Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:59 PM JST

PDB ID	:	6J40
EMDB ID	:	EMD-9777
Title	:	Structure of C2S2M2-type PSII-FCPII supercomplex from diatom
Authors	:	Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on	:	2019-01-07
Resolution	:	3.80 Å(reported)
Based on initial models	:	3WU2, 3JCU

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

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

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

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

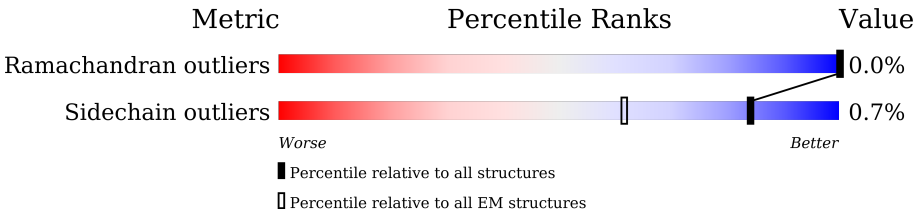
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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)
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	344	97%
1	a	344	97%
2	B	509	94% 5%
2	b	509	94% 5%
3	C	471	95%
3	c	471	95%
4	D	351	95%
4	d	351	96%
5	E	84	7% 89% 11%

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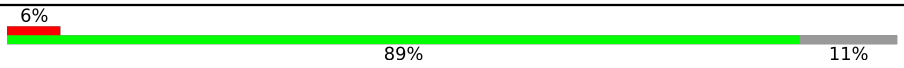
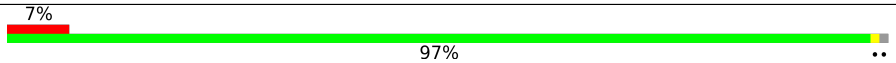
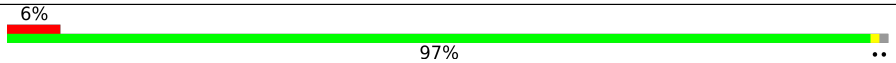
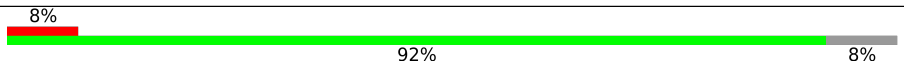
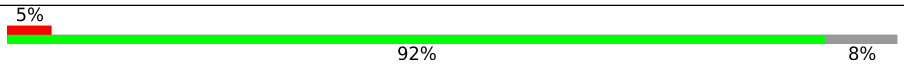
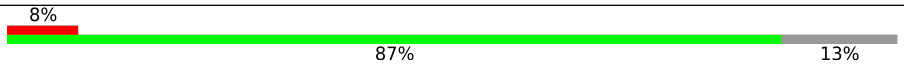
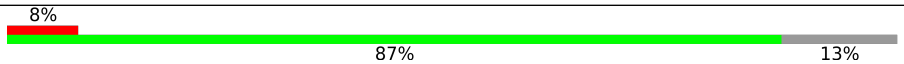
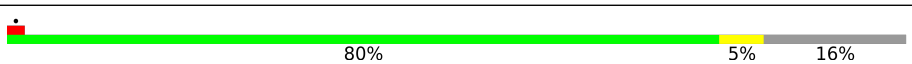
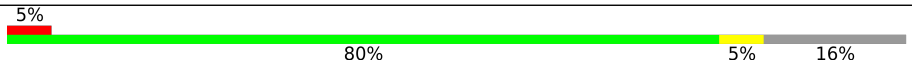
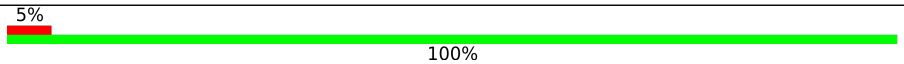
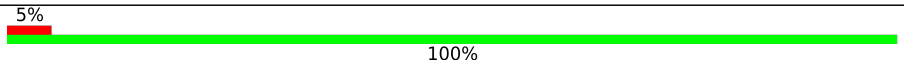
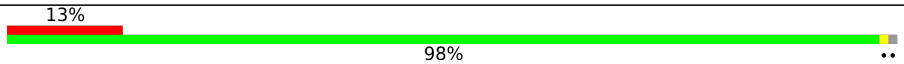
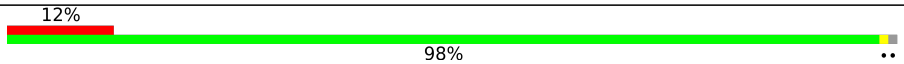
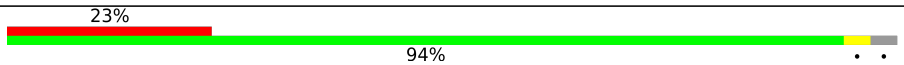
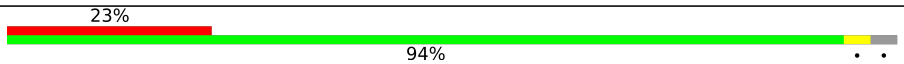
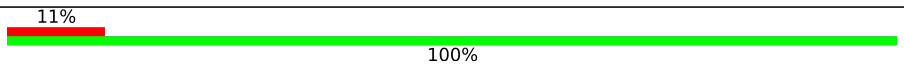
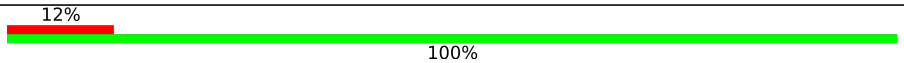
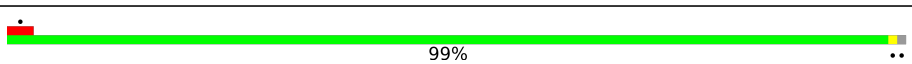
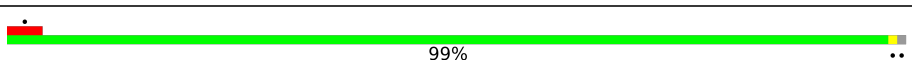
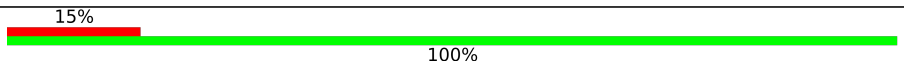
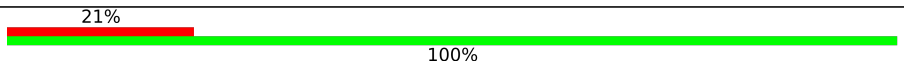
Mol	Chain	Length	Quality of chain
5	e	84	
6	F	43	
6	f	43	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	44	
10	k	44	
11	L	38	
11	l	38	
12	M	131	
12	m	131	
13	O	248	
13	o	248	
14	T	31	
14	t	31	
15	U	93	
15	u	93	
16	V	137	
16	v	137	
17	Y	34	
17	y	34	

