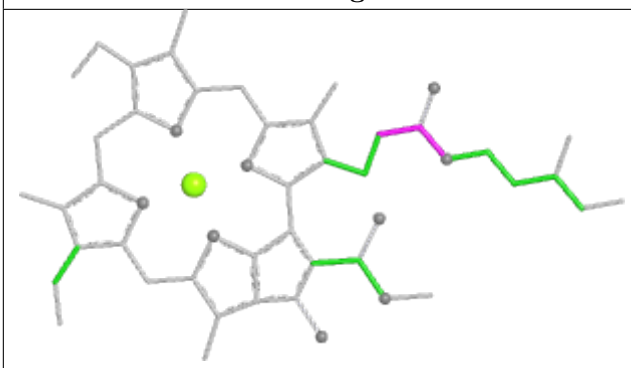
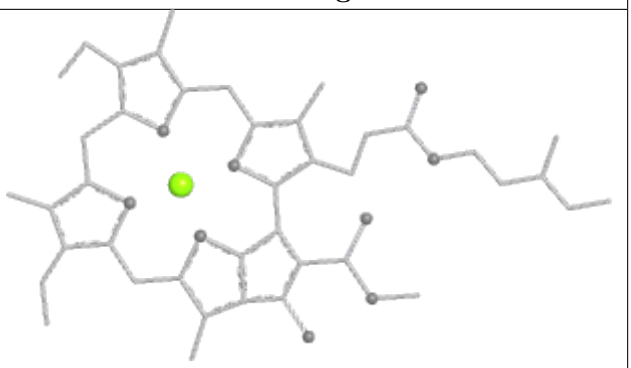
Ligand CLA B1 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

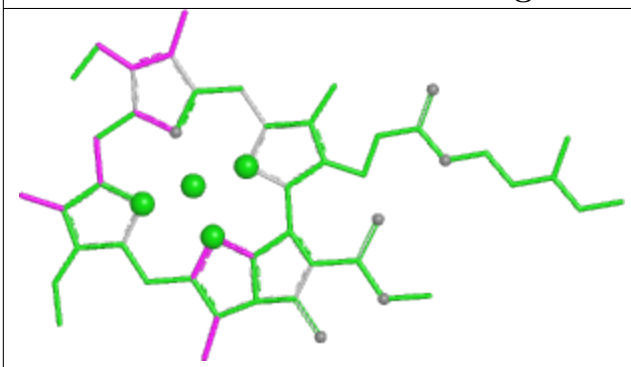
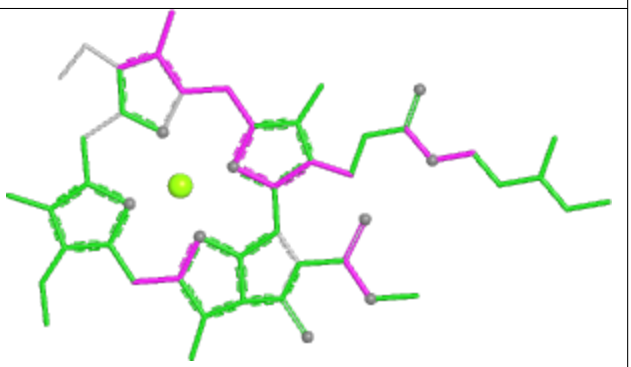
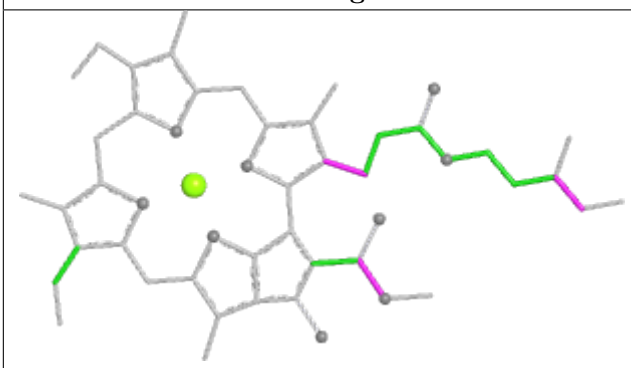
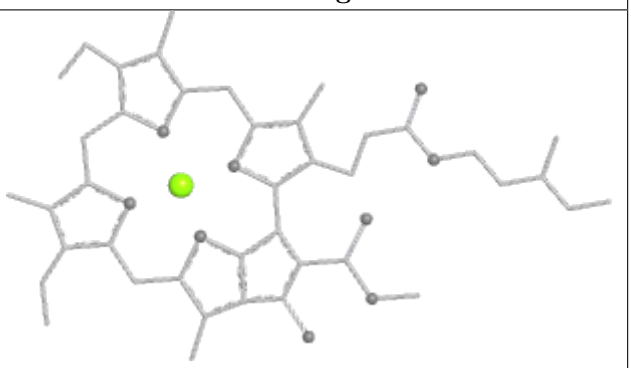
Ligand BCR A2 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

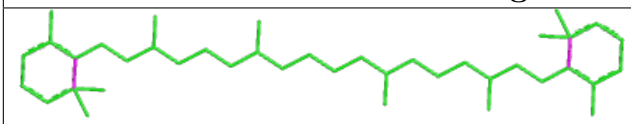
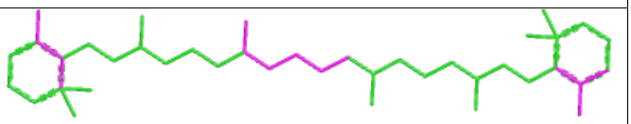
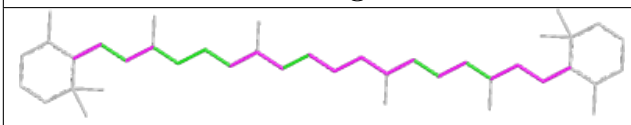
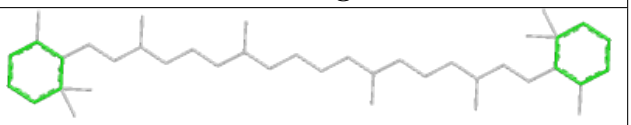
Ligand BCR K1 106	
	
Bond lengths	Bond angles
	
Torsions	Rings

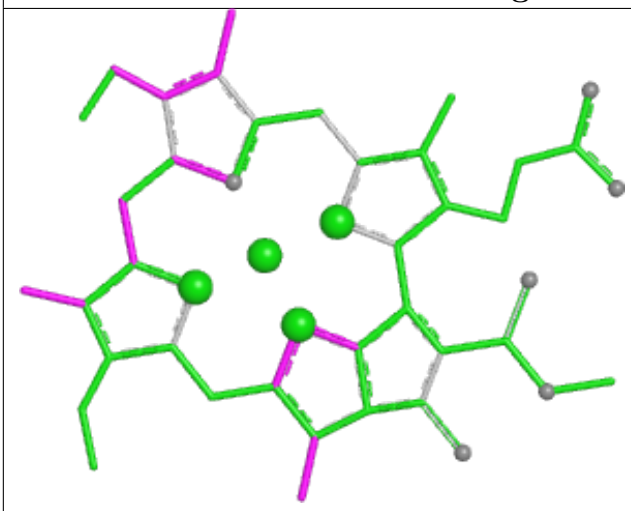
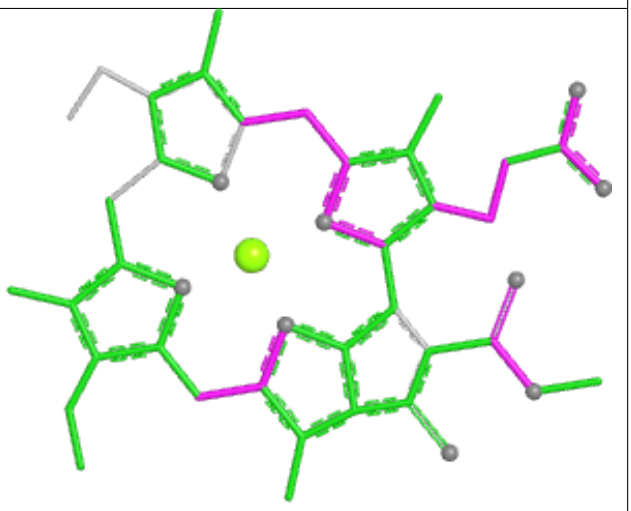
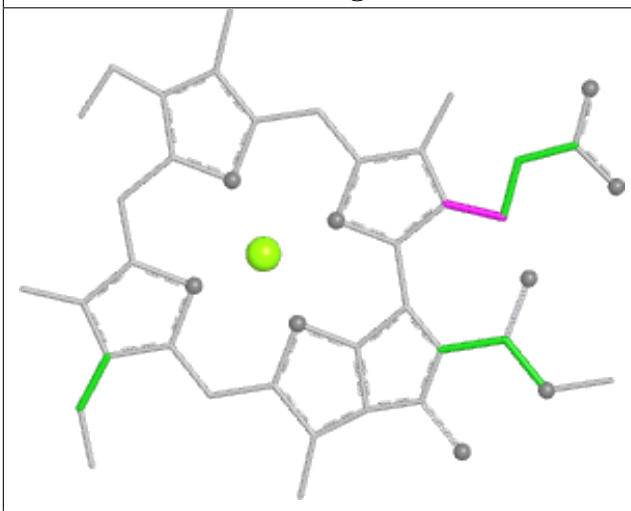
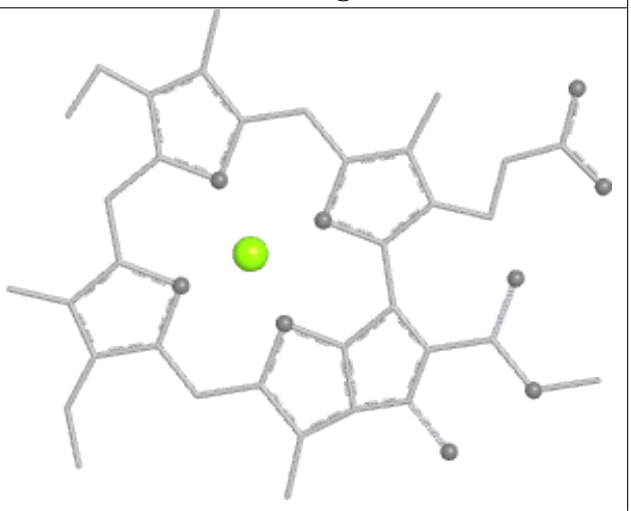
Ligand CLA B2 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

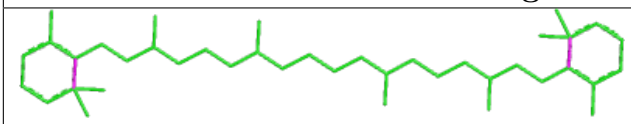
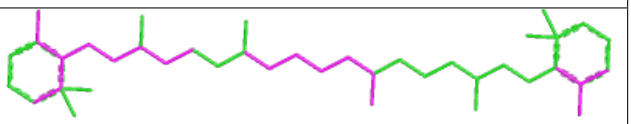
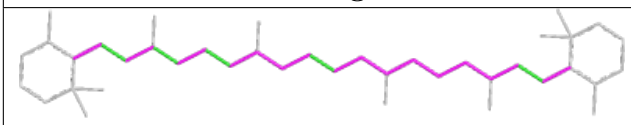
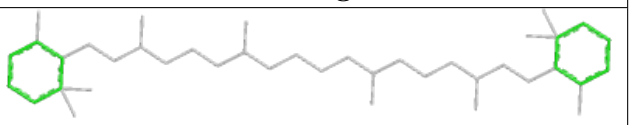
Ligand CLA BB 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

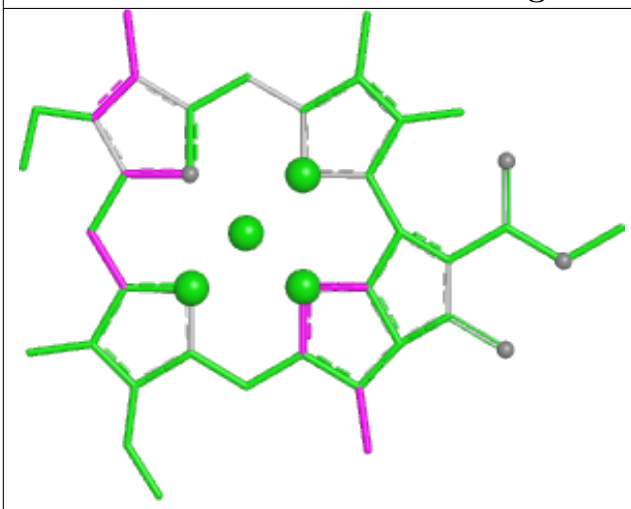
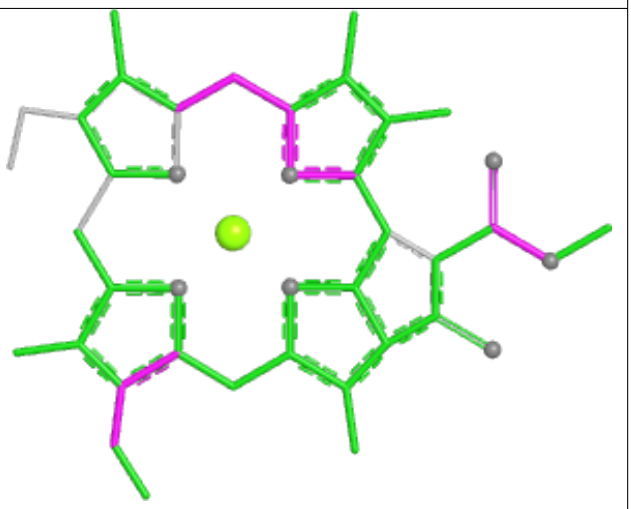
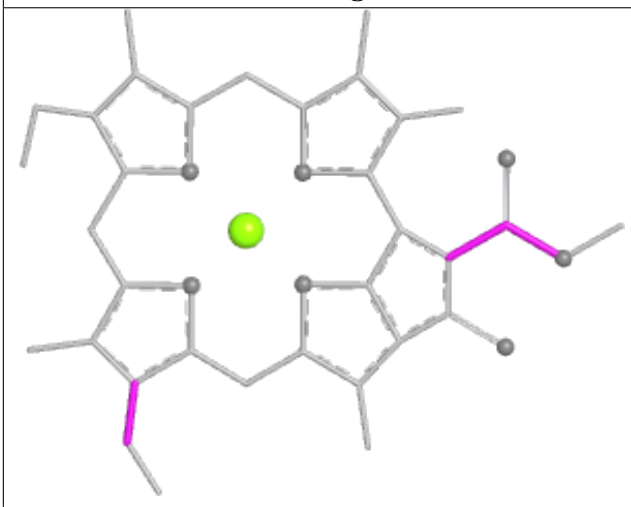
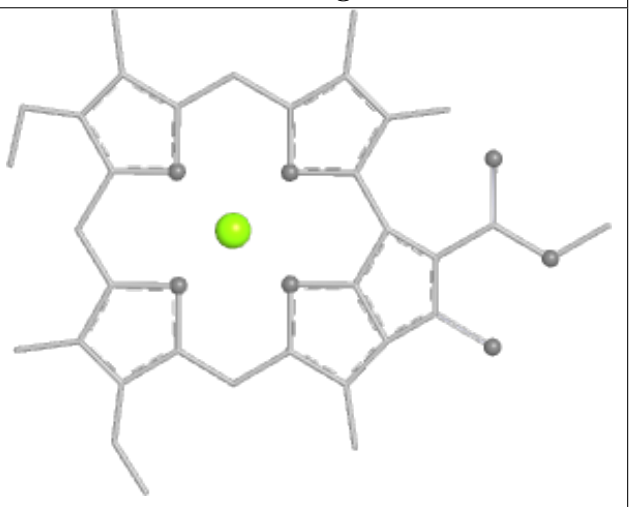
Ligand CLA A1 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

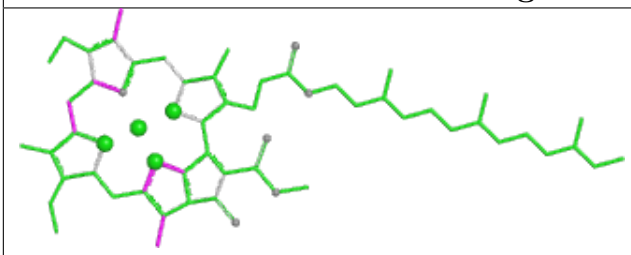
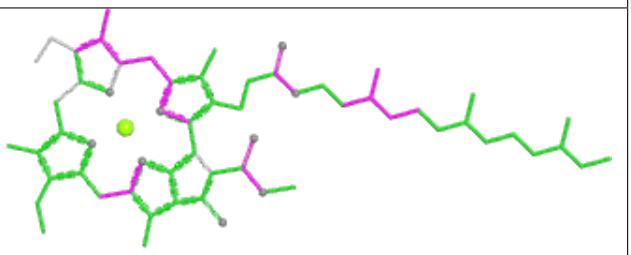
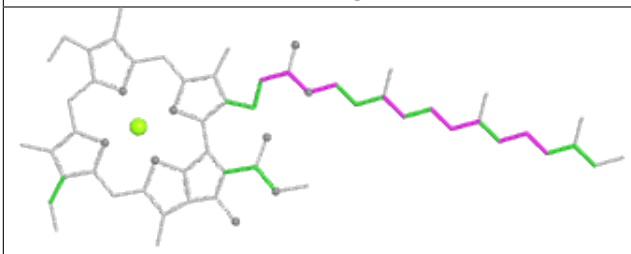
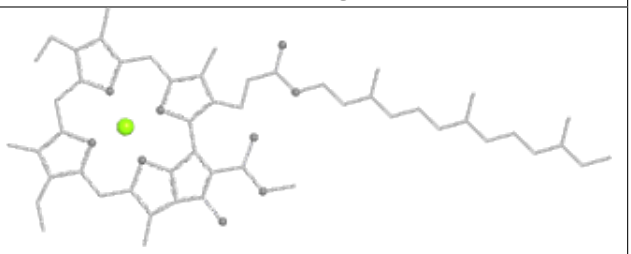
Ligand CLA A2 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR BB 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L1 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

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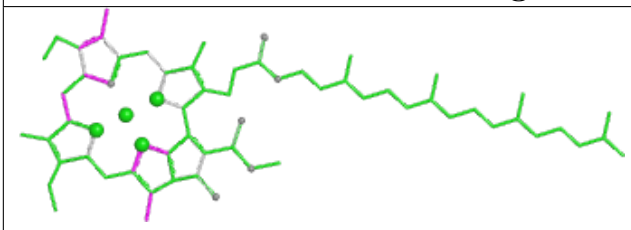
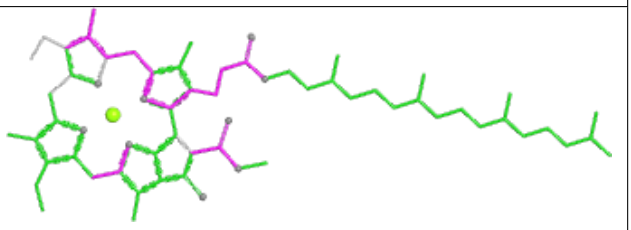
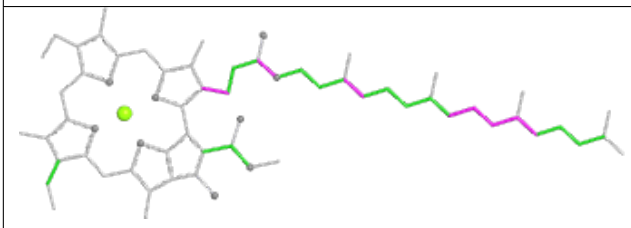
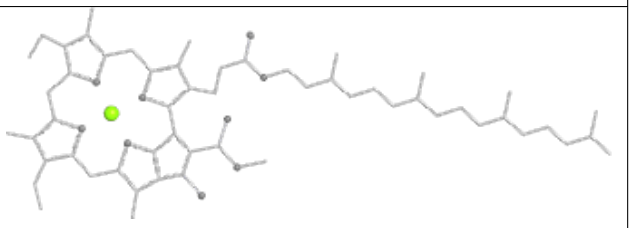
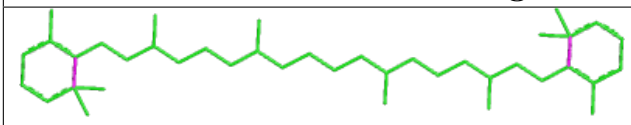
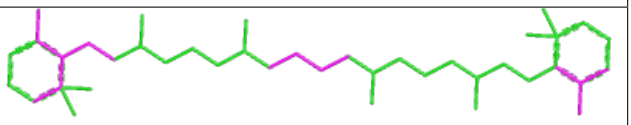
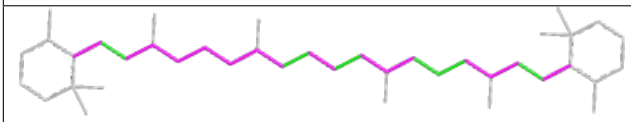
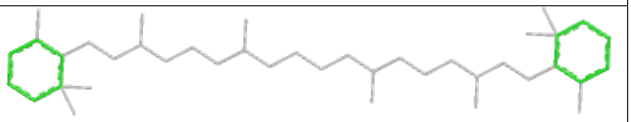
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR AA 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