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Mol	Chain	Length	Quality of chain
18	X	38	13% 97%
18	x	38	13% 97%
19	Z	61	97%
19	z	61	97%
20	Q	155	14% 88% 12%
20	q	155	12% 88% 12%
21	W	72	14% 71% 28%
21	w	72	15% 71% 28%
22	0	31	6% 100%
22	5	31	6% 100%
23	1	30	7% 100%
23	6	30	7% 100%
24	2	10	100%
24	7	10	10% 100%
25	11	207	84% 15%
25	12	207	6% 84% 15%
25	13	207	9% 84% 15%
25	14	207	7% 84% 15%
25	15	207	23% 85% 15%
25	16	207	5% 84% 15%
25	17	207	10% 84% 15%
25	18	207	24% 84% 15%
25	31	207	85% 15%
25	32	207	6% 85% 15%
25	33	207	10% 85% 15%

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Mol	Chain	Length	Quality of chain
25	34	207	6% 85% 15%
25	35	207	24% 85% 15%
25	36	207	5% 84% 15%
25	37	207	8% 84% 15%
25	38	207	23% 84% 15%
26	19	215	98%
26	39	215	98%
27	20	143	7% 98%
27	40	143	8% 98%
28	21	155	53% 100%
28	41	155	54% 100%

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
30	CLA	11	301	X	-	-	-
30	CLA	11	302	X	-	-	-
30	CLA	11	303	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	305	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	307	X	-	-	-
30	CLA	11	309	X	-	-	-
30	CLA	11	315	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	305	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	309	X	-	-	-
30	CLA	12	310	X	-	-	-
30	CLA	12	311	X	-	-	-
30	CLA	12	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	12	314	X	-	-	-
30	CLA	13	302	X	-	-	-
30	CLA	13	303	X	-	-	-
30	CLA	13	304	X	-	-	-
30	CLA	13	305	X	-	-	-
30	CLA	13	306	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	308	X	-	-	-
30	CLA	13	310	X	-	-	-
30	CLA	14	301	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	306	X	-	-	-
30	CLA	14	307	X	-	-	-
30	CLA	14	308	X	-	-	-
30	CLA	14	310	X	-	-	-
30	CLA	15	301	X	-	-	-
30	CLA	15	302	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-
30	CLA	15	308	X	-	-	-
30	CLA	15	309	X	-	-	-
30	CLA	16	301	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-
30	CLA	16	304	X	-	-	-
30	CLA	16	306	X	-	-	-
30	CLA	16	307	X	-	-	-
30	CLA	16	309	X	-	-	-
30	CLA	17	301	X	-	-	-
30	CLA	17	303	X	-	-	-
30	CLA	17	305	X	-	-	-
30	CLA	17	307	X	-	-	-
30	CLA	17	308	X	-	-	-
30	CLA	17	309	X	-	-	-
30	CLA	17	310	X	-	-	-
30	CLA	18	301	X	-	-	-
30	CLA	18	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	18	304	X	-	-	-
30	CLA	18	305	X	-	-	-
30	CLA	18	307	X	-	-	-
30	CLA	18	308	X	-	-	-
30	CLA	18	309	X	-	-	-
30	CLA	18	310	X	-	-	-
30	CLA	18	311	X	-	-	-
30	CLA	18	312	X	-	-	-
30	CLA	19	302	X	-	-	-
30	CLA	19	303	X	-	-	-
30	CLA	19	304	X	-	-	-
30	CLA	19	305	X	-	-	-
30	CLA	19	306	X	-	-	-
30	CLA	19	307	X	-	-	-
30	CLA	19	308	X	-	-	-
30	CLA	20	203	X	-	-	-
30	CLA	20	204	X	-	-	-
30	CLA	20	206	X	-	-	-
30	CLA	20	207	X	-	-	-
30	CLA	20	209	X	-	-	-
30	CLA	21	303	X	-	-	-
30	CLA	21	304	X	-	-	-
30	CLA	21	305	X	-	-	-
30	CLA	21	306	X	-	-	-
30	CLA	21	307	X	-	-	-
30	CLA	21	308	X	-	-	-
30	CLA	21	309	X	-	-	-
30	CLA	31	301	X	-	-	-
30	CLA	31	302	X	-	-	-
30	CLA	31	303	X	-	-	-
30	CLA	31	304	X	-	-	-
30	CLA	31	305	X	-	-	-
30	CLA	31	306	X	-	-	-
30	CLA	31	307	X	-	-	-
30	CLA	31	309	X	-	-	-
30	CLA	31	315	X	-	-	-
30	CLA	32	303	X	-	-	-
30	CLA	32	305	X	-	-	-
30	CLA	32	306	X	-	-	-
30	CLA	32	307	X	-	-	-
30	CLA	32	308	X	-	-	-
30	CLA	32	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	32	310	X	-	-	-
30	CLA	32	311	X	-	-	-
30	CLA	32	313	X	-	-	-
30	CLA	33	301	X	-	-	-
30	CLA	33	303	X	-	-	-
30	CLA	33	304	X	-	-	-
30	CLA	33	305	X	-	-	-
30	CLA	33	306	X	-	-	-
30	CLA	33	307	X	-	-	-
30	CLA	33	308	X	-	-	-
30	CLA	33	309	X	-	-	-
30	CLA	33	311	X	-	-	-
30	CLA	34	301	X	-	-	-
30	CLA	34	302	X	-	-	-
30	CLA	34	303	X	-	-	-
30	CLA	34	304	X	-	-	-
30	CLA	34	305	X	-	-	-
30	CLA	34	306	X	-	-	-
30	CLA	34	307	X	-	-	-
30	CLA	34	308	X	-	-	-
30	CLA	34	310	X	-	-	-
30	CLA	35	301	X	-	-	-
30	CLA	35	302	X	-	-	-
30	CLA	35	303	X	-	-	-
30	CLA	35	305	X	-	-	-
30	CLA	35	306	X	-	-	-
30	CLA	35	307	X	-	-	-
30	CLA	35	308	X	-	-	-
30	CLA	35	309	X	-	-	-
30	CLA	36	301	X	-	-	-
30	CLA	36	302	X	-	-	-
30	CLA	36	303	X	-	-	-
30	CLA	36	304	X	-	-	-
30	CLA	36	306	X	-	-	-
30	CLA	36	307	X	-	-	-
30	CLA	36	309	X	-	-	-
30	CLA	37	301	X	-	-	-
30	CLA	37	303	X	-	-	-
30	CLA	37	305	X	-	-	-
30	CLA	37	307	X	-	-	-
30	CLA	37	308	X	-	-	-
30	CLA	37	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	37	310	X	-	-	-
30	CLA	38	301	X	-	-	-
30	CLA	38	303	X	-	-	-
30	CLA	38	304	X	-	-	-
30	CLA	38	305	X	-	-	-
30	CLA	38	307	X	-	-	-
30	CLA	38	308	X	-	-	-
30	CLA	38	309	X	-	-	-
30	CLA	38	310	X	-	-	-
30	CLA	38	311	X	-	-	-
30	CLA	38	312	X	-	-	-
30	CLA	39	302	X	-	-	-
30	CLA	39	303	X	-	-	-
30	CLA	39	304	X	-	-	-
30	CLA	39	305	X	-	-	-
30	CLA	39	306	X	-	-	-
30	CLA	39	307	X	-	-	-
30	CLA	39	308	X	-	-	-
30	CLA	40	203	X	-	-	-
30	CLA	40	204	X	-	-	-
30	CLA	40	206	X	-	-	-
30	CLA	40	207	X	-	-	-
30	CLA	40	209	X	-	-	-
30	CLA	41	303	X	-	-	-
30	CLA	41	304	X	-	-	-
30	CLA	41	305	X	-	-	-
30	CLA	41	306	X	-	-	-
30	CLA	41	307	X	-	-	-
30	CLA	41	308	X	-	-	-
30	CLA	41	309	X	-	-	-
30	CLA	A	402	X	-	-	-
30	CLA	A	404	X	-	-	-
30	CLA	B	601	X	-	-	-
30	CLA	B	602	X	-	-	-
30	CLA	B	603	X	-	-	-
30	CLA	B	604	X	-	-	-
30	CLA	B	605	X	-	-	-
30	CLA	B	606	X	-	-	-
30	CLA	B	607	X	-	-	-
30	CLA	B	608	X	-	-	-
30	CLA	B	609	X	-	-	-
30	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	B	611	X	-	-	-
30	CLA	B	612	X	-	-	-
30	CLA	B	613	X	-	-	-
30	CLA	B	614	X	-	-	-
30	CLA	B	615	X	-	-	-
30	CLA	B	623	X	-	-	-
30	CLA	C	502	X	-	-	-
30	CLA	C	503	X	-	-	-
30	CLA	C	504	X	-	-	-
30	CLA	C	505	X	-	-	-
30	CLA	C	506	X	-	-	-
30	CLA	C	507	X	-	-	-
30	CLA	C	508	X	-	-	-
30	CLA	C	509	X	-	-	-
30	CLA	C	510	X	-	-	-
30	CLA	C	511	X	-	-	-
30	CLA	C	512	X	-	-	-
30	CLA	C	513	X	-	-	-
30	CLA	C	514	X	-	-	-
30	CLA	C	520	X	-	-	-
30	CLA	C	521	X	-	-	-
30	CLA	D	401	X	-	-	-
30	CLA	D	402	X	-	-	-
30	CLA	D	405	X	-	-	-
30	CLA	D	406	X	-	-	-
30	CLA	M	101	X	-	-	-
30	CLA	W	102	X	-	-	-
30	CLA	Z	102	X	-	-	-
30	CLA	a	402	X	-	-	-
30	CLA	a	403	X	-	-	-
30	CLA	b	601	X	-	-	-
30	CLA	b	602	X	-	-	-
30	CLA	b	603	X	-	-	-
30	CLA	b	604	X	-	-	-
30	CLA	b	605	X	-	-	-
30	CLA	b	606	X	-	-	-
30	CLA	b	607	X	-	-	-
30	CLA	b	608	X	-	-	-
30	CLA	b	609	X	-	-	-
30	CLA	b	610	X	-	-	-
30	CLA	b	611	X	-	-	-
30	CLA	b	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	b	613	X	-	-	-
30	CLA	b	614	X	-	-	-
30	CLA	b	615	X	-	-	-
30	CLA	b	622	X	-	-	-
30	CLA	c	502	X	-	-	-
30	CLA	c	503	X	-	-	-
30	CLA	c	504	X	-	-	-
30	CLA	c	505	X	-	-	-
30	CLA	c	506	X	-	-	-
30	CLA	c	507	X	-	-	-
30	CLA	c	508	X	-	-	-
30	CLA	c	509	X	-	-	-
30	CLA	c	510	X	-	-	-
30	CLA	c	511	X	-	-	-
30	CLA	c	512	X	-	-	-
30	CLA	c	513	X	-	-	-
30	CLA	c	514	X	-	-	-
30	CLA	c	522	X	-	-	-
30	CLA	c	523	X	-	-	-
30	CLA	c	524	X	-	-	-
30	CLA	d	401	X	-	-	-
30	CLA	d	402	X	-	-	-
30	CLA	d	406	X	-	-	-
30	CLA	d	407	X	-	-	-
30	CLA	m	101	X	-	-	-
30	CLA	w	102	X	-	-	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 96390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II reaction center protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		