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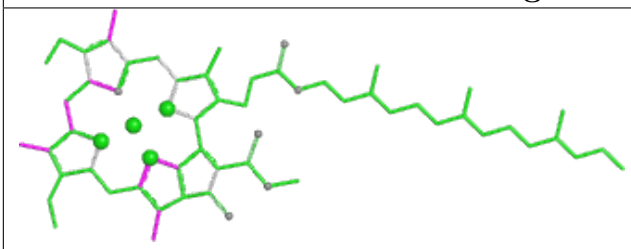
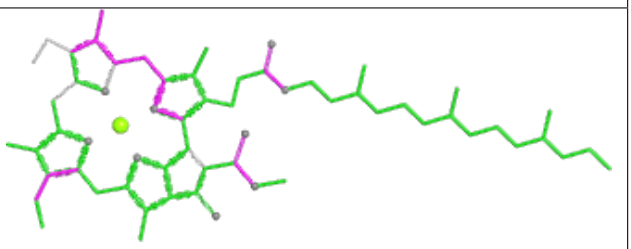
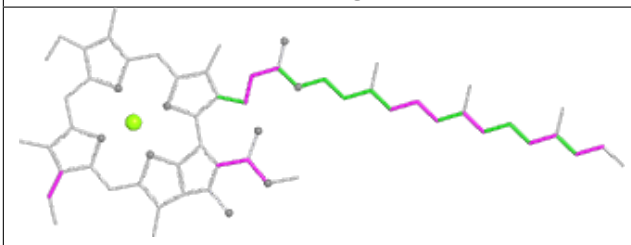
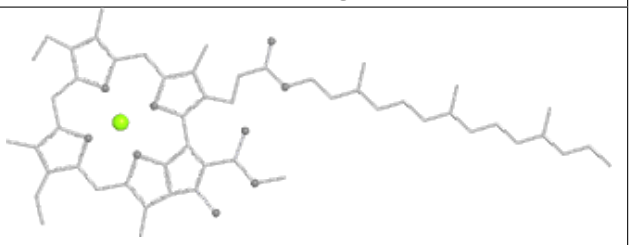
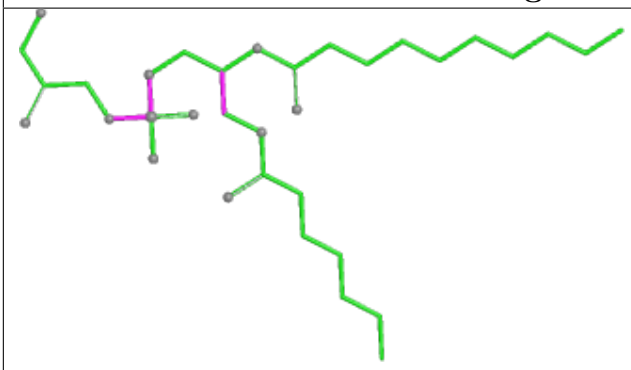
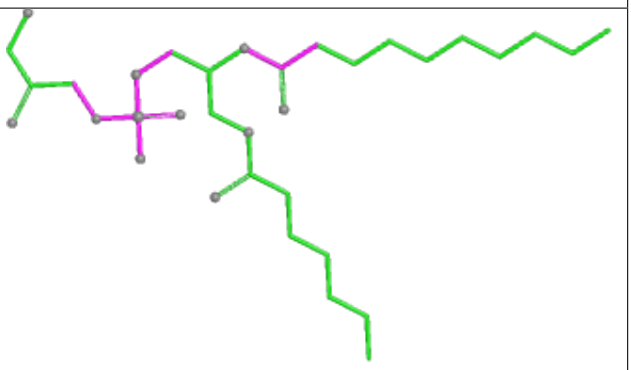
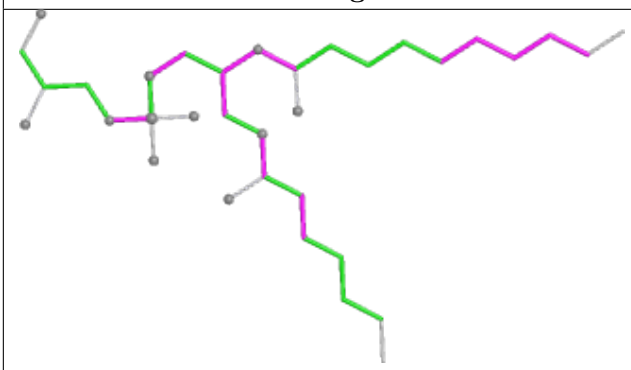
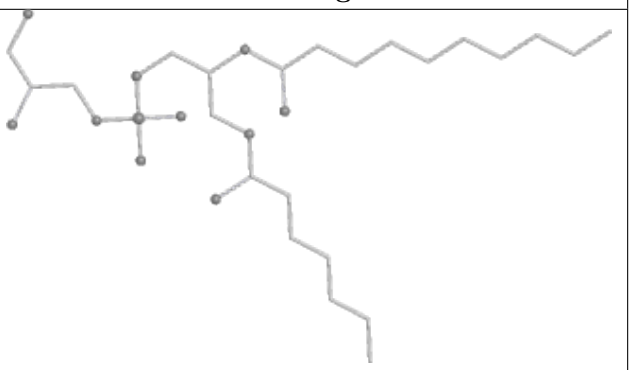
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG L 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

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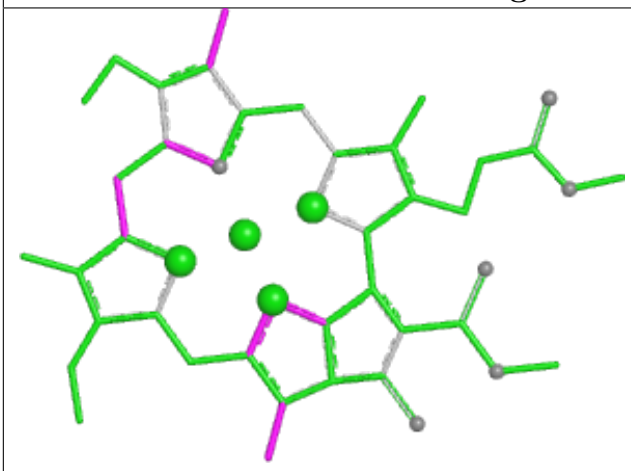
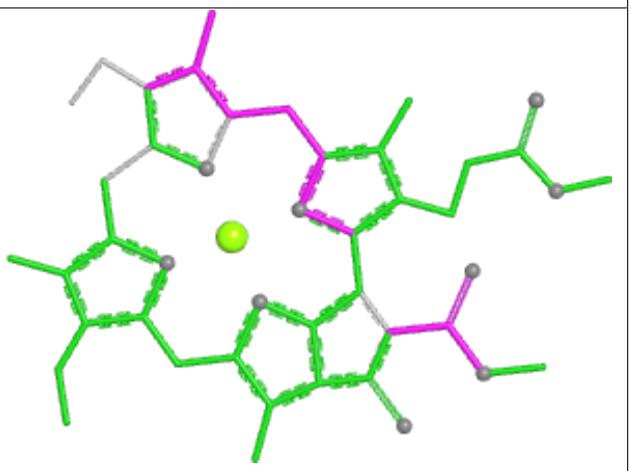
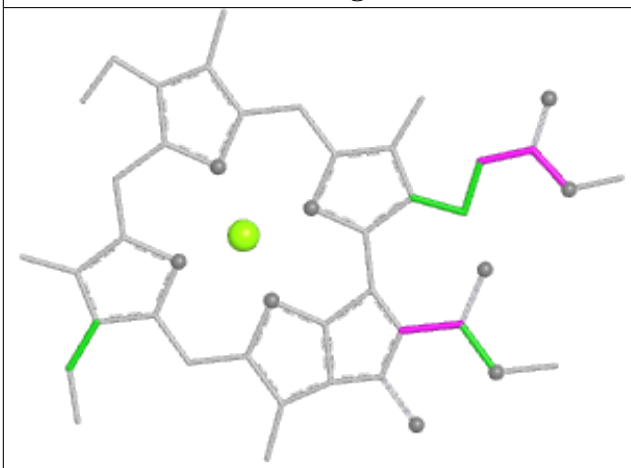
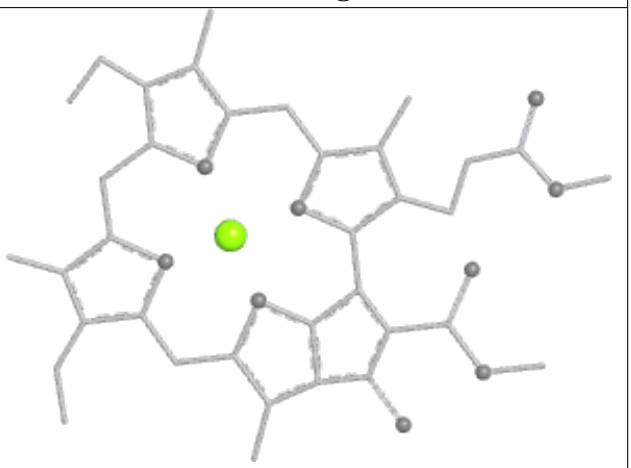
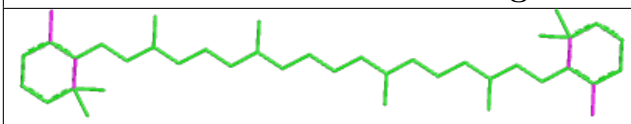
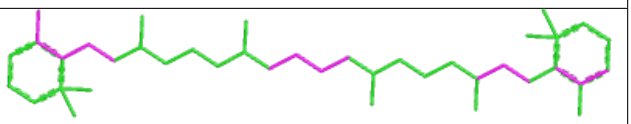
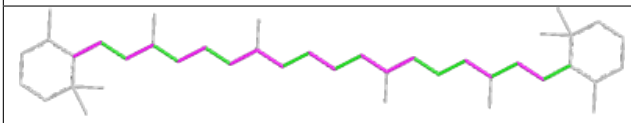
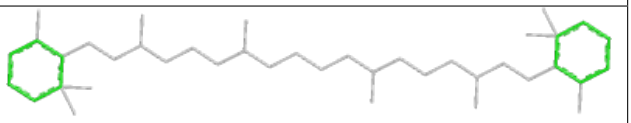
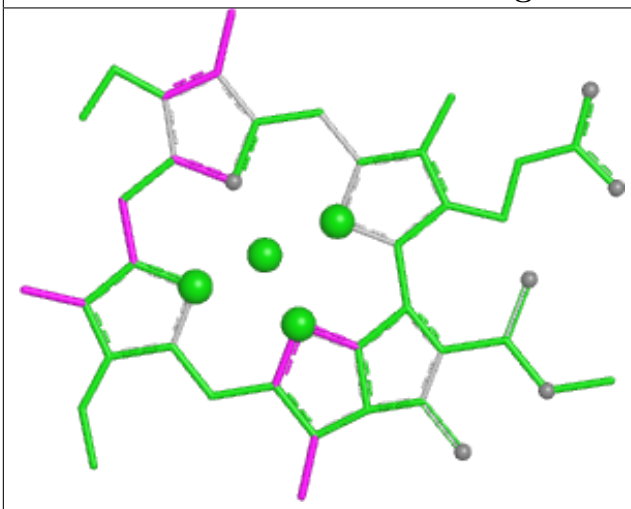
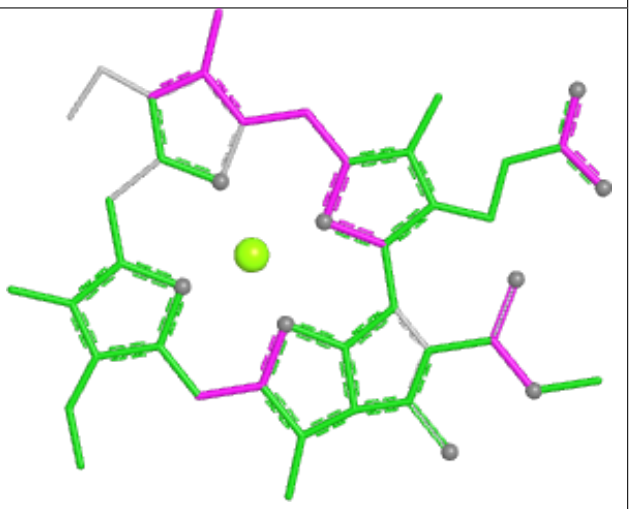
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR BB 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

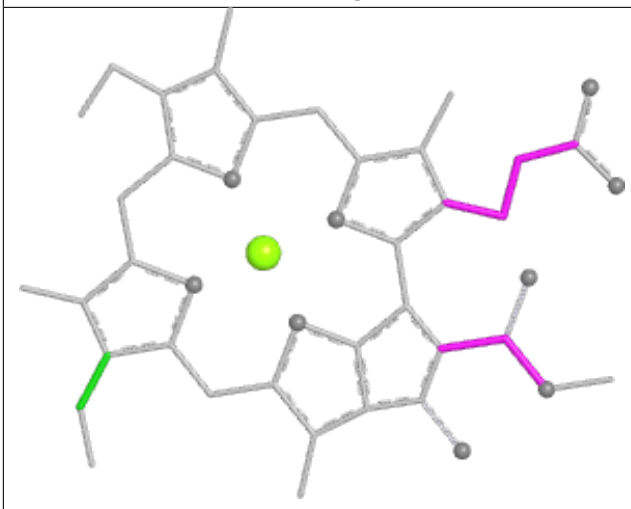
Ligand CLA A2 826



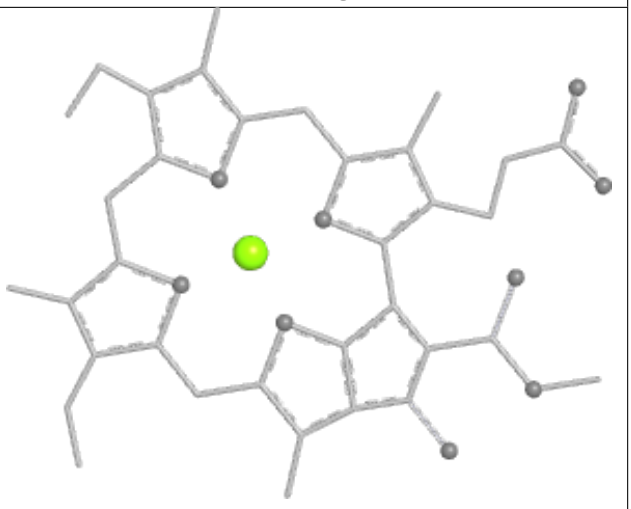
Bond lengths



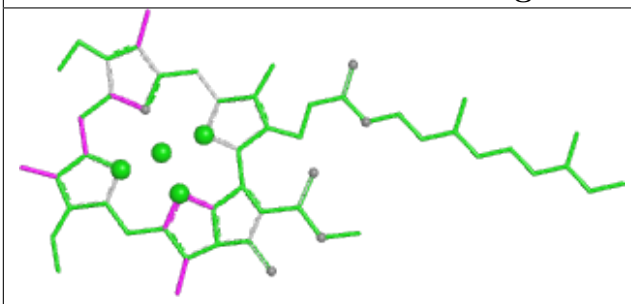
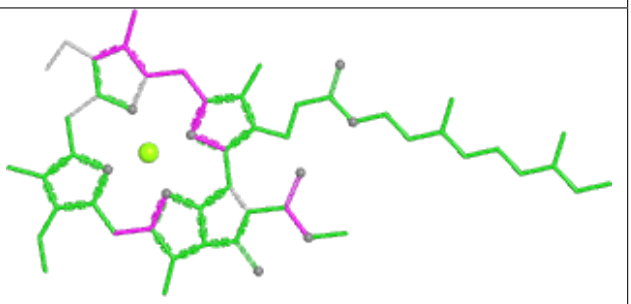
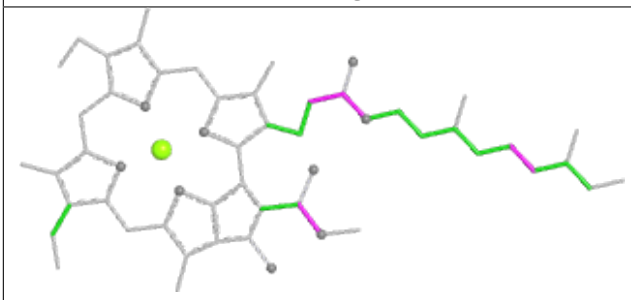
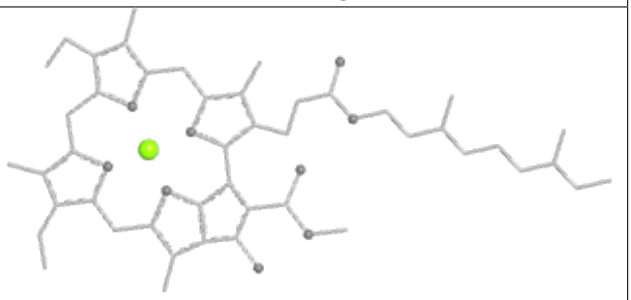
Bond angles



Torsions



Rings

Ligand CLA A1 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

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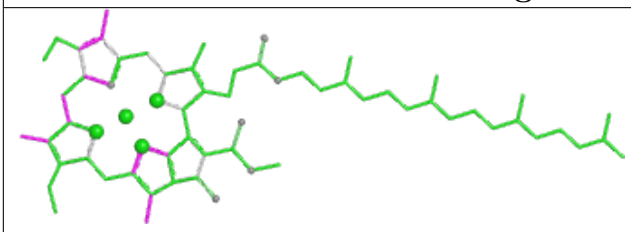
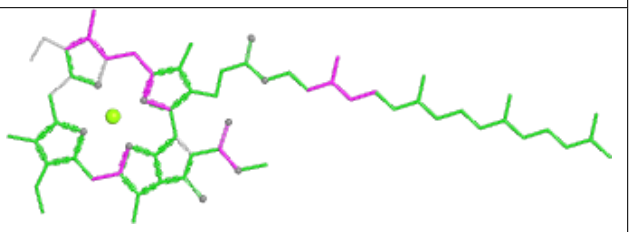
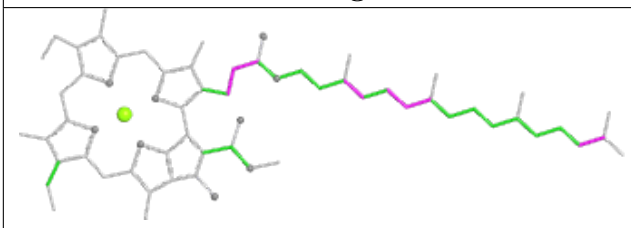
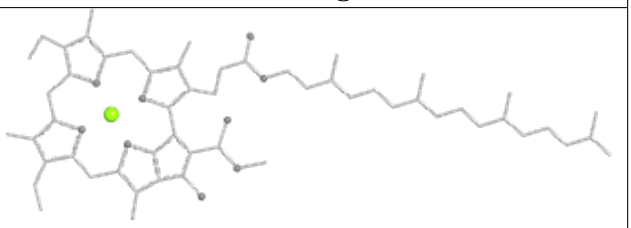
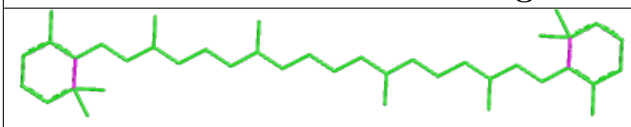
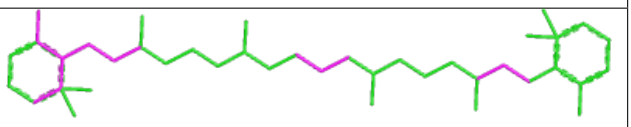
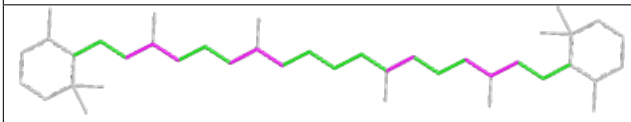
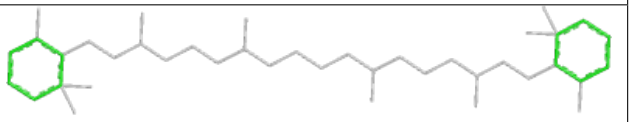
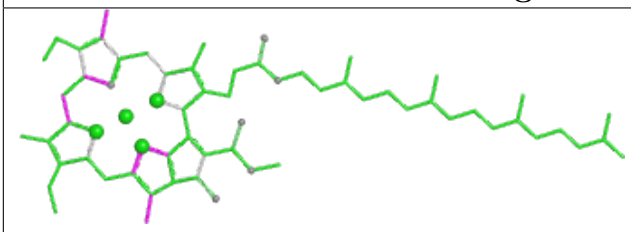
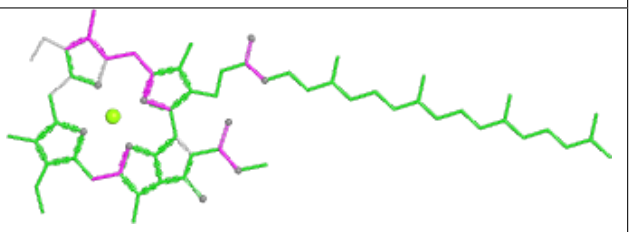
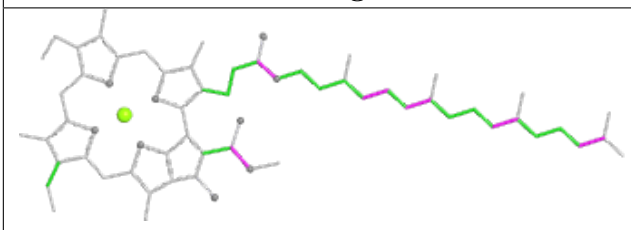
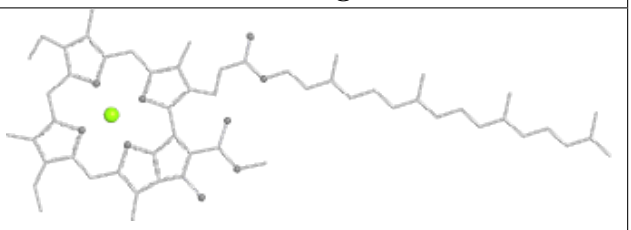
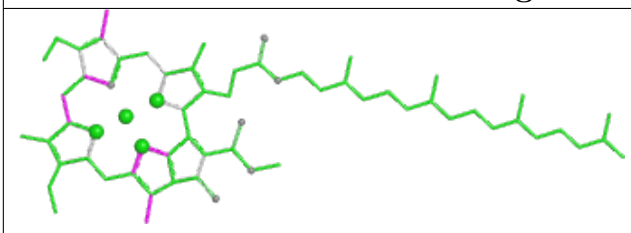
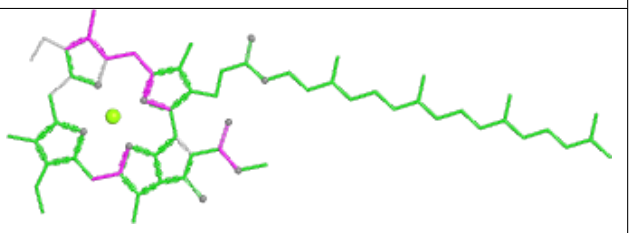
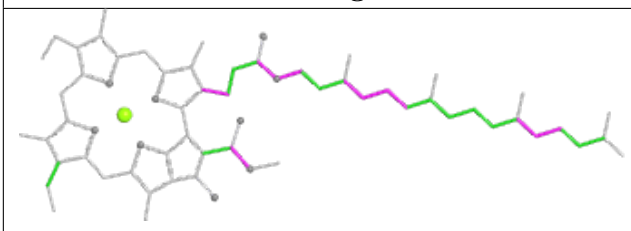
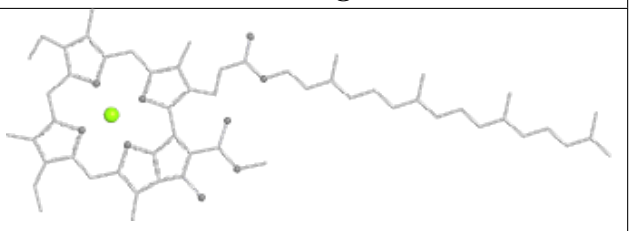
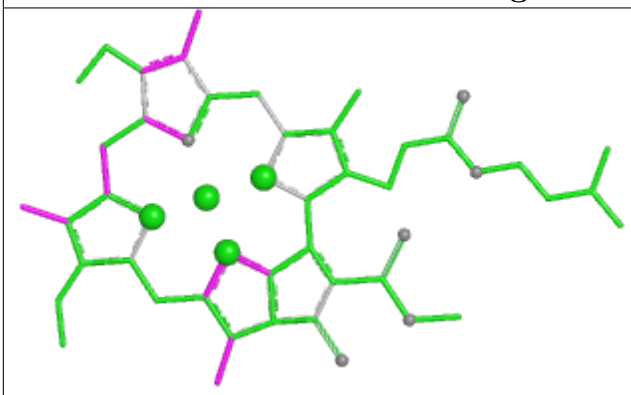
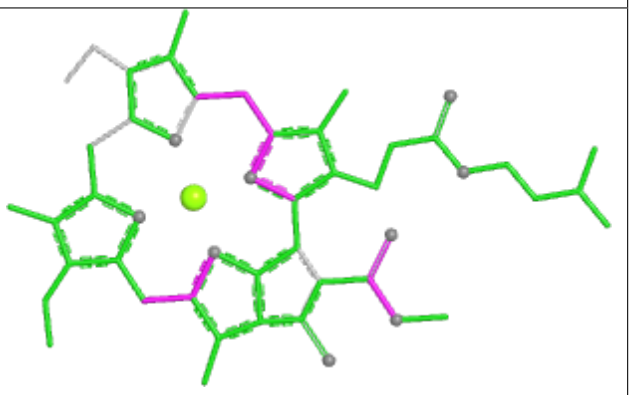
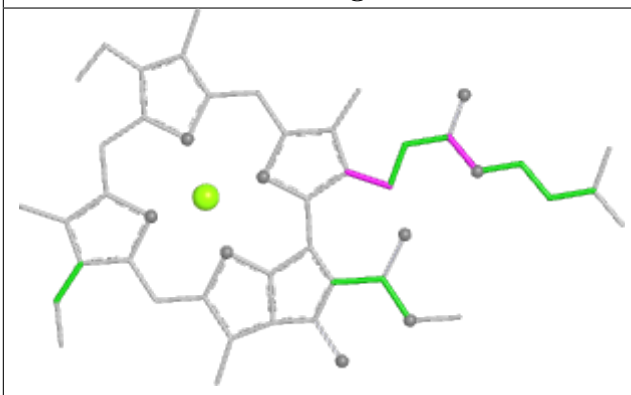
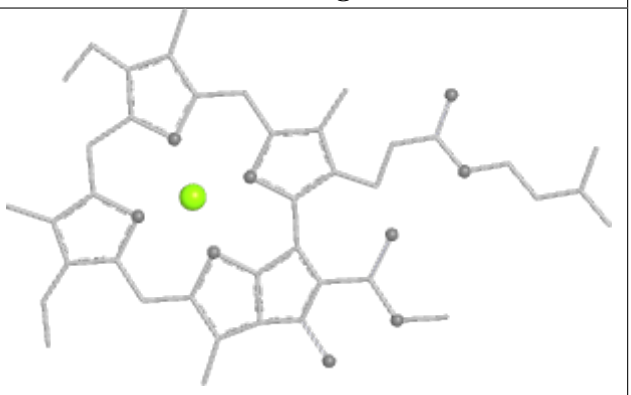
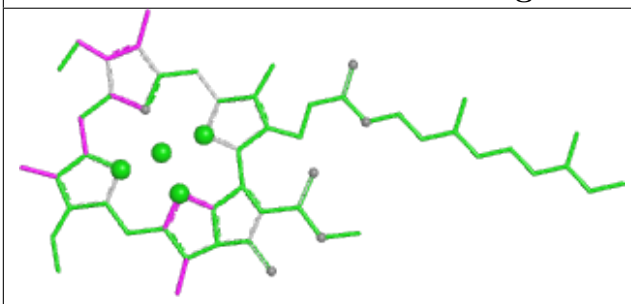
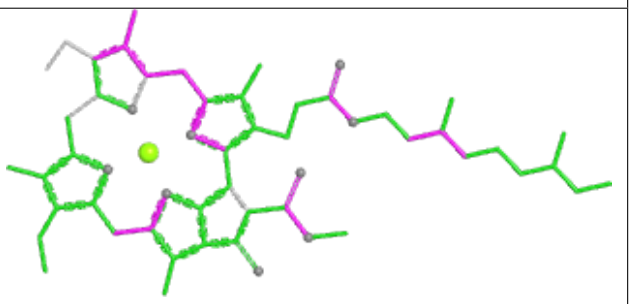
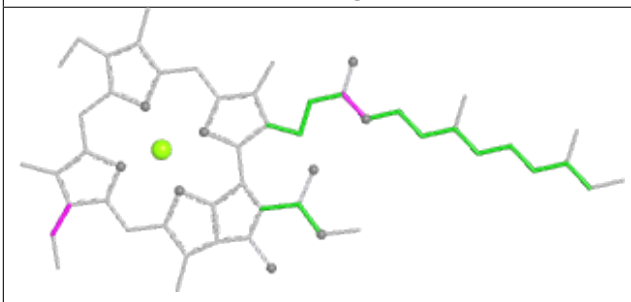
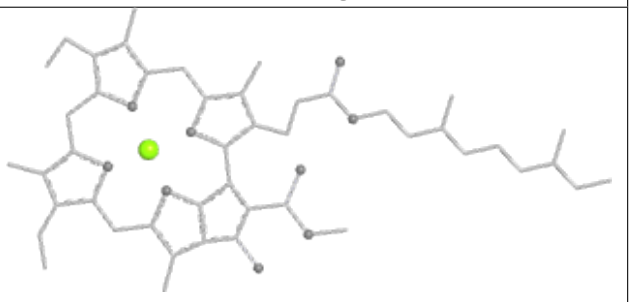
 Bond lengths	 Bond angles
 Torsions	 Rings

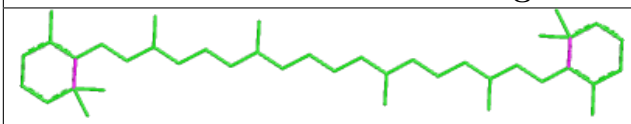
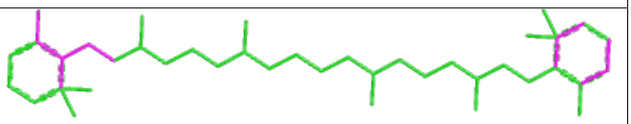
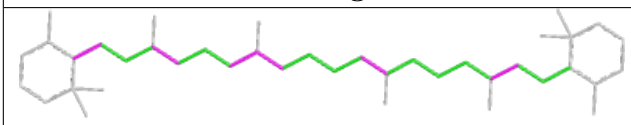
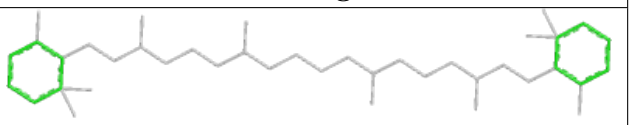
Ligand BCR L1 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

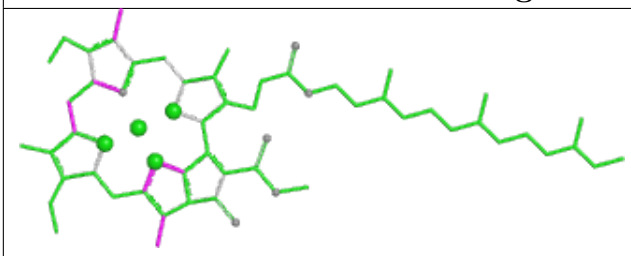
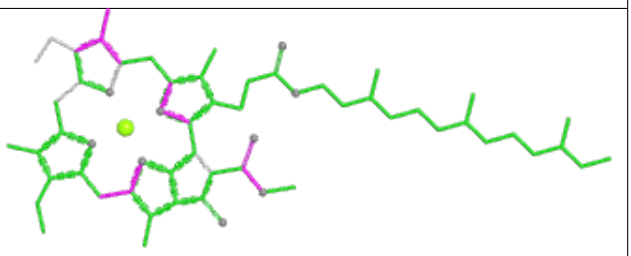
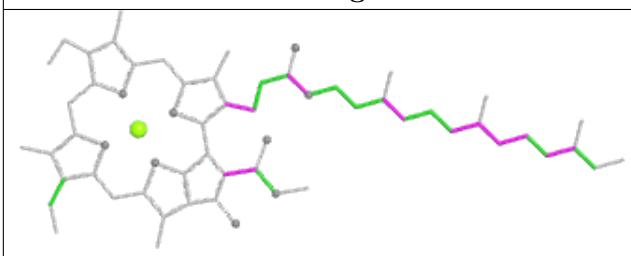
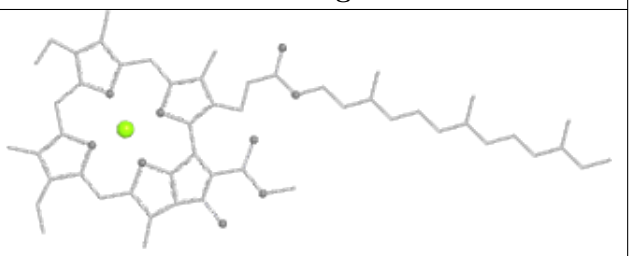
Ligand CLA A2 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

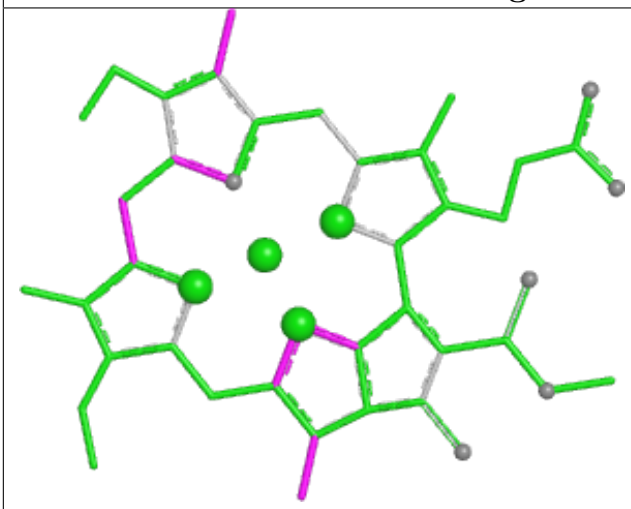
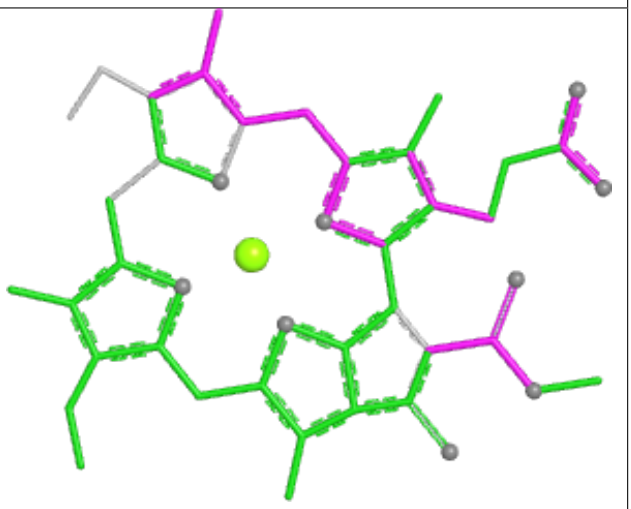
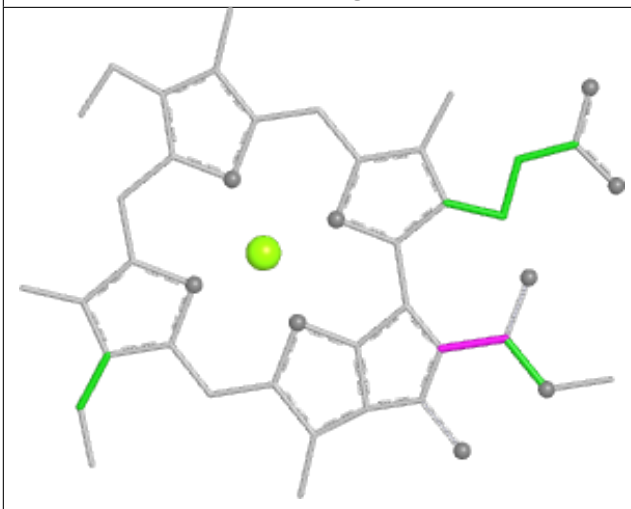
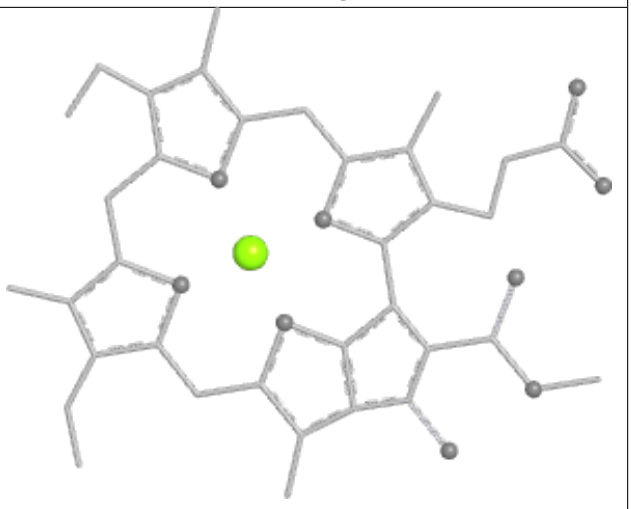
Ligand CLA B2 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

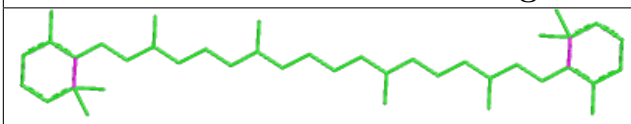
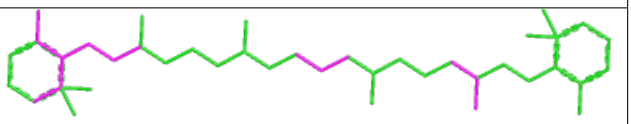
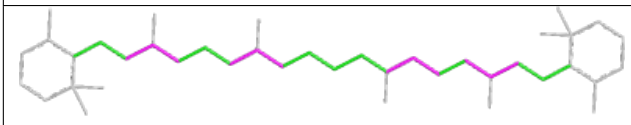
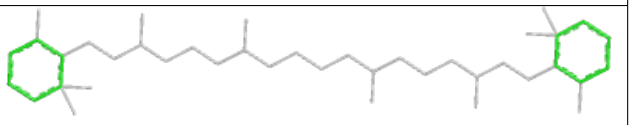
Ligand CLA AA 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

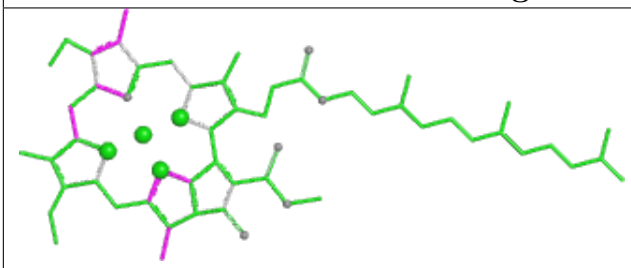
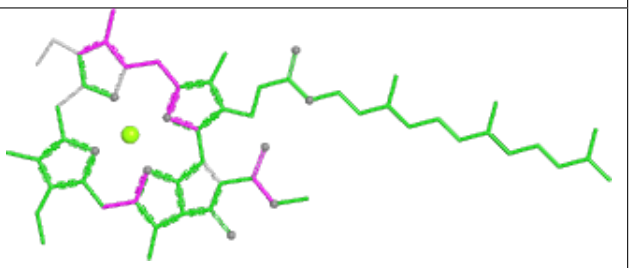
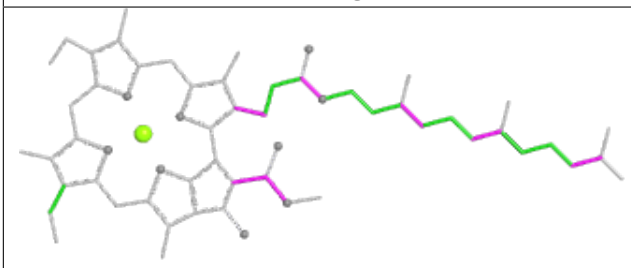
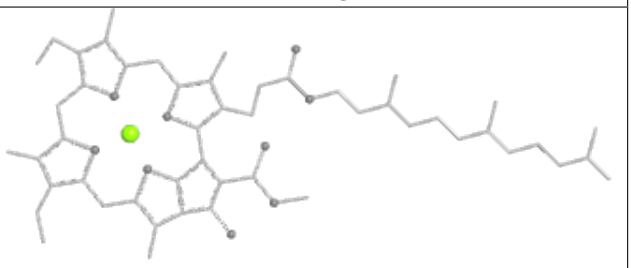
Ligand CLA B2 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

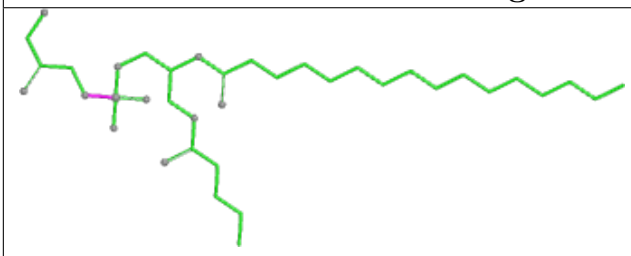
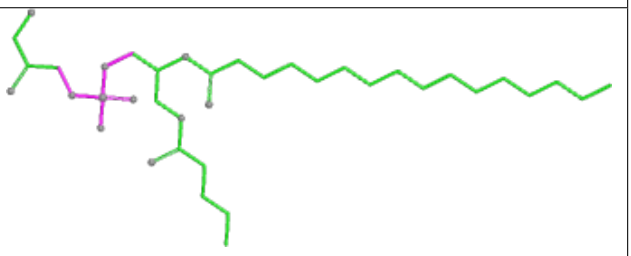
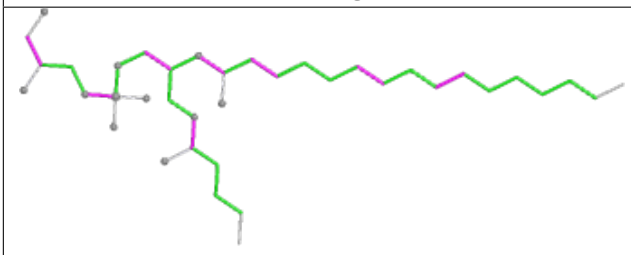
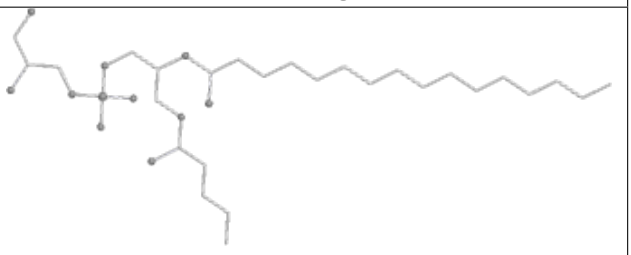
Ligand BCR B2 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

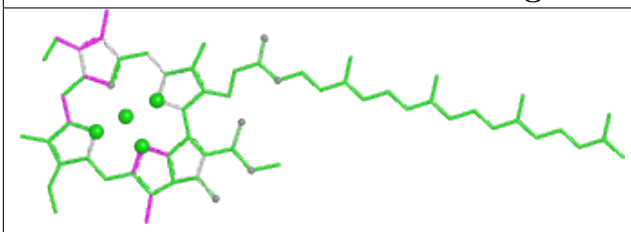
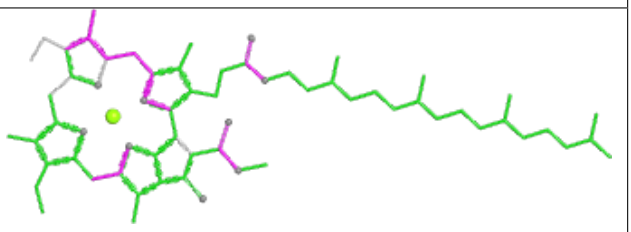
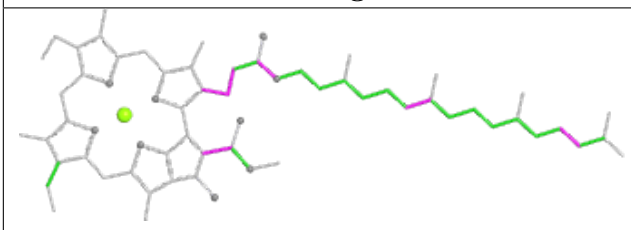
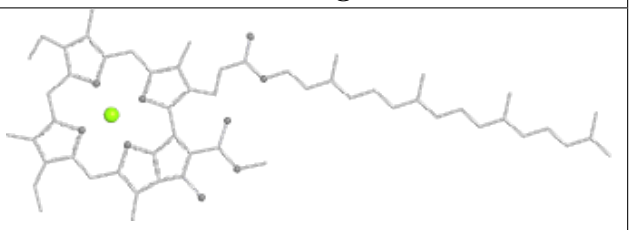
Ligand CLA B1 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