- Molecule 2 is a protein called Photosystem II chlorophyll protein CP47.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		
2	b	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		

- Molecule 3 is a protein called Photosystem II chlorophyll protein CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		
3	c	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		

- Molecule 4 is a protein called Photosystem II reaction center protein D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		
4	d	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total 616	C 401	N 102	O 113	0	0
5	e	75	Total 616	C 401	N 102	O 113	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	28	Total 228	C 155	N 39	O 33	S 1	0	0
6	f	28	Total 228	C 155	N 39	O 33	S 1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	66	Total 513	C 340	N 83	O 88	S 2	0	0
7	h	66	Total 513	C 340	N 83	O 88	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total 287	C 194	N 45	O 47	S 1	0	0
8	i	35	Total 287	C 194	N 45	O 47	S 1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total 254	C 172	N 38	O 43	S 1	0	0
9	j	34	Total 254	C 172	N 38	O 43	S 1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total 302	C 212	N 45	O 45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total 302	C 212	N 45	O 45	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total 310	C 208	N 48	O 53	S 1	0	0
11	l	38	Total 310	C 208	N 48	O 53	S 1	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	42	Total 316	C 207	N 51	O 58	0	0
12	m	42	Total 316	C 207	N 51	O 58	0	0

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	245	Total 1845	C 1166	N 306	O 365	S 8	0	0
13	o	245	Total 1845	C 1166	N 306	O 365	S 8	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total 250	C 174	N 36	O 38	S 2	0	0
14	t	30	Total 250	C 174	N 36	O 38	S 2	0	0

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	93	Total 713	C 455	N 119	O 137	S 2	0	0
15	u	93	Total 713	C 455	N 119	O 137	S 2	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		
16	v	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		
17	y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	37	Total	C	N	O	S	0	0
			263	171	45	46	1		
18	x	37	Total	C	N	O	S	0	0
			263	171	45	46	1		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		
19	z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		
20	q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		