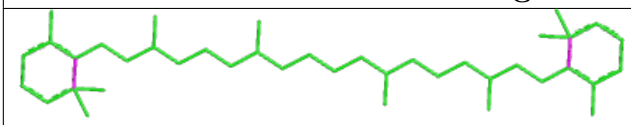
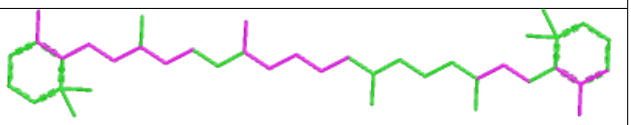
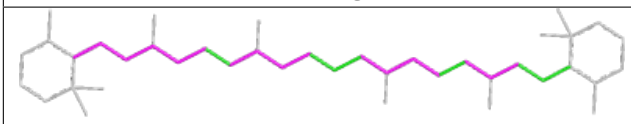
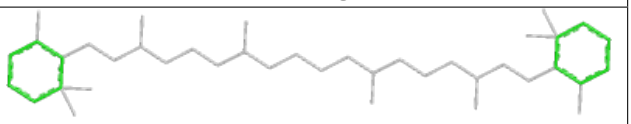
Ligand CLA KK 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

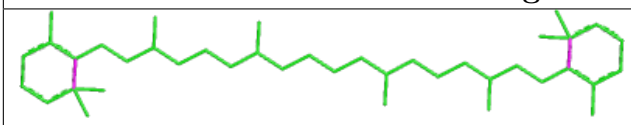
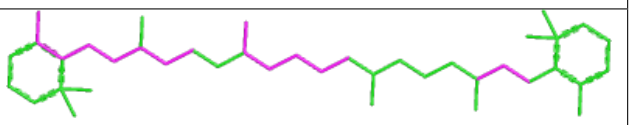
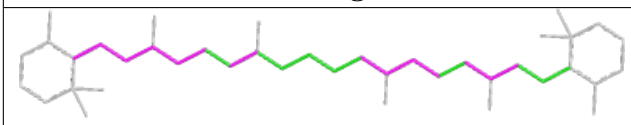
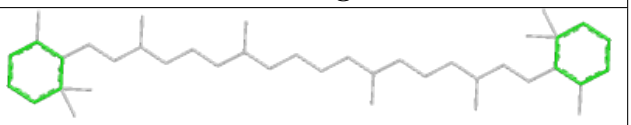
Ligand BCR I2 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BB 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

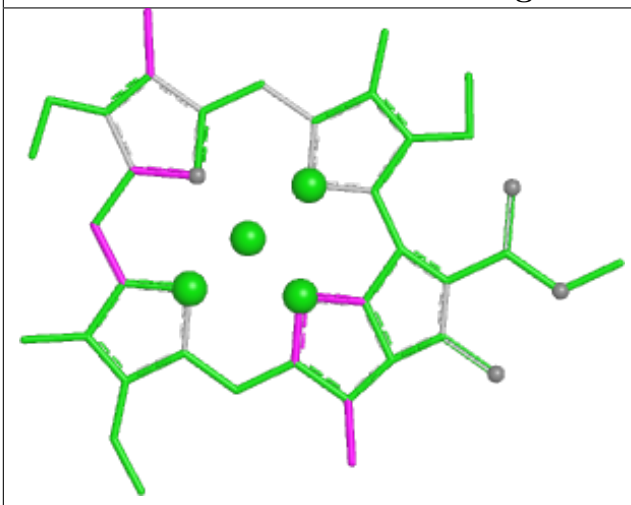
Ligand LHG AA 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

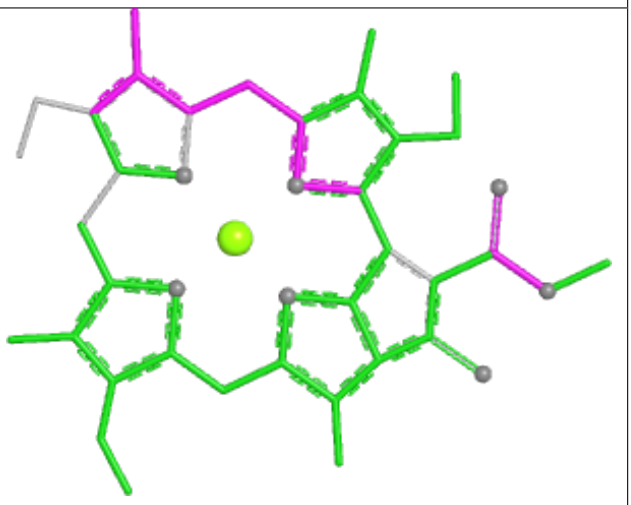
Ligand BCR B1 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

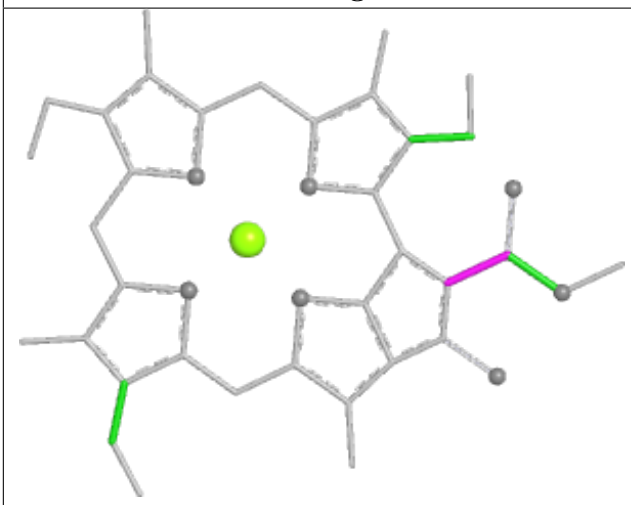
Ligand CLA B1 817



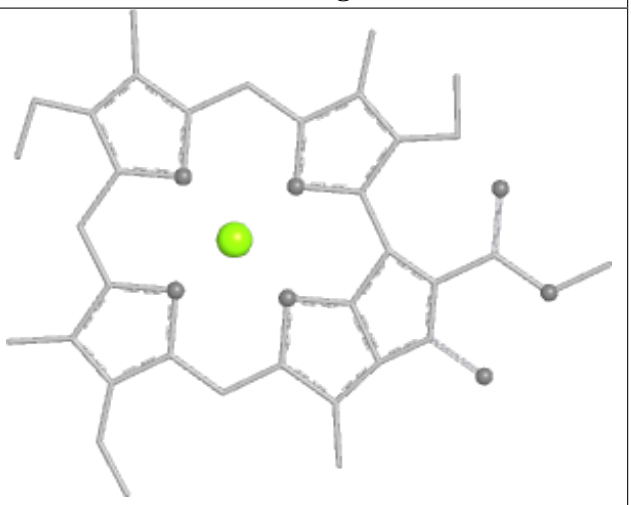
Bond lengths



Bond angles

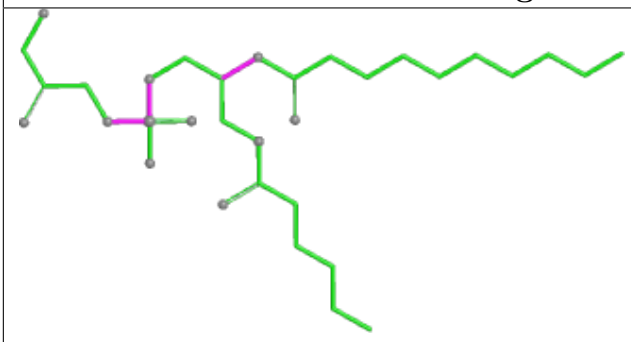


Torsions

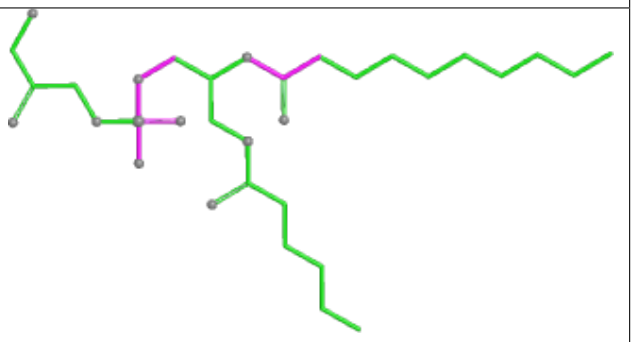


Rings

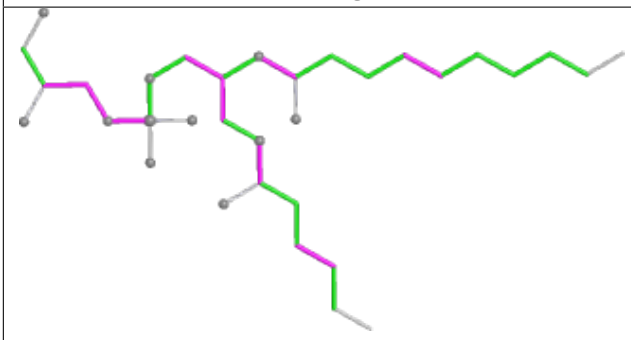
Ligand LHG L1 211



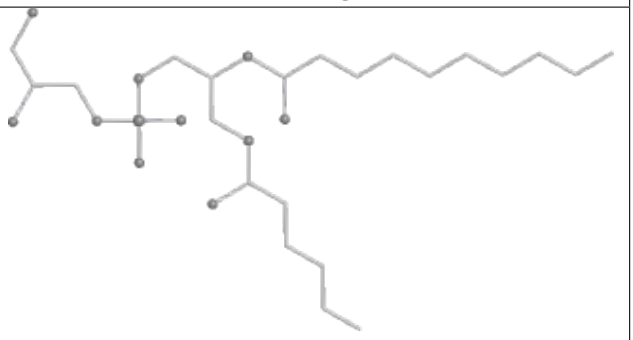
Bond lengths



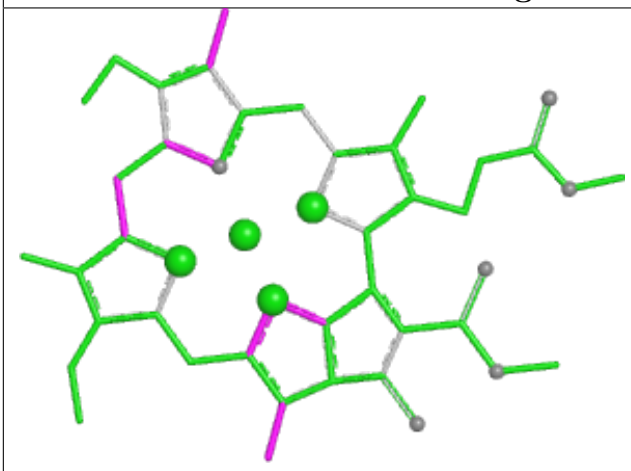
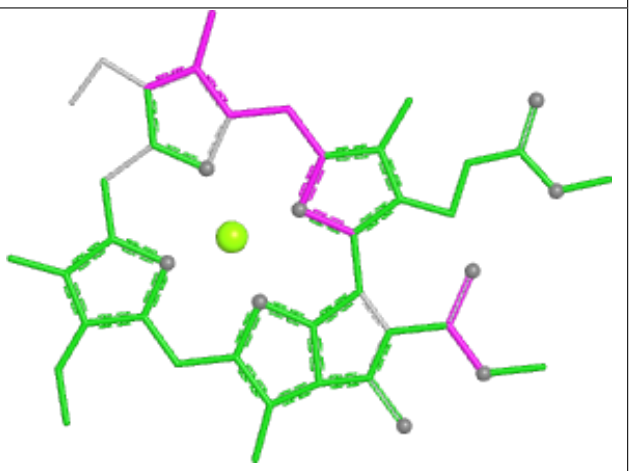
Bond angles



Torsions



Rings

Ligand CLA A1 840	
	
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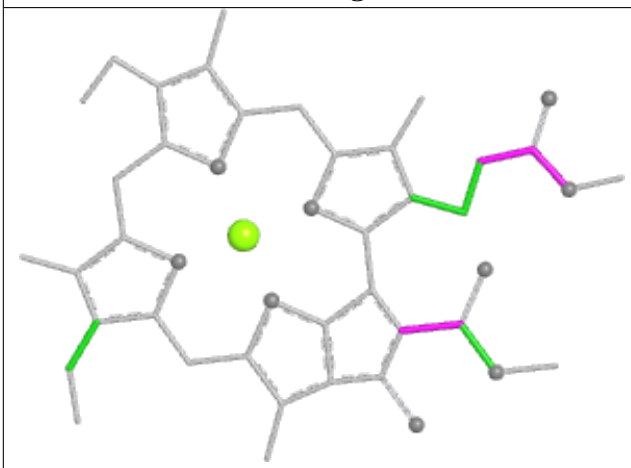	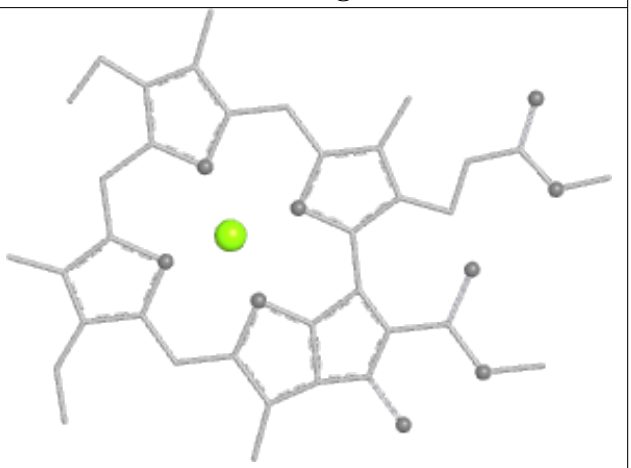
Torsions	Rings

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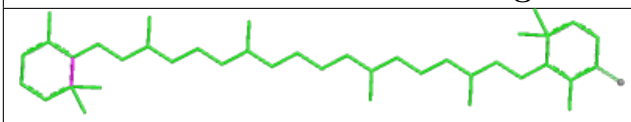
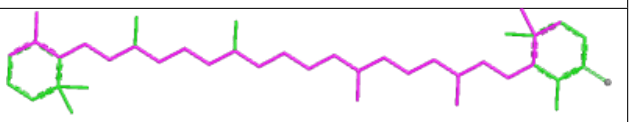
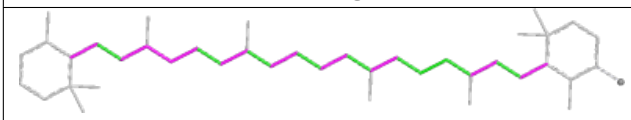
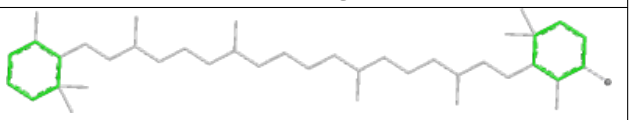
	
Bond lengths	Bond angles
	
Torsions	Rings

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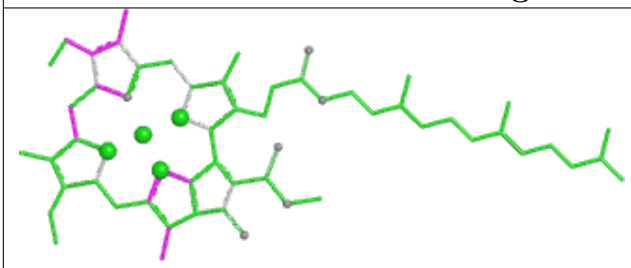	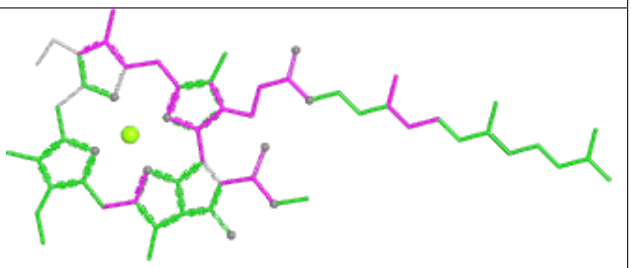
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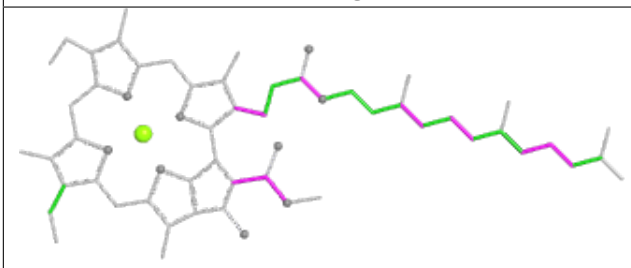	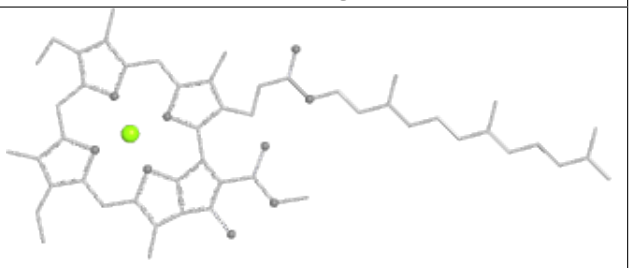
Torsions	Rings