- Molecule 21 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	52	Total	C	N	O	0	0
			422	273	65	84		
21	w	52	Total	C	N	O	0	0
			422	273	65	84		

- Molecule 22 is a protein called Unknown protein 0.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	0	31	Total	C	N	O	0	0
			155	93	31	31		
22	5	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 23 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	30	Total	C	N	O	0	0
			150	90	30	30		
23	6	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 24 is a protein called Unknown protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	10	Total	C	N	O	0	0
			50	30	10	10		
24	7	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	12	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	13	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	14	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	15	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	16	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	17	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	18	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	31	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	32	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	33	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	34	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	35	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	36	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	37	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	38	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	19	215	Total	C	N	O	0	0
			1075	645	215	215		
26	39	215	Total	C	N	O	0	0
			1075	645	215	215		

- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	20	143	Total	C	N	O	0	0
			715	429	143	143		
27	40	143	Total	C	N	O	0	0
			715	429	143	143		

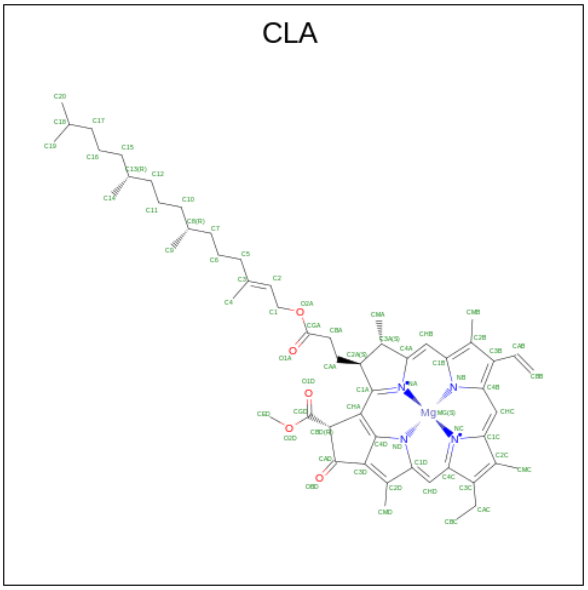
- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	21	155	Total 775	C 465	N 155	O 155	0	0
28	41	155	Total 775	C 465	N 155	O 155	0	0

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total 1	Fe 1	0
29	a	1	Total 1	Fe 1	0

- Molecule 30 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total 130	C 110	Mg 2	N 8	O 10	0
30	A	1	Total 130	C 110	Mg 2	N 8	O 10	0
30	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
30	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
30	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
30	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	C	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	D	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	D	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	D	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	D	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	W	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
30	W	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
30	a	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
30	a	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	c	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
30	d	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	d	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	d	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	d	1	Total	C	Mg	N	O	0
			260	220	4	16	20	
30	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	w	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
30	w	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	11	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	12	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	13	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	14	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
30	15	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	16	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	17	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	

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Mol	Chain	Residues	Atoms					AltConf
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	18	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	19	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	20	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	21	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	31	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	32	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
30	33	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	35	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	36	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	37	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	

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Mol	Chain	Residues	Atoms					AltConf
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	38	1	Total	C	Mg	N	O	0
			595	485	11	44	55	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	39	1	Total	C	Mg	N	O	0
			400	320	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	

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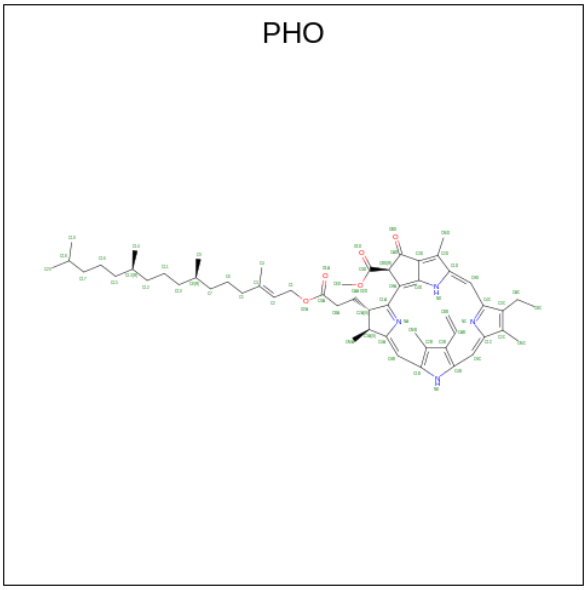
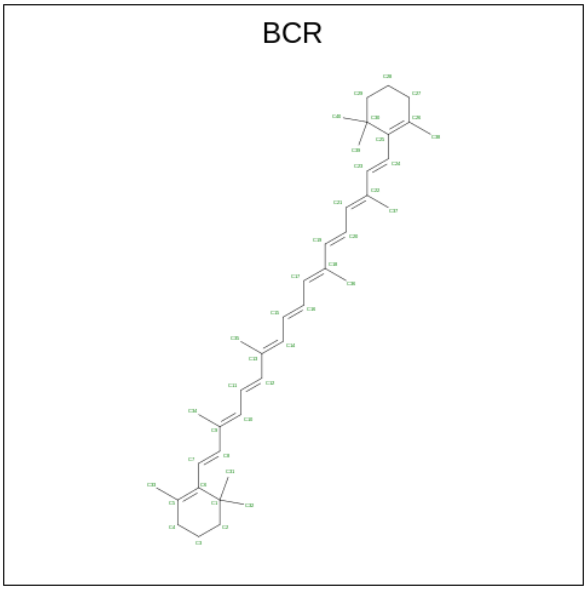
Mol	Chain	Residues	Atoms					AltConf
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	40	1	Total	C	Mg	N	O	0
			420	340	8	32	40	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	
30	41	1	Total	C	Mg	N	O	0
			485	395	9	36	45	