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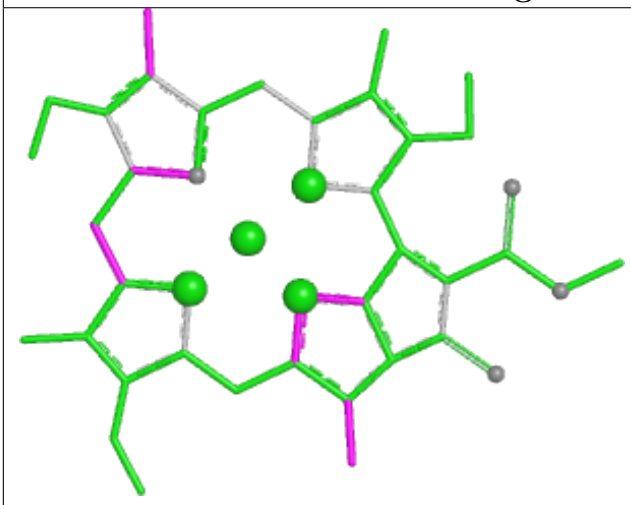
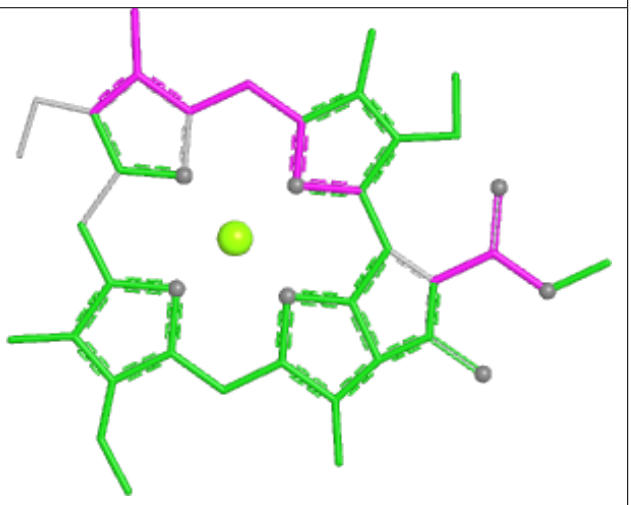
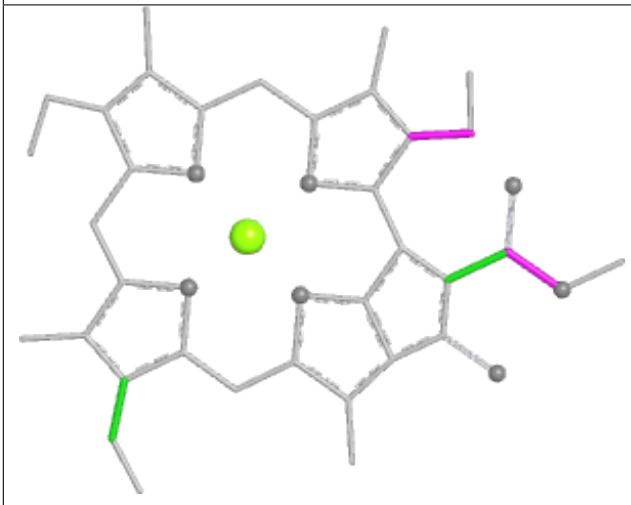
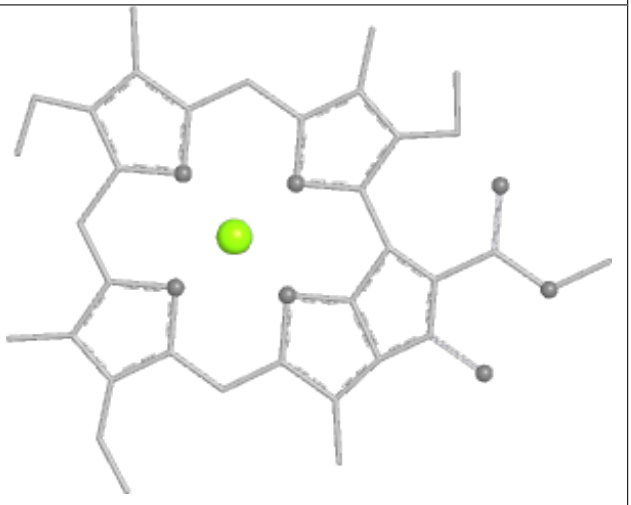
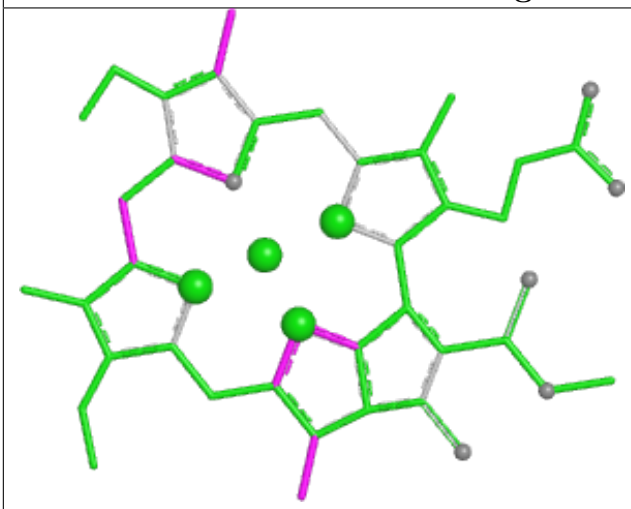
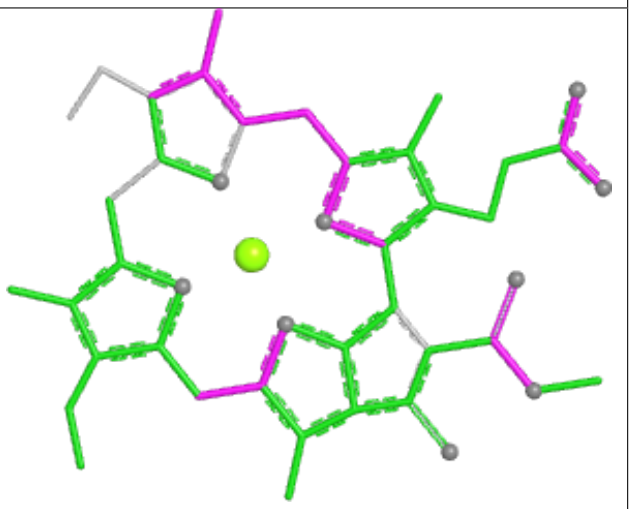
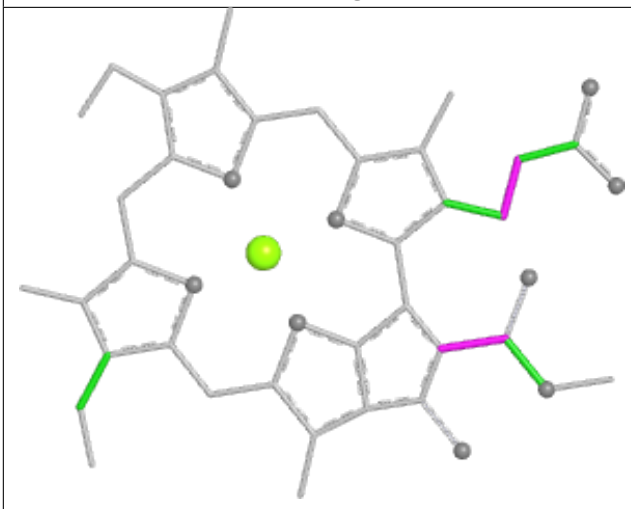
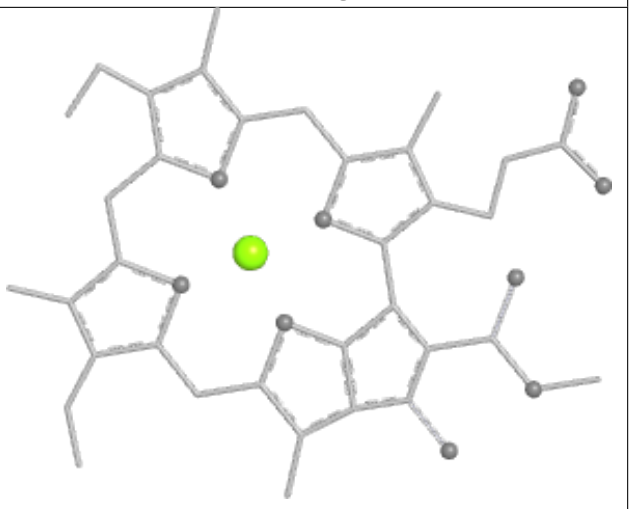
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

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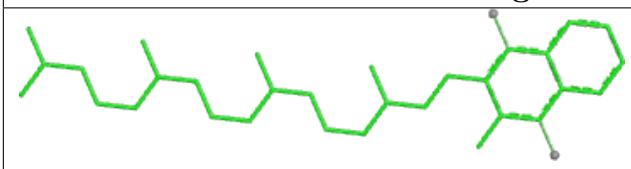
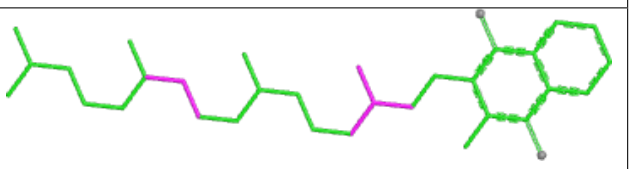
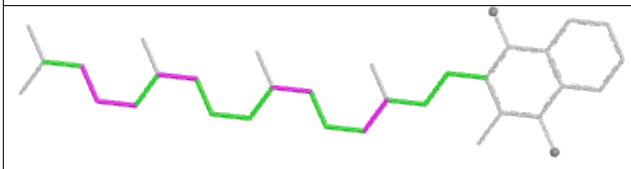
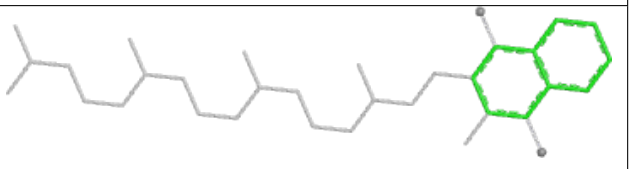
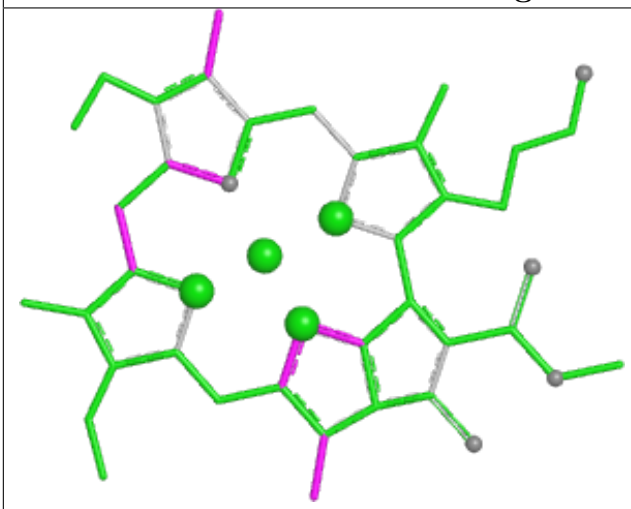
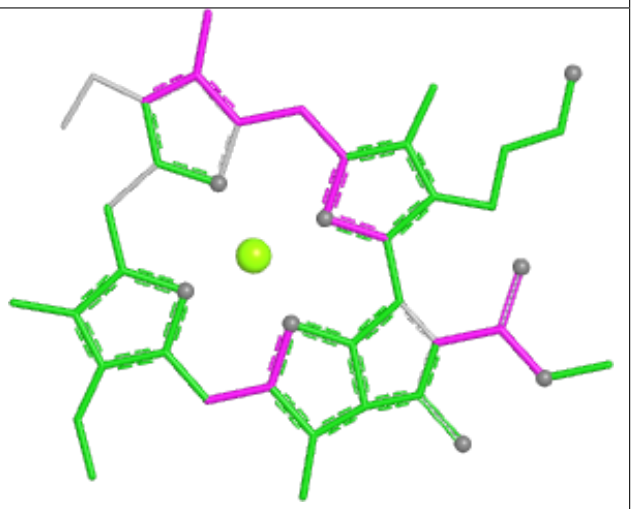
 Bond lengths	 Bond angles
 Torsions	 Rings

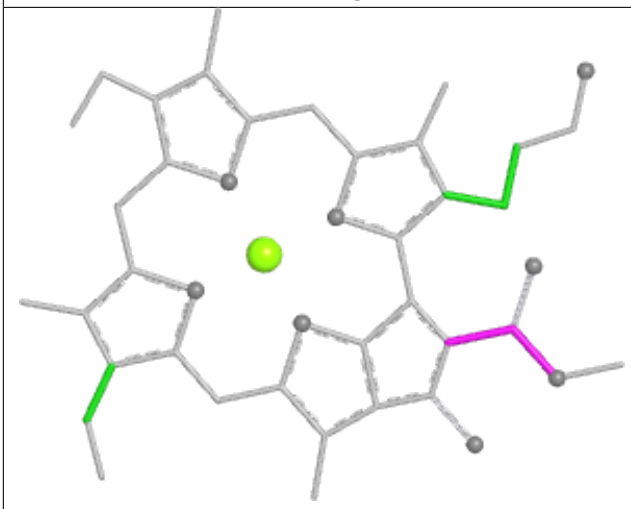
Ligand CLA A1 837



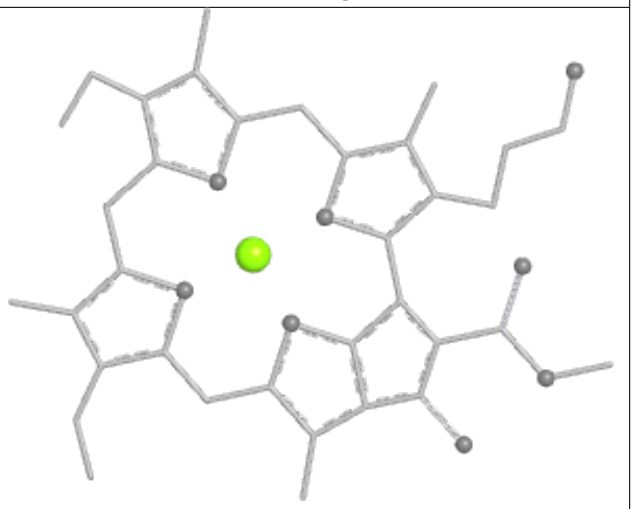
Bond lengths



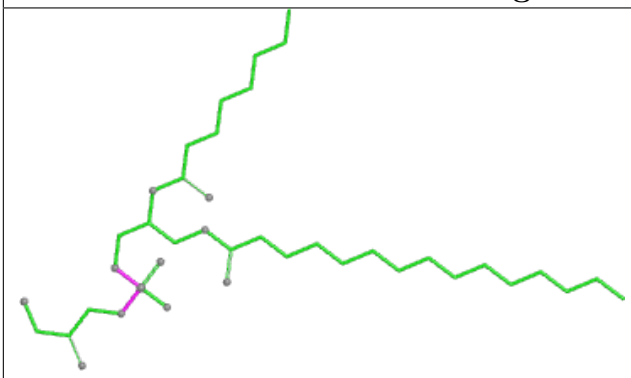
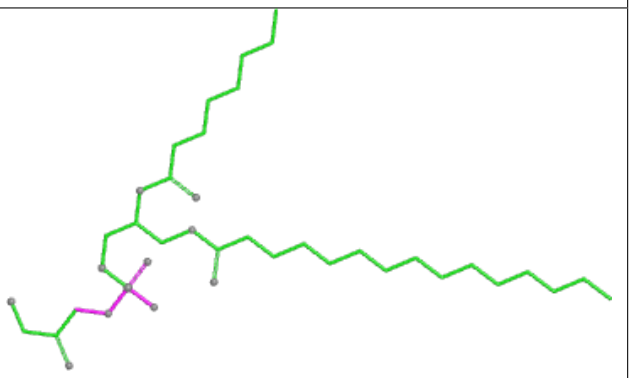
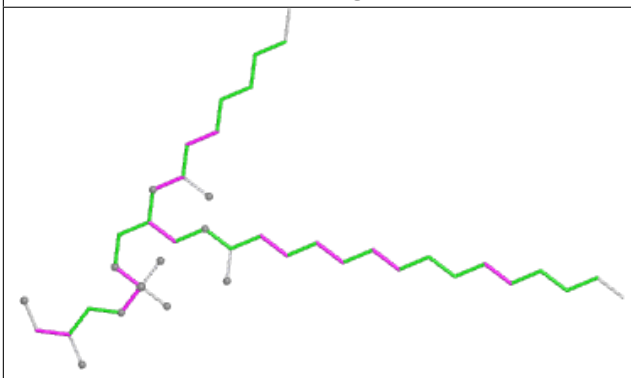
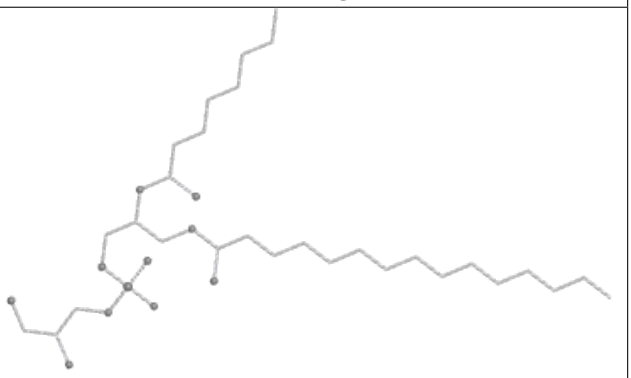
Bond angles



Torsions



Rings

Ligand LHG X2 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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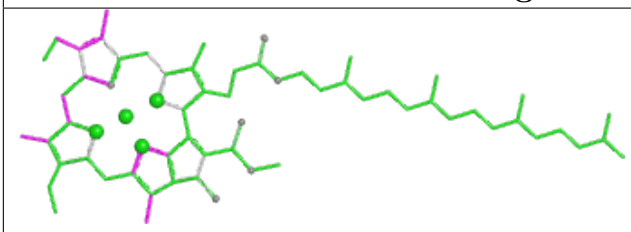
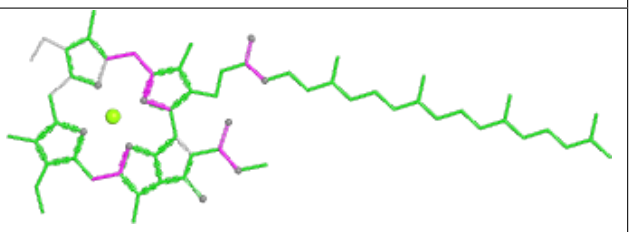
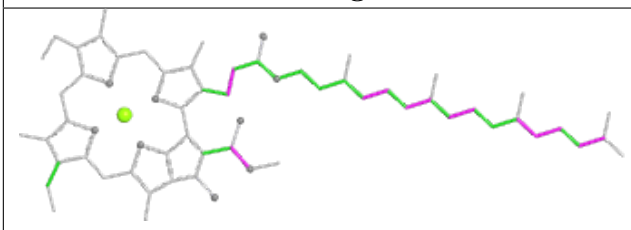
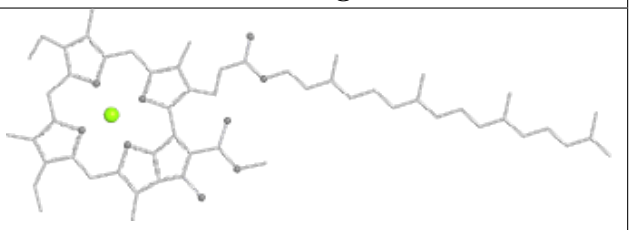
 Bond lengths	 Bond angles
 Torsions	 Rings

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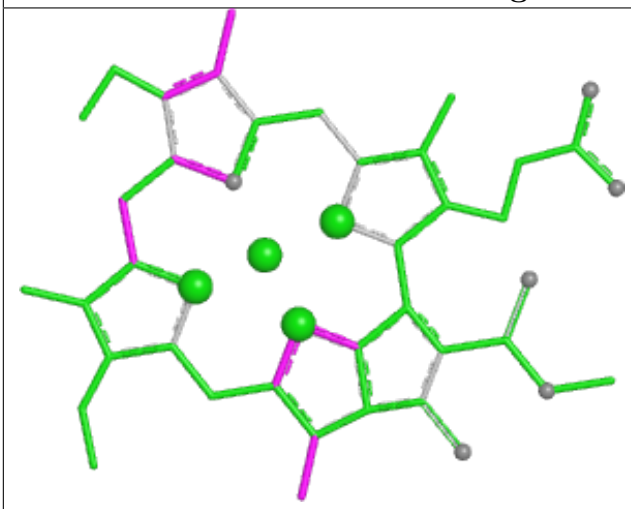
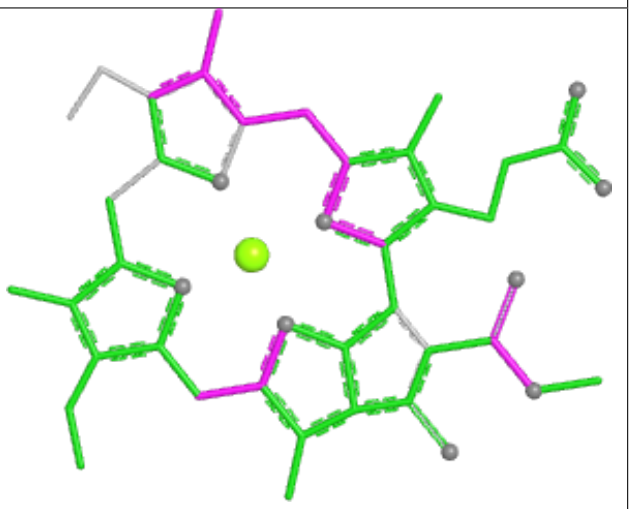
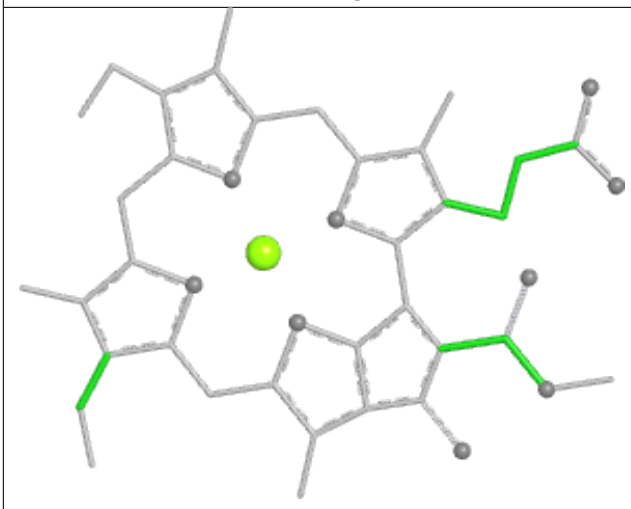
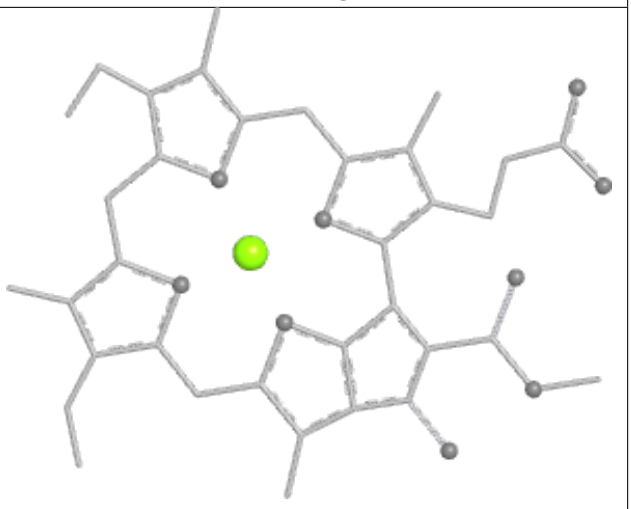
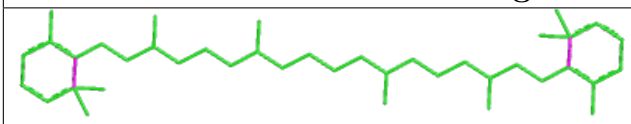
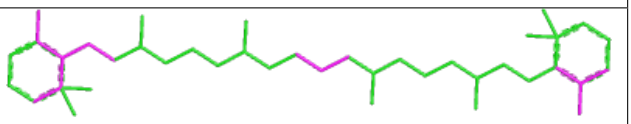
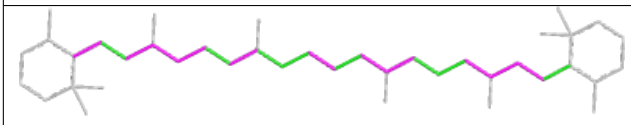
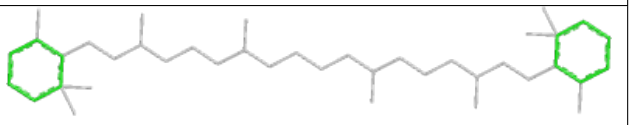
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A1 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

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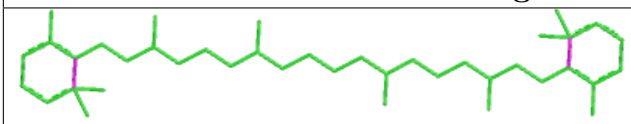
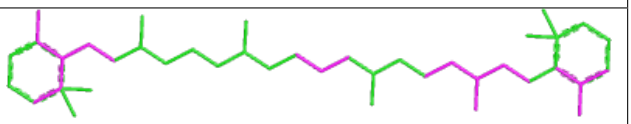
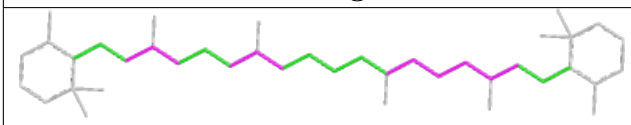
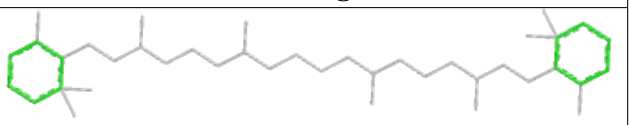
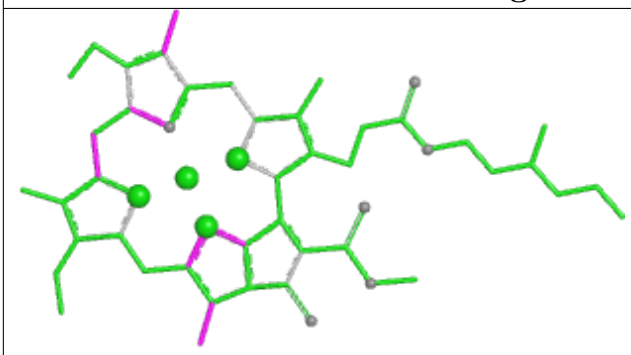
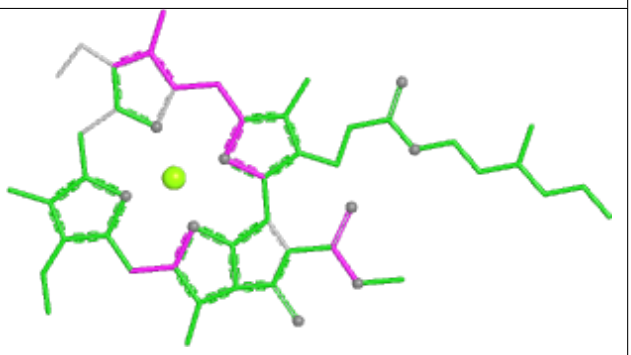
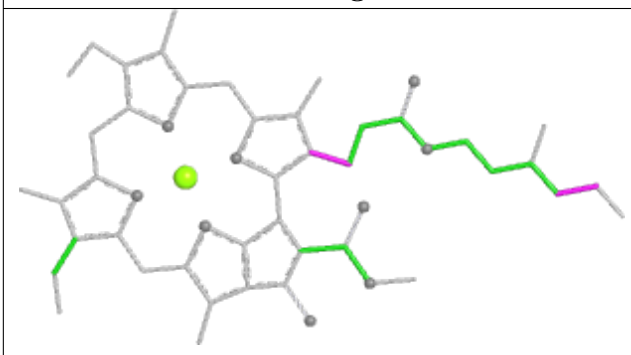
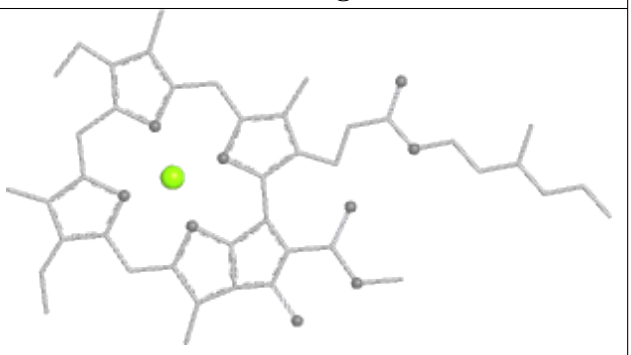
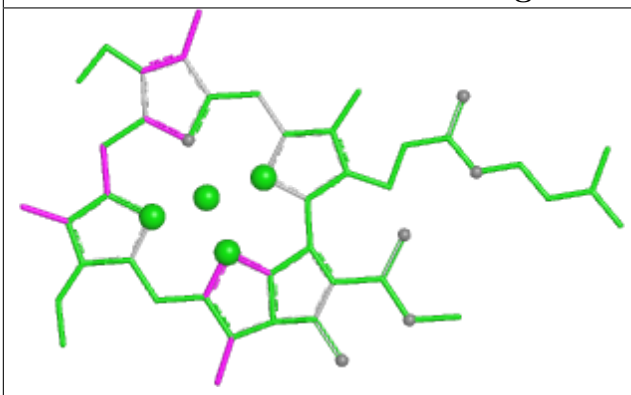
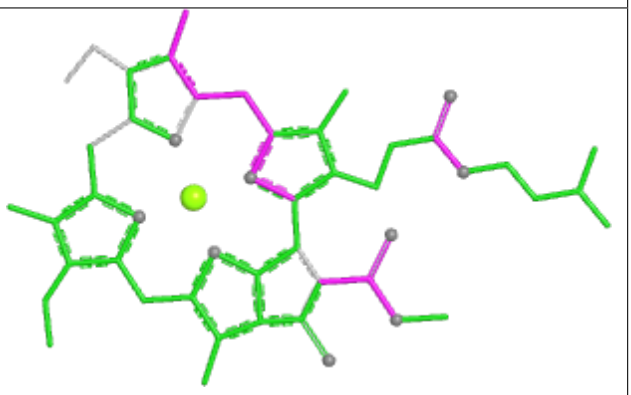
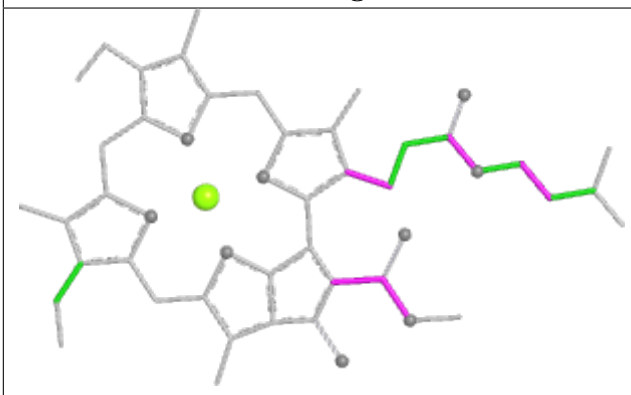
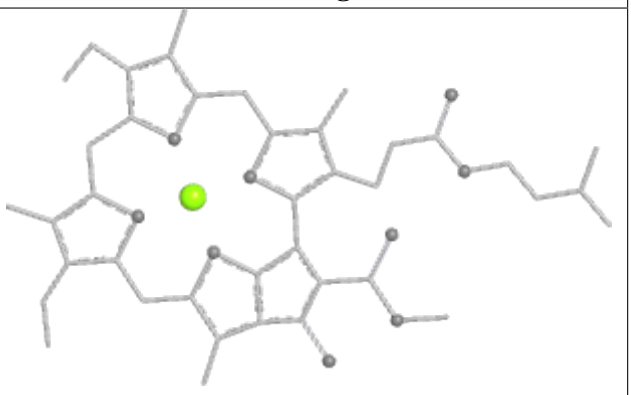
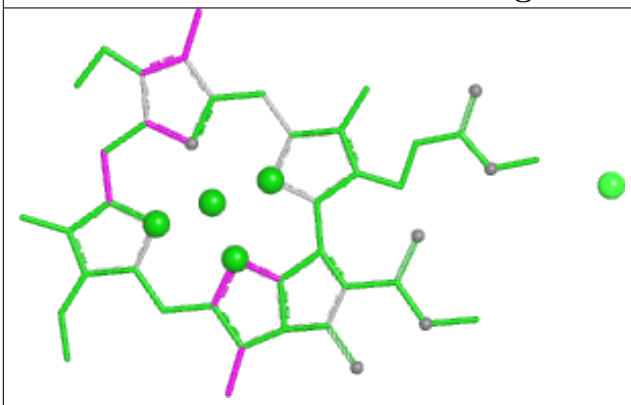
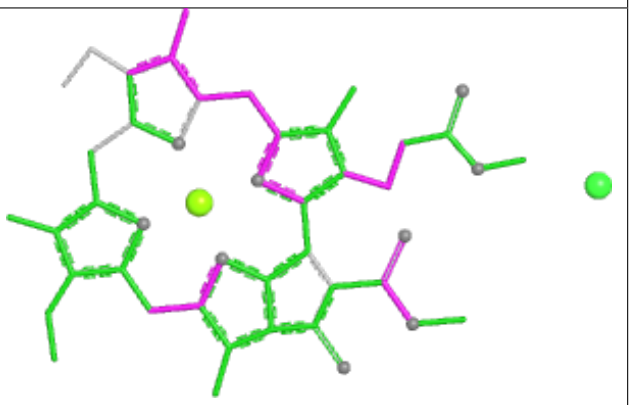
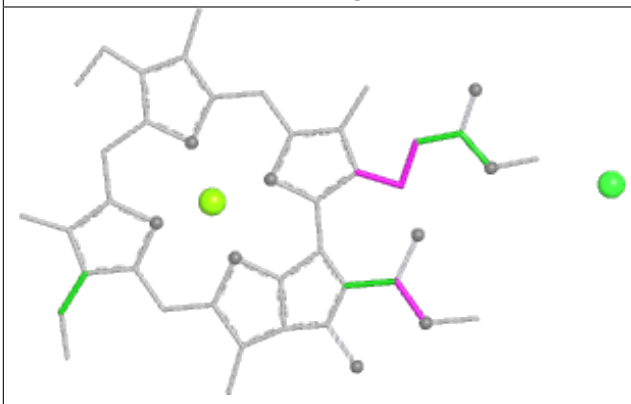
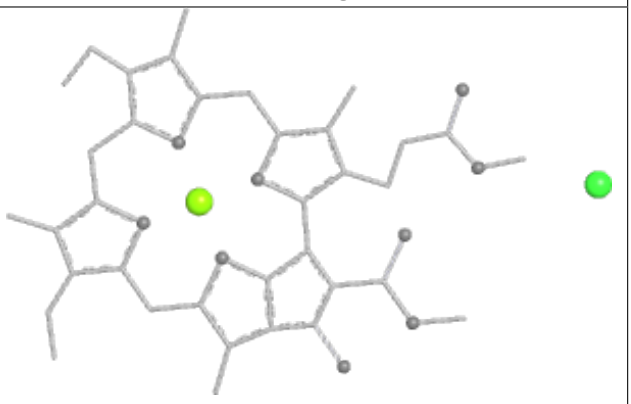
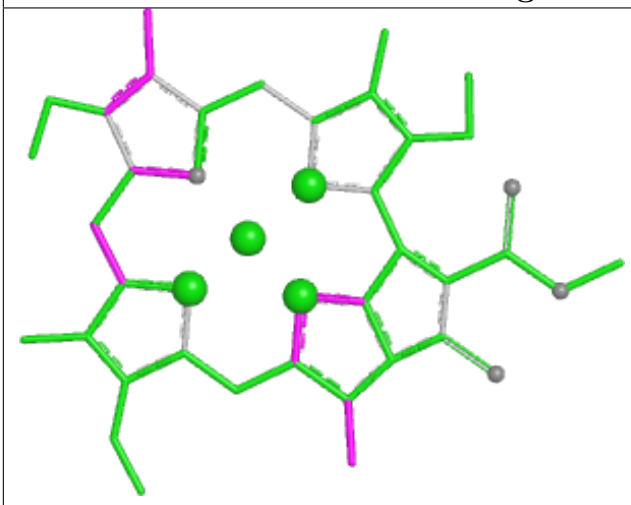
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

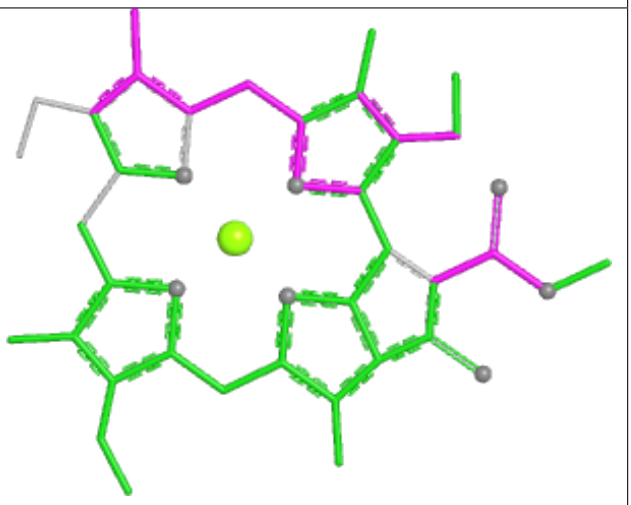
Ligand CLA A1 832	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A1 811	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

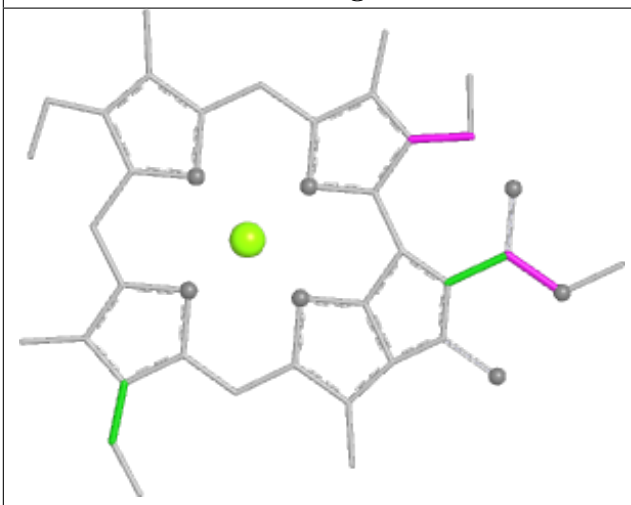
Ligand CLA F1 302



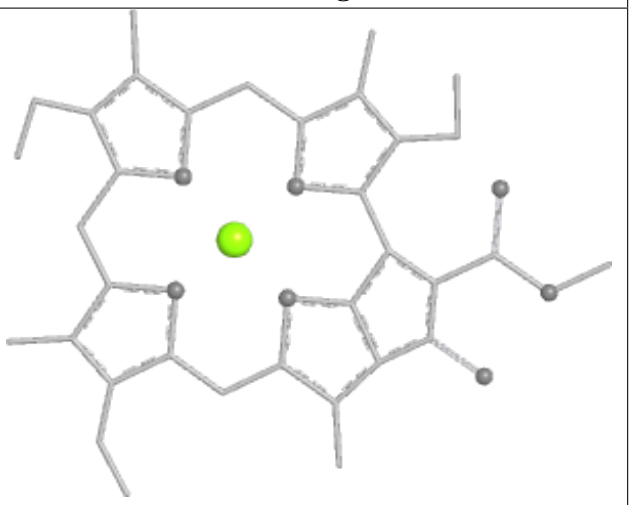
Bond lengths



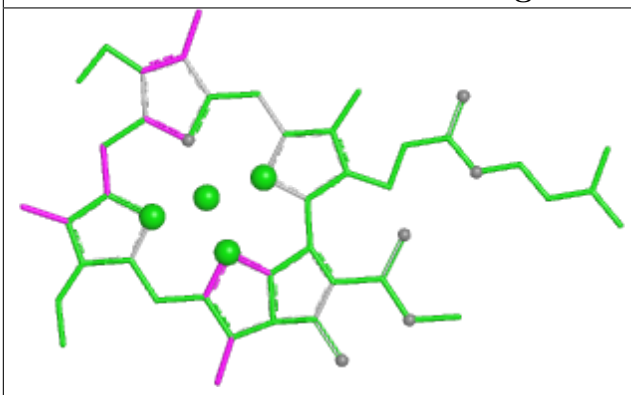
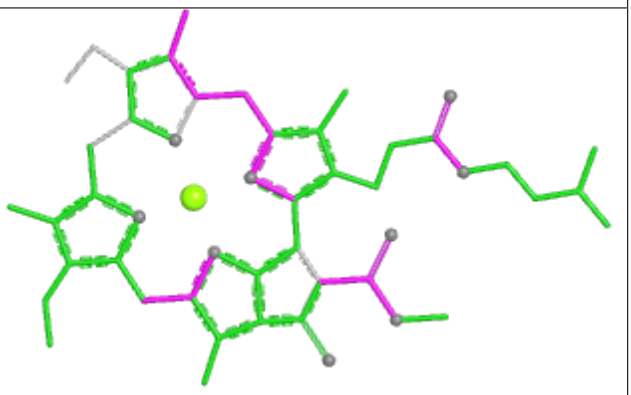
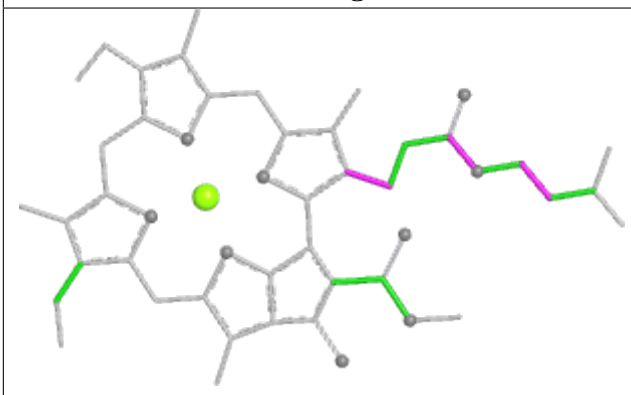
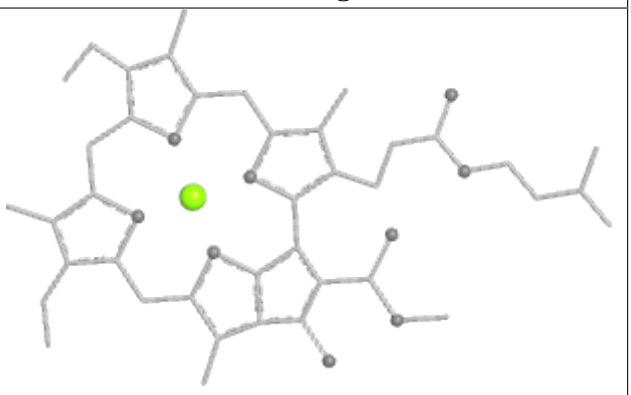
Bond angles

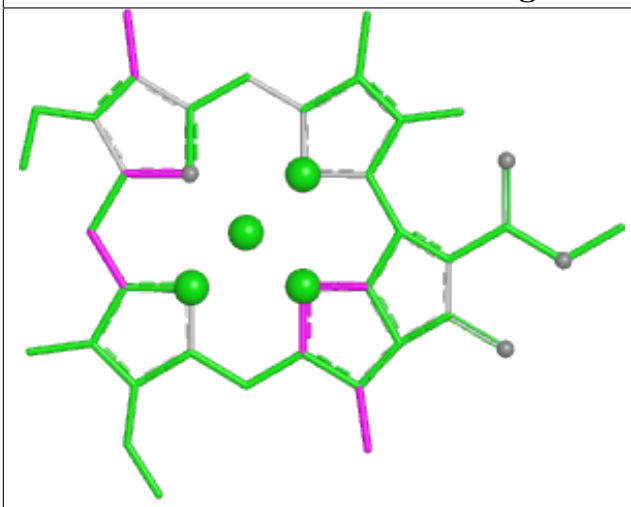
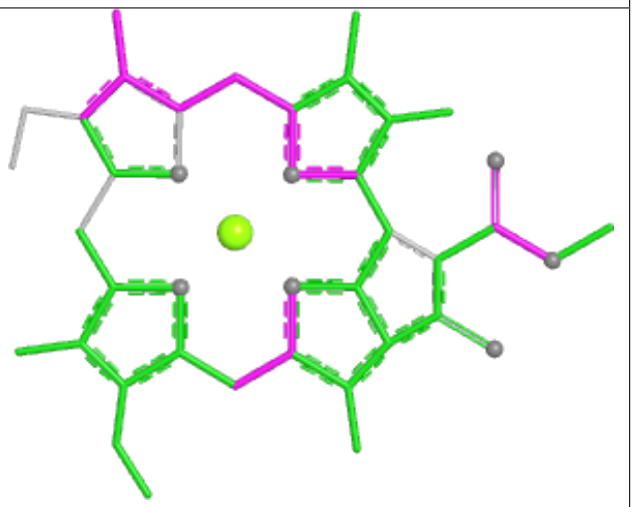
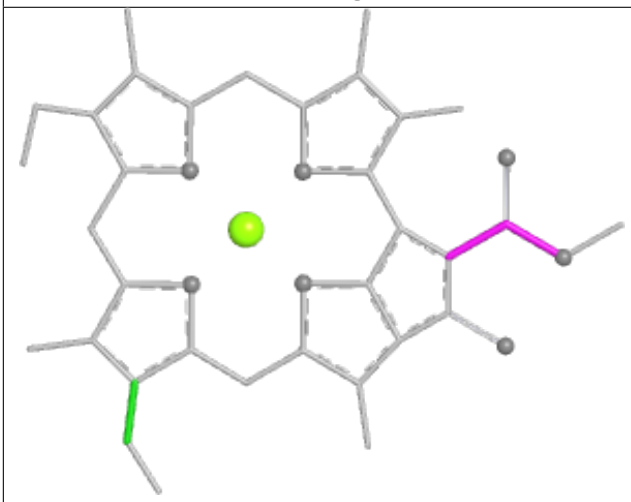
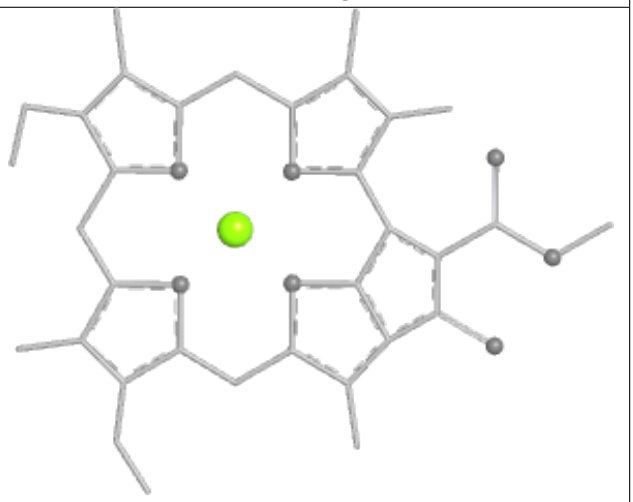