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	N	O	0
			64	55	4	5	
31	D	1	Total	C	N	O	0
			64	55	4	5	
31	d	1	Total	C	N	O	0
			128	110	8	10	
31	d	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 32 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	C	0
			80	80	
32	A	1	Total	C	0
			80	80	
32	B	1	Total	C	0
			160	160	
32	B	1	Total	C	0
			160	160	
32	B	1	Total	C	0
			160	160	
32	B	1	Total	C	0
			160	160	
32	C	1	Total	C	0
			80	80	
32	C	1	Total	C	0
			80	80	

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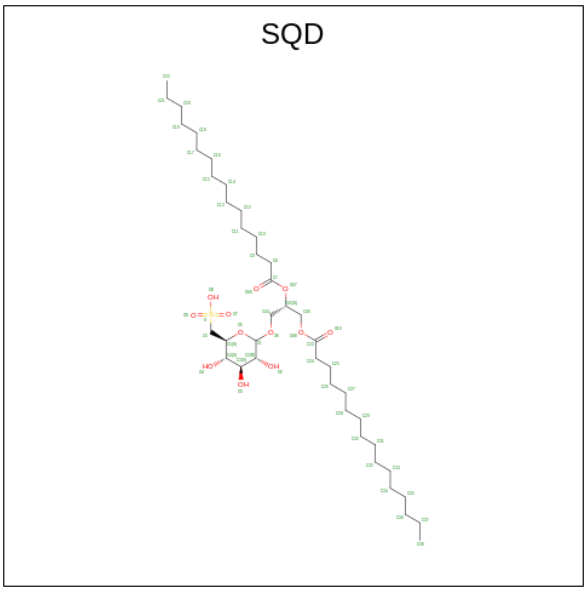
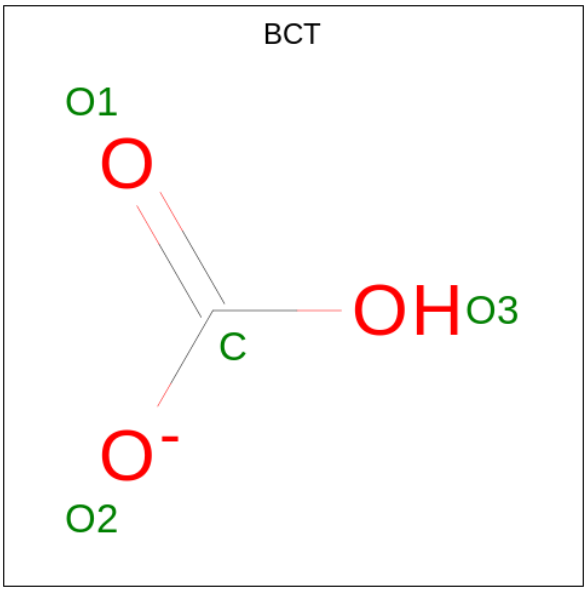
Mol	Chain	Residues	Atoms	AltConf
32	F	1	Total C 40 40	0
32	H	1	Total C 40 40	0
32	Y	1	Total C 40 40	0
32	Z	1	Total C 40 40	0
32	a	1	Total C 80 80	0
32	a	1	Total C 80 80	0
32	b	1	Total C 120 120	0
32	b	1	Total C 120 120	0
32	b	1	Total C 120 120	0
32	c	1	Total C 160 160	0
32	c	1	Total C 160 160	0
32	c	1	Total C 160 160	0
32	c	1	Total C 160 160	0
32	f	1	Total C 40 40	0
32	h	1	Total C 40 40	0
32	m	1	Total C 40 40	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



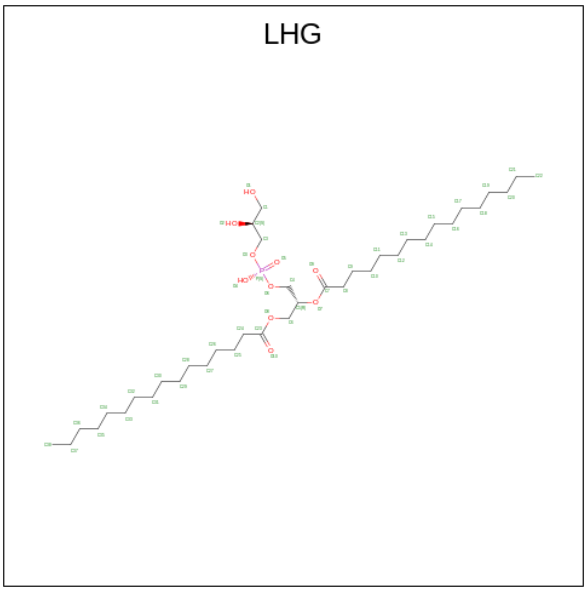
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			54	41	12	1	
33	B	1	Total	C	O	S	0
			37	24	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	b	1	Total	C	O	S	0
			37	24	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	a	1	Total	C	O	0
			4	1	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			46	35	10	1	