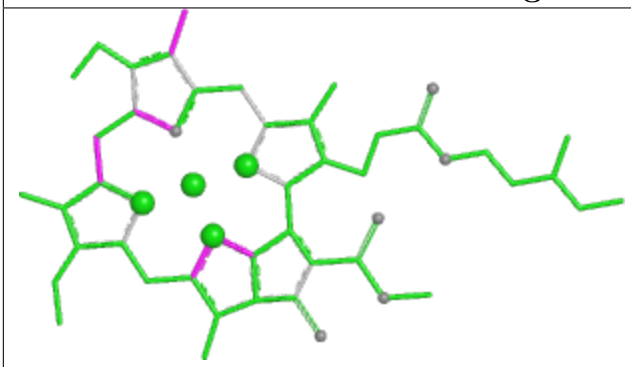
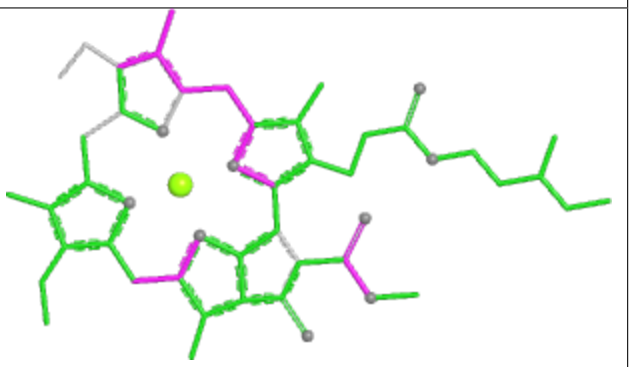
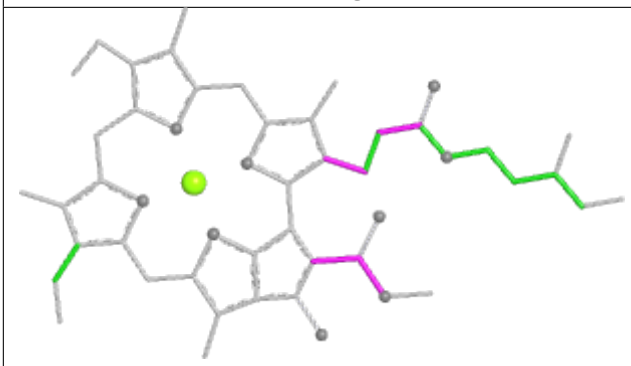
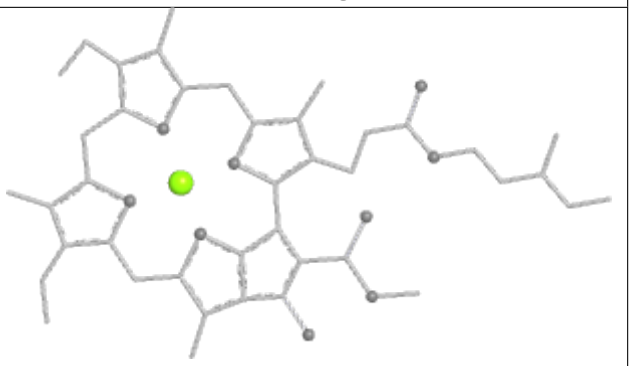
Torsions

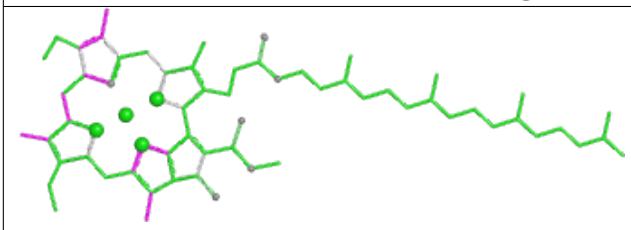
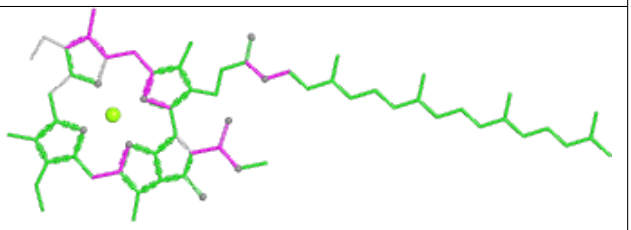
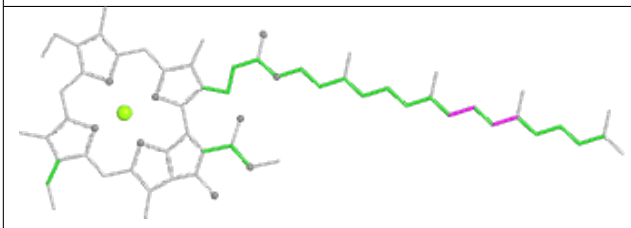
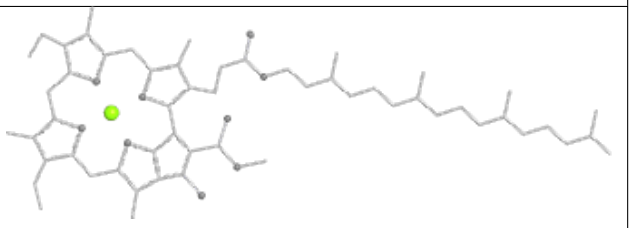


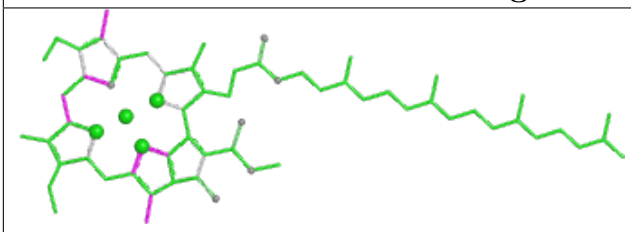
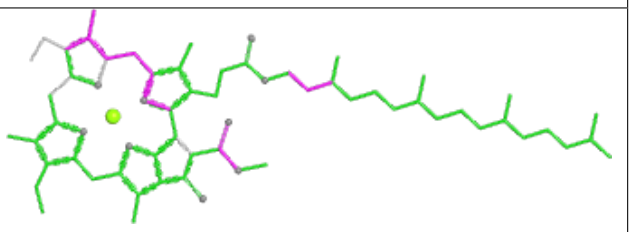
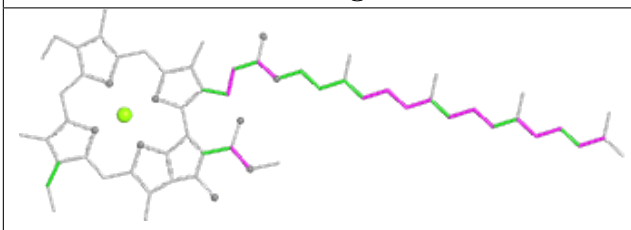
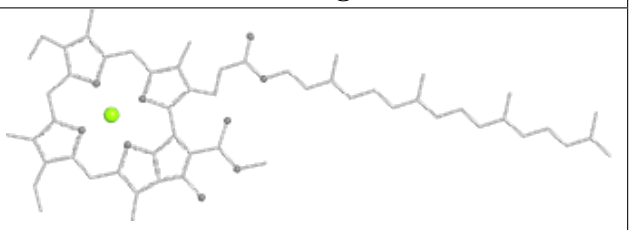
Rings

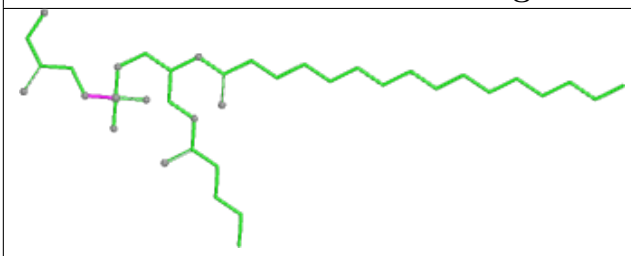
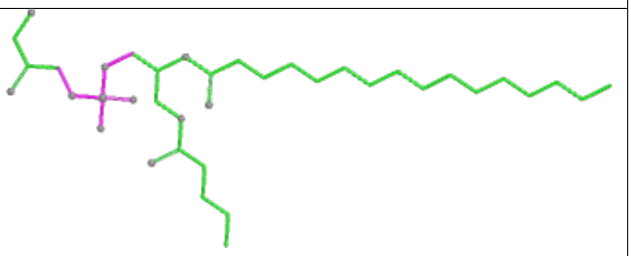
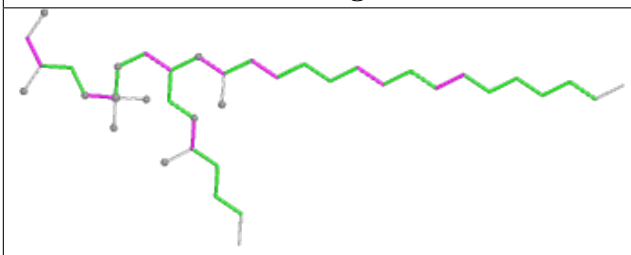
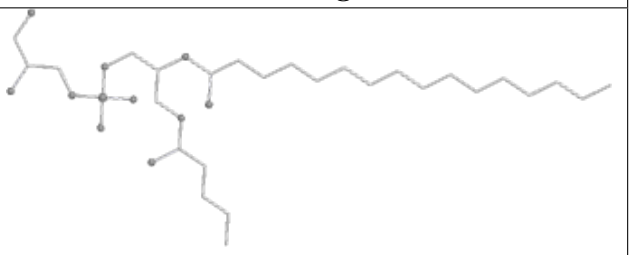
Ligand CLA A2 833	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA JJ 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L1 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A2 846	
 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.

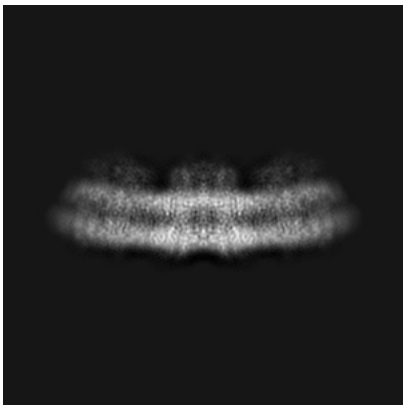
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10461. These allow visual inspection of the internal detail of the map and identification of artifacts.

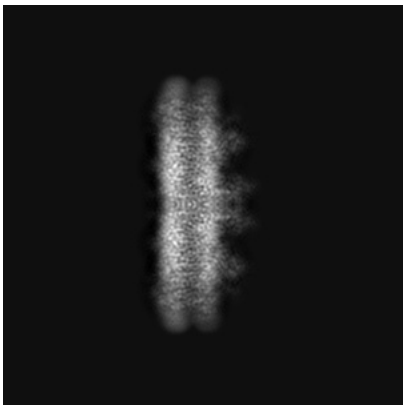
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

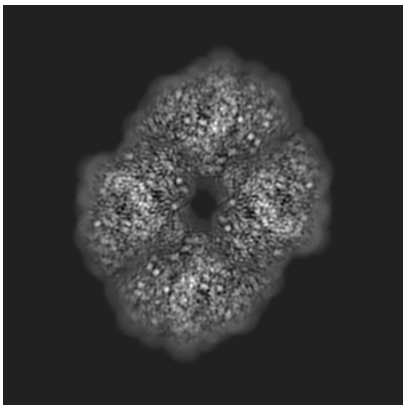
6.1.1 Primary map



X

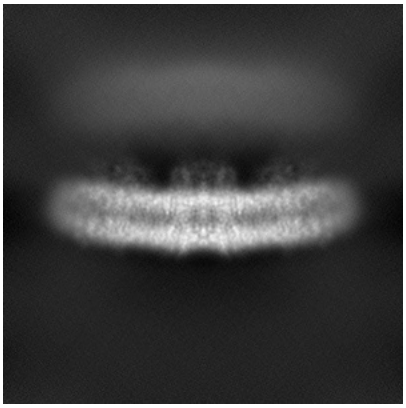


Y

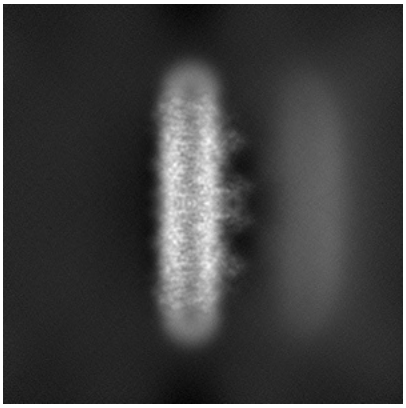


Z

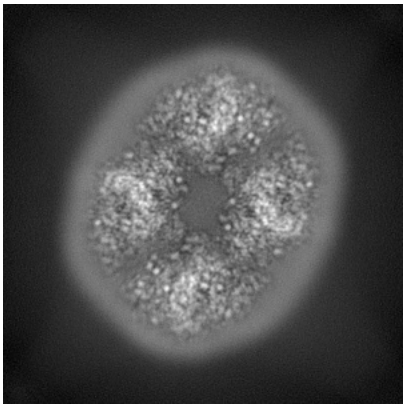
6.1.2 Raw map



X



Y

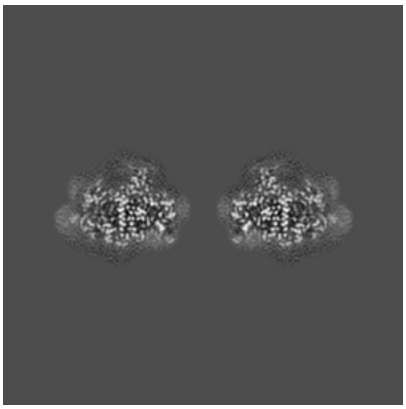


Z

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

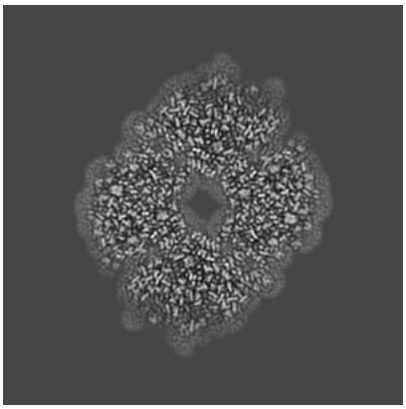
6.2 Central slices (i)

6.2.1 Primary map



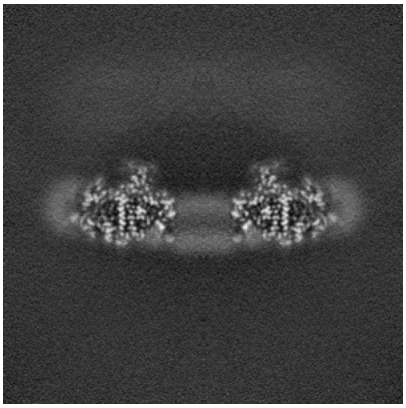
X Index: 185

Y Index: 185

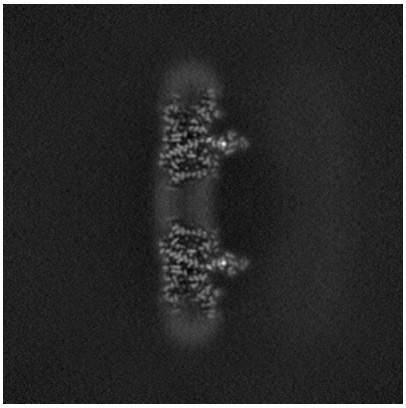


Z Index: 185

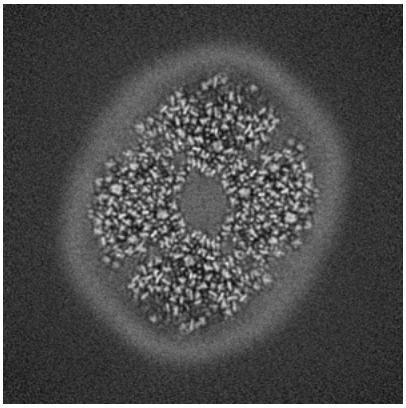
6.2.2 Raw map



X Index: 185



Y Index: 185

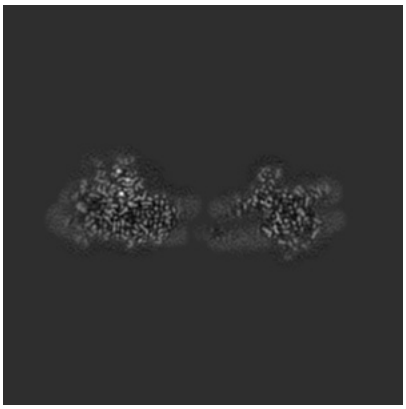


Z Index: 185

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

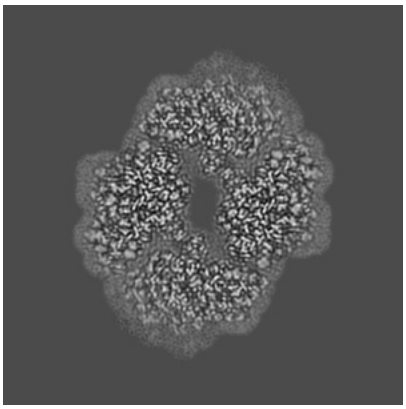
6.3 Largest variance slices (i)

6.3.1 Primary map



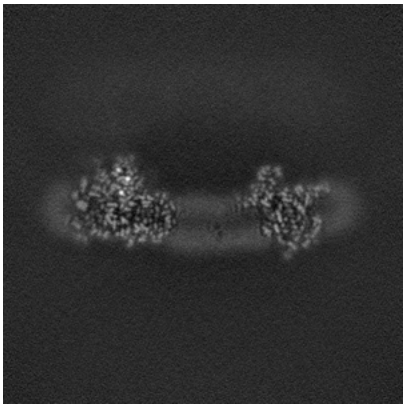
X Index: 173

Y Index: 168

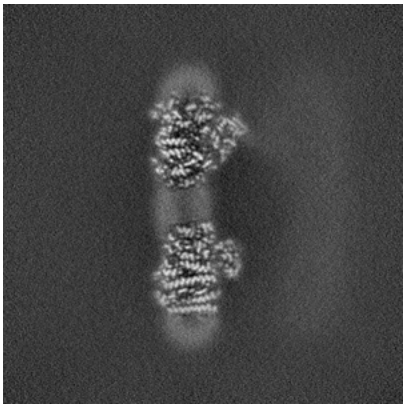


Z Index: 160

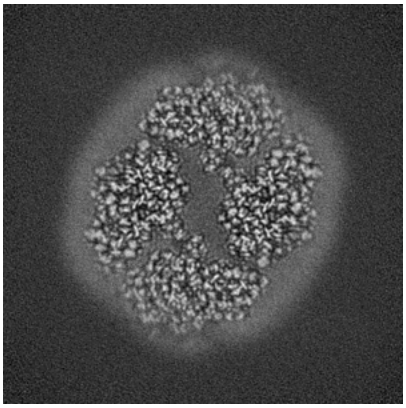
6.3.2 Raw map



X Index: 174



Y Index: 168



Z Index: 160

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 0.434. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

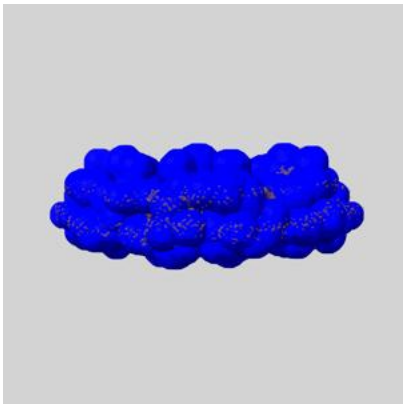
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

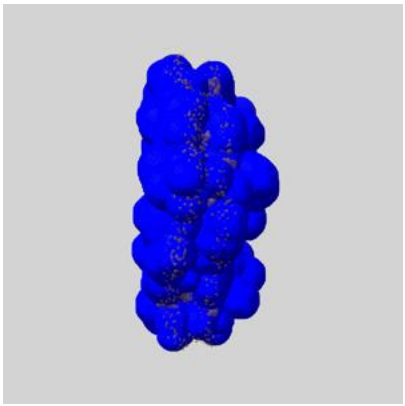
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