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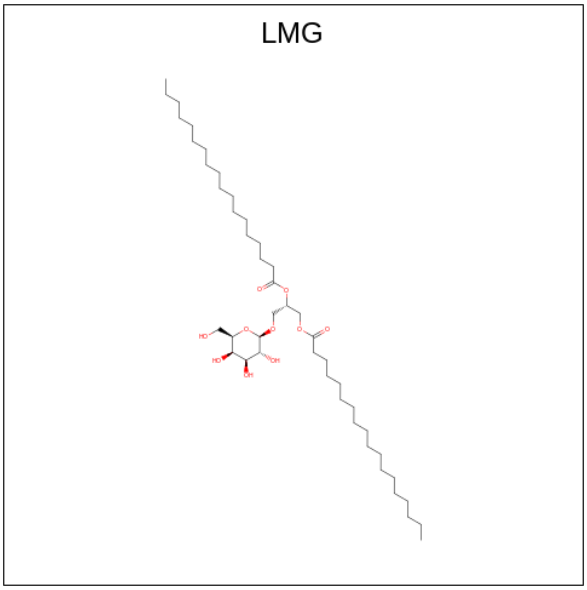
Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			98	76	20	2	
35	L	1	Total	C	O	P	0
			98	76	20	2	
35	a	1	Total	C	O	P	0
			46	35	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			102	82	20	
36	B	1	Total	C	O	0
			102	82	20	
36	D	1	Total	C	O	0
			51	41	10	
36	M	1	Total	C	O	0
			40	30	10	

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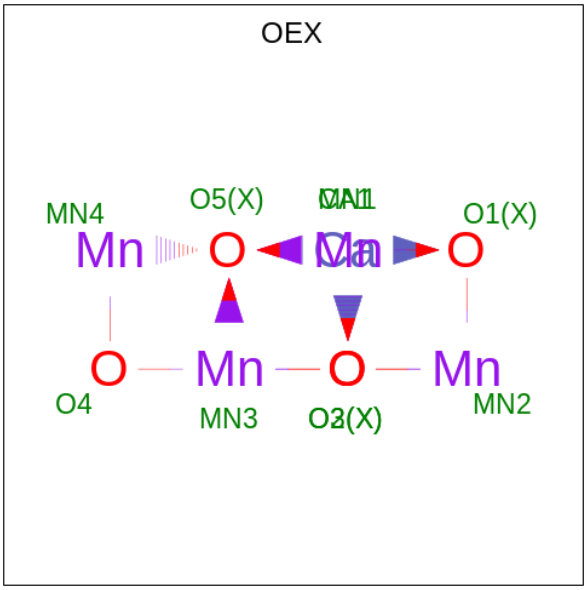
Mol	Chain	Residues	Atoms	AltConf
36	Q	1	Total C O 51 41 10	0
36	W	1	Total C O 51 41 10	0
36	b	1	Total C O 102 82 20	0
36	b	1	Total C O 102 82 20	0
36	c	1	Total C O 51 41 10	0
36	d	1	Total C O 51 41 10	0
36	m	1	Total C O 40 30 10	0
36	w	1	Total C O 51 41 10	0
36	12	1	Total C O 39 29 10	0
36	32	1	Total C O 39 29 10	0

- Molecule 37 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
37	C	1	Total Ca Mn O 10 1 4 5	0

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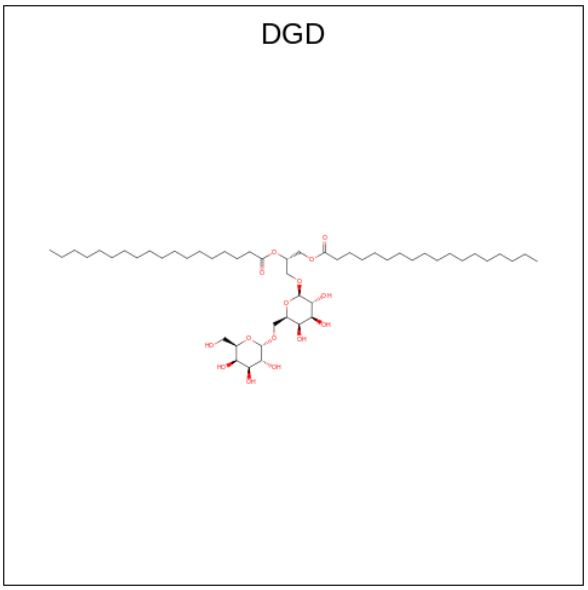
Mol	Chain	Residues	Atoms				AltConf
37	c	1	Total	Ca	Mn	O	0
			10	1	4	5	