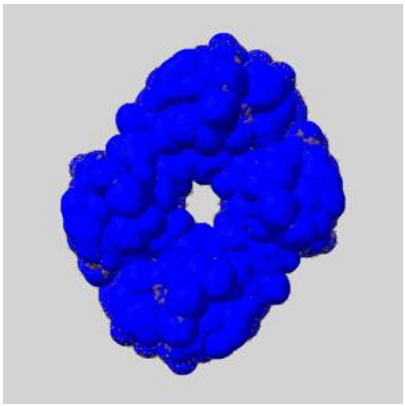
6.5.1 emd_10461_msk_1.map



X



Y

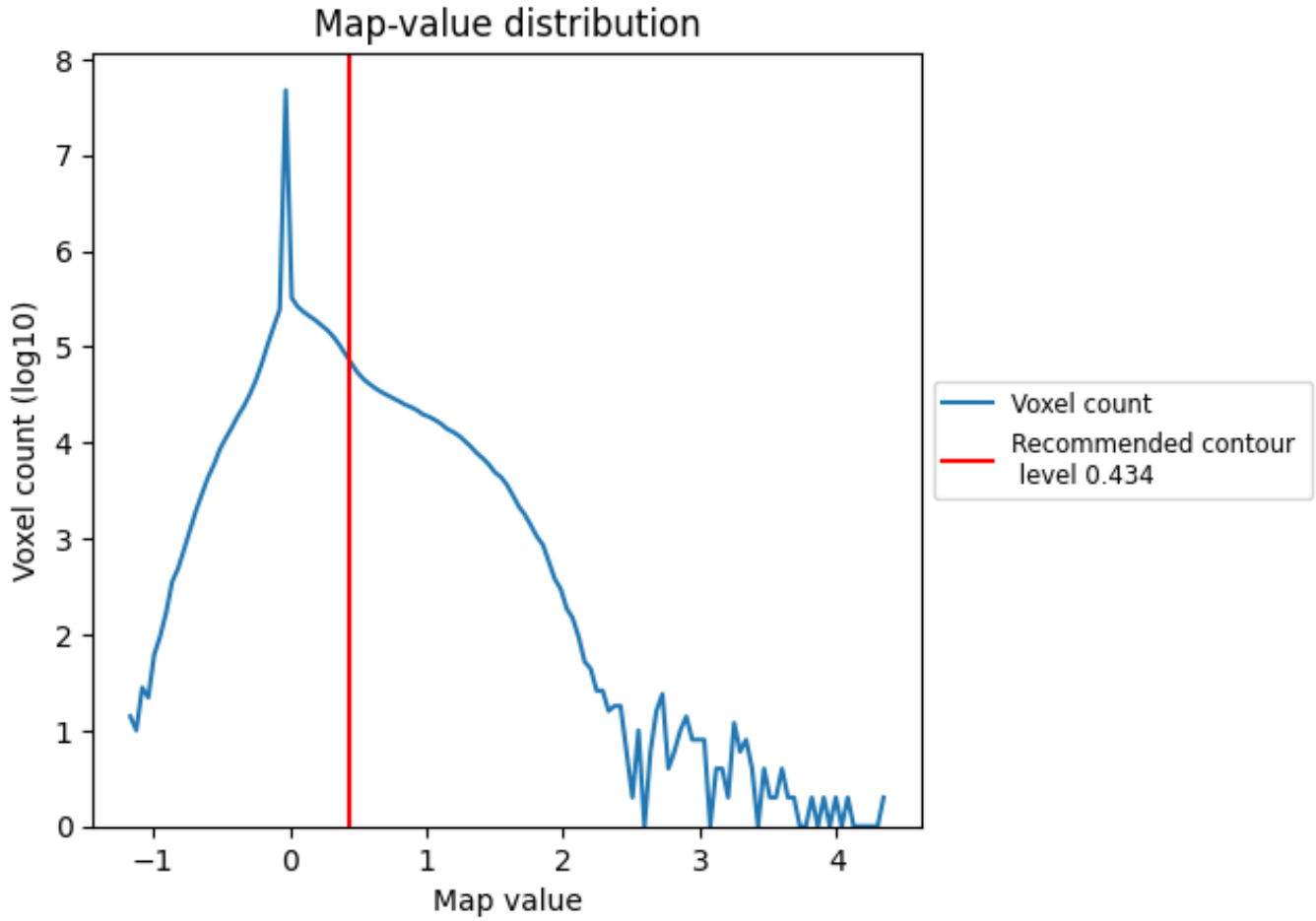


Z

7 Map analysis

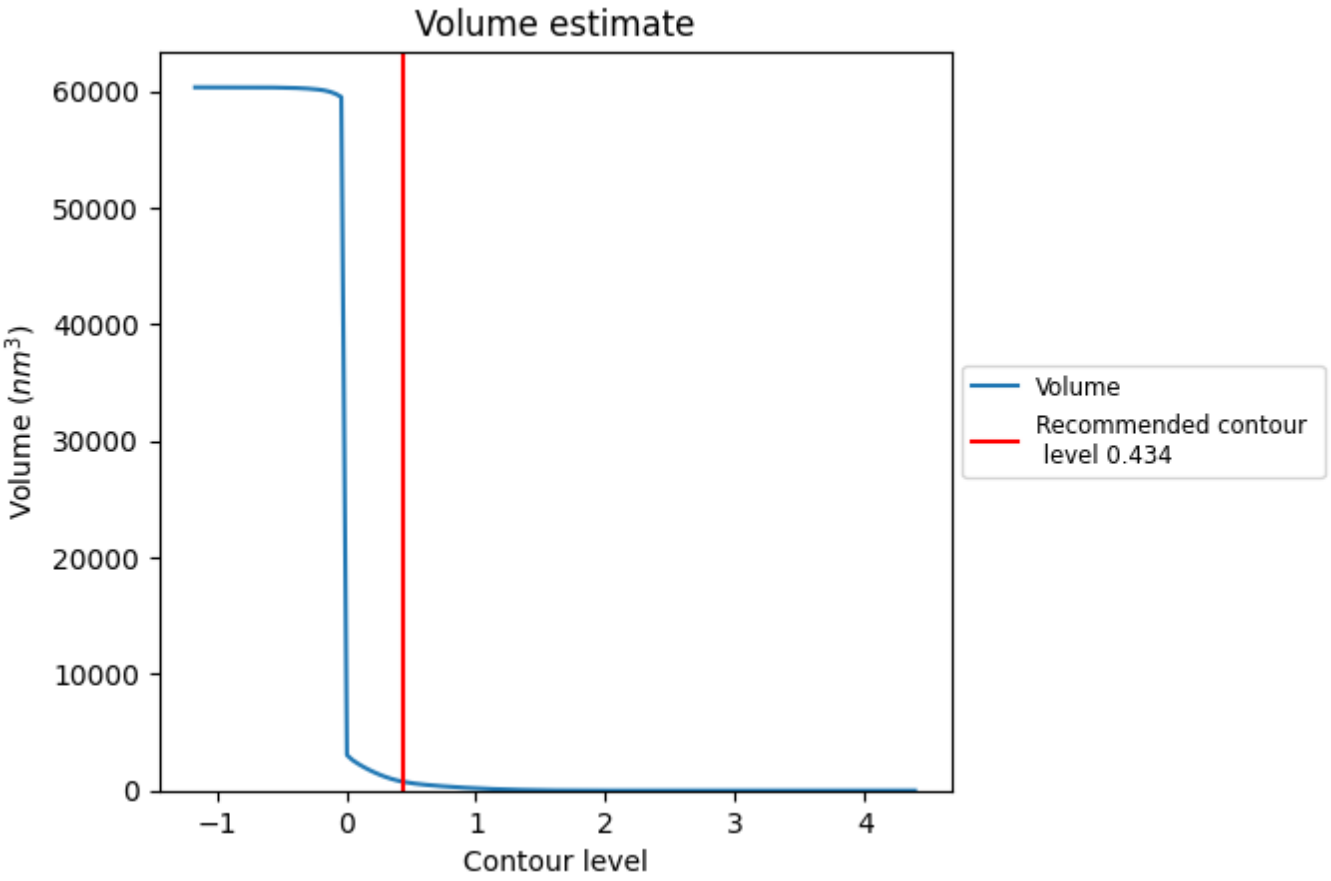
This section contains the results of statistical analysis of the map.

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.

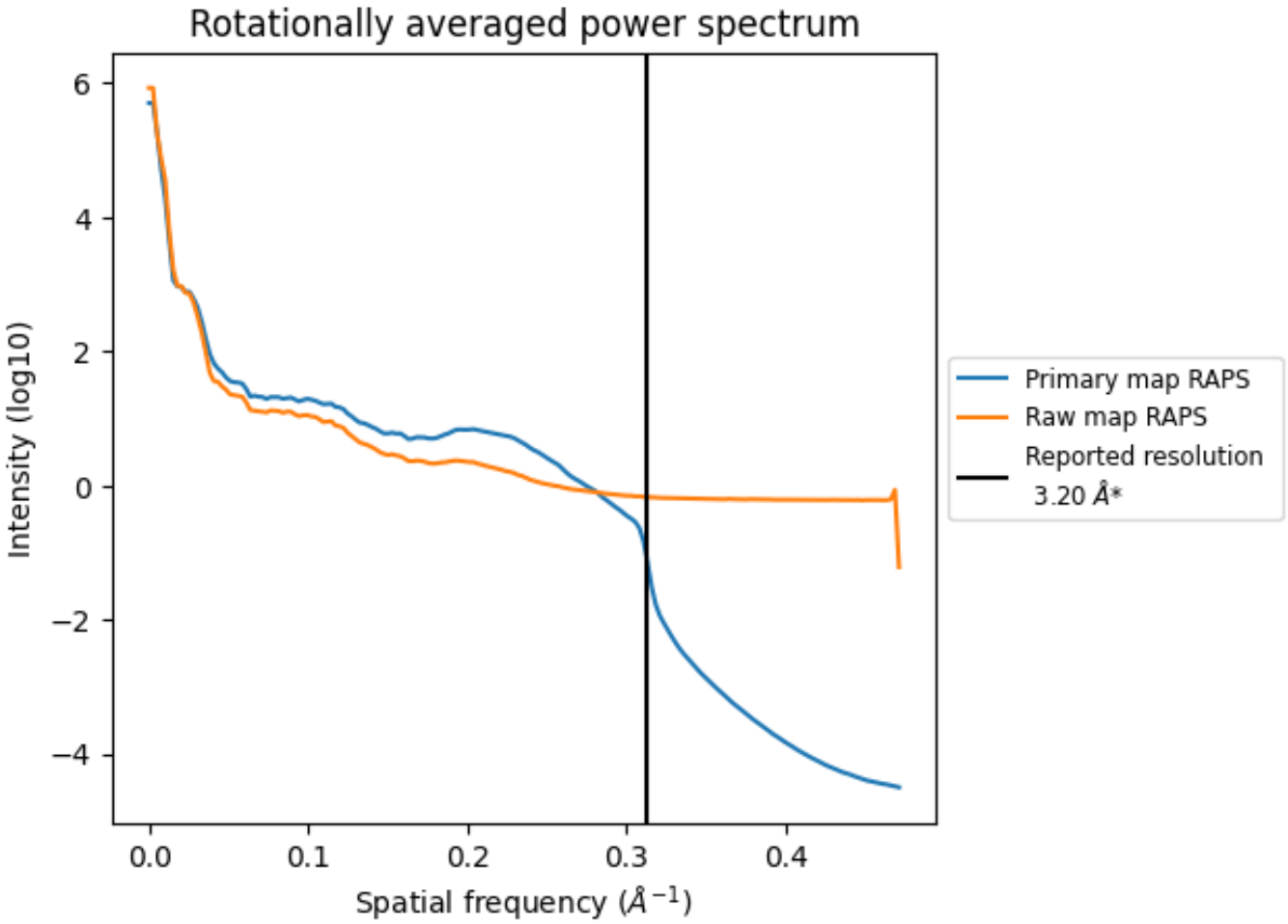
7.2 Volume estimate



The volume at the recommended contour level is 765 nm^3; this corresponds to an approximate mass of 691 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)

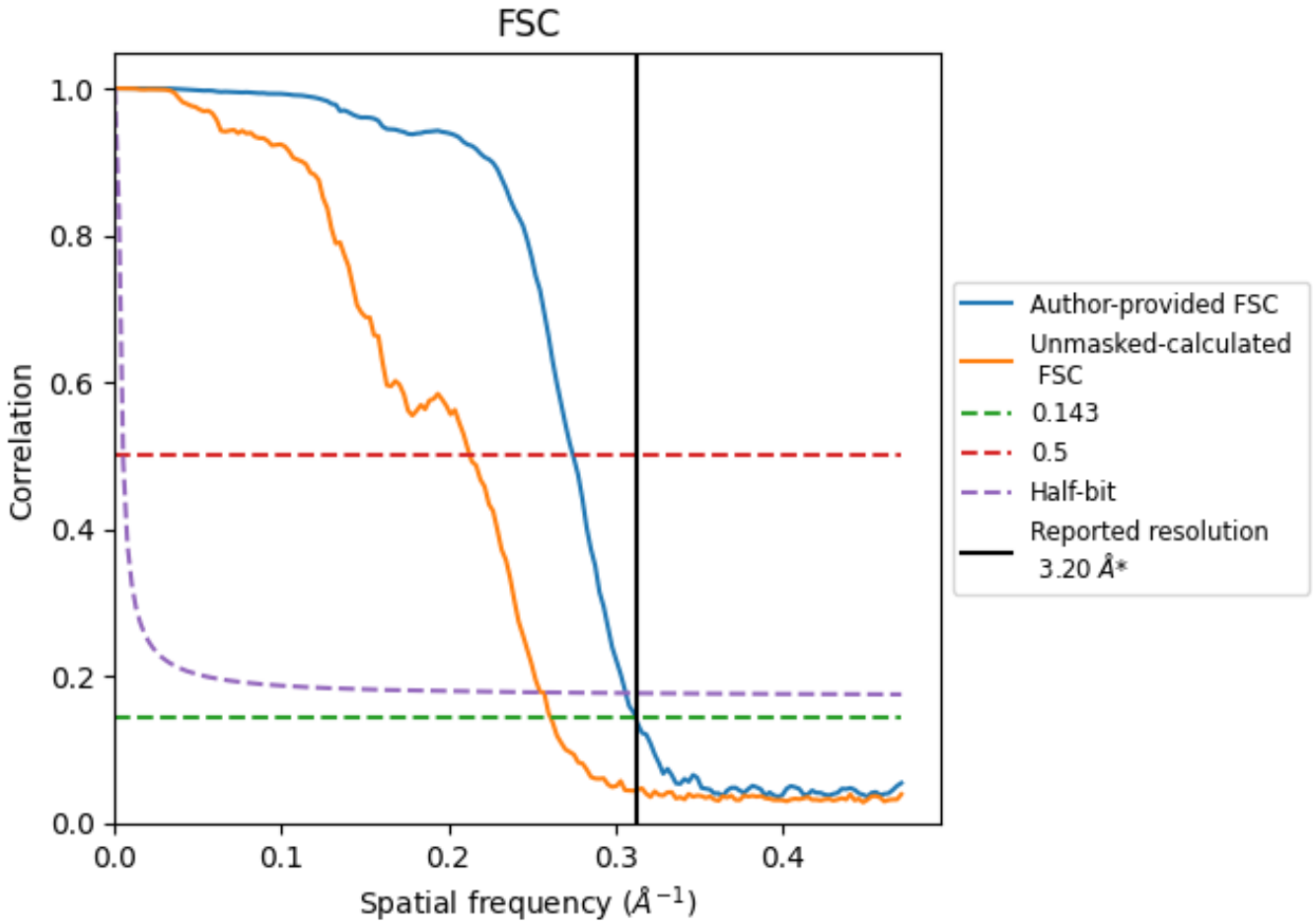


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

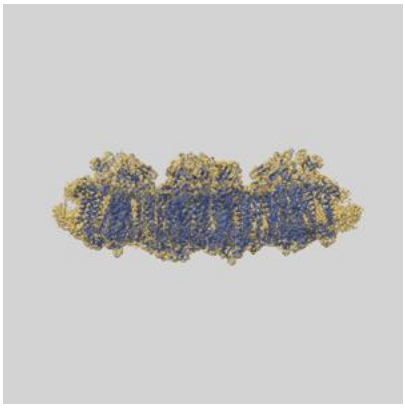
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.64	3.26
Unmasked-calculated*	3.83	4.69	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.2 by more than 10 %

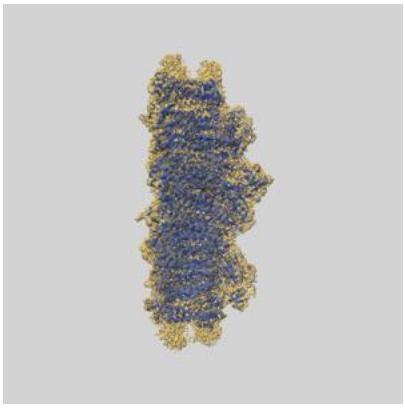
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10461 and PDB model 6TCL. Per-residue inclusion information can be found in section 3 on page 51.

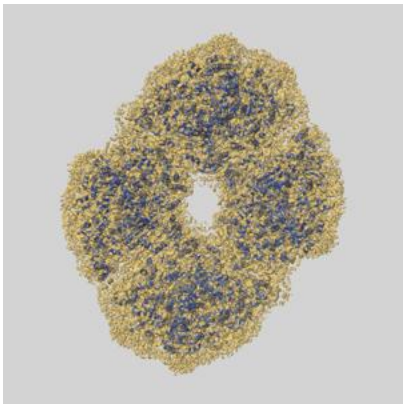
9.1 Map-model overlay



X



Y



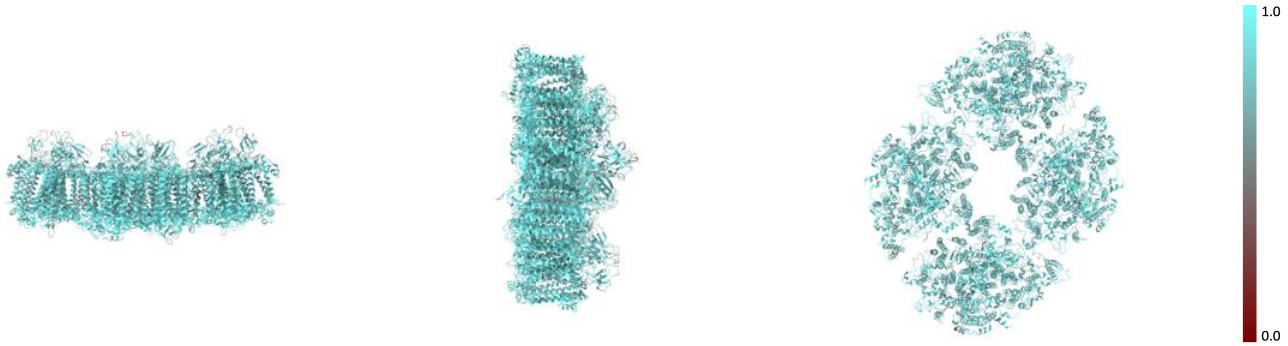
Z

The images above show the 3D surface view of the map at the recommended contour level 0.434 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

This section was not generated.

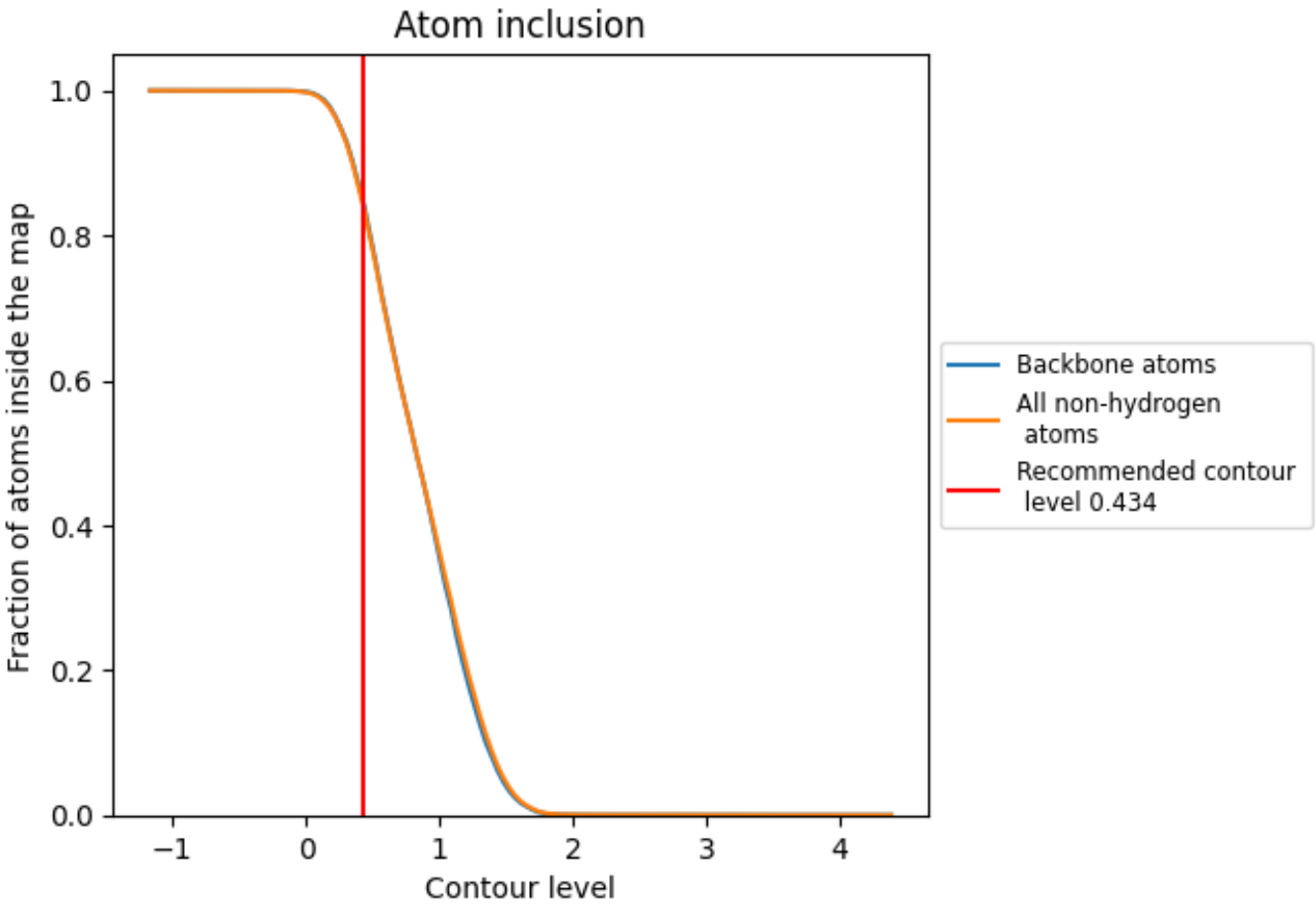
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.434).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8386
A	0.8613
A1	0.8531
A2	0.8530
AA	0.8600
B	0.8668
B1	0.8288
B2	0.8314
BB	0.8730
C	0.8502
C1	0.8336
C2	0.8253
CC	0.8336
D	0.8260
D1	0.7876
D2	0.7906
DD	0.8142
E	0.7796
E1	0.7569
E2	0.7505
EE	0.7837
F	0.8438
F1	0.7870
F2	0.7882
FF	0.8381
I	0.8571
I1	0.8488
I2	0.8125
II	0.8326
J	0.8569
J1	0.7843
J2	0.8024
JJ	0.8508
K	0.7085
K1	0.8086

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Chain	Atom inclusion
K2	0.8070
KK	0.7203
L	0.8203
L1	0.8200
L2	0.8361
LL	0.8361
M	0.8100
M1	0.7309
M2	0.7204
MM	0.8255
X	0.7891
X1	0.6721
X2	0.6767
XX	0.7839