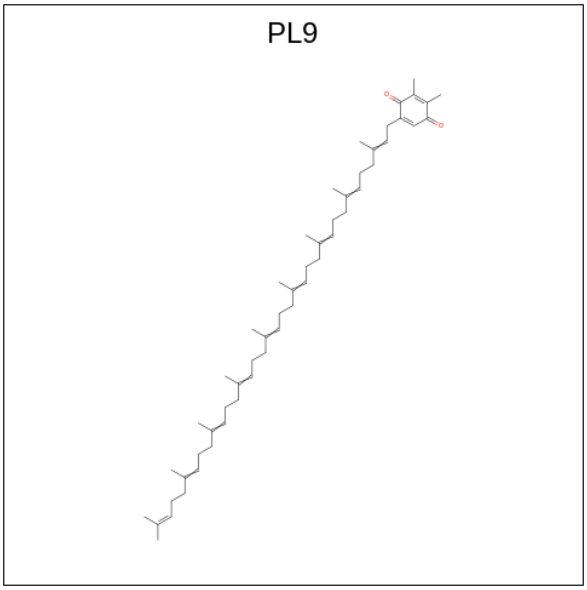
- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
38	C	1	Total	C	O	0
			124	94	30	
38	C	1	Total	C	O	0
			124	94	30	
38	H	1	Total	C	O	0
			62	47	15	
38	J	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			124	94	30	
38	c	1	Total	C	O	0
			124	94	30	
38	h	1	Total	C	O	0
			62	47	15	
38	j	1	Total	C	O	0
			62	47	15	

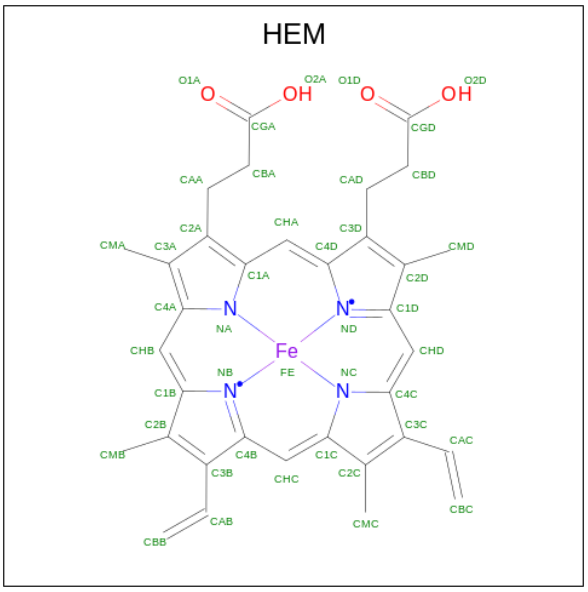
- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

$C_{53}H_{80}O_2$).



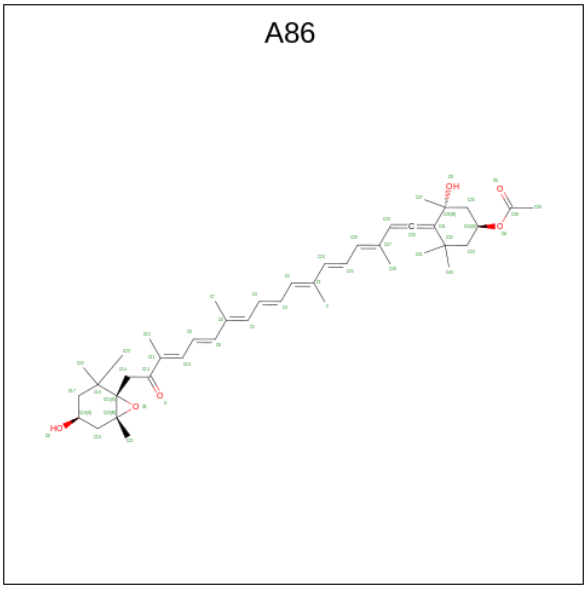
Mol	Chain	Residues	Atoms			AltConf
39	D	1	Total	C	O	0
			110	106	4	
39	D	1	Total	C	O	0
			110	106	4	
39	d	1	Total	C	O	0
			110	106	4	
39	d	1	Total	C	O	0
			110	106	4	

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
40	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
40	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
40	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
40	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 41 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7 ,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
41	11	1	Total	C	O	0
			288	252	36	
41	11	1	Total	C	O	0
			288	252	36	
41	11	1	Total	C	O	0
			288	252	36	
41	11	1	Total	C	O	0
			288	252	36	
41	11	1	Total	C	O	0
			288	252	36	
41	11	1	Total	C	O	0
			288	252	36	
41	12	1	Total	C	O	0
			288	252	36	
41	12	1	Total	C	O	0
			288	252	36	
41	12	1	Total	C	O	0
			288	252	36	
41	12	1	Total	C	O	0
			288	252	36	
41	12	1	Total	C	O	0
			288	252	36	
41	12	1	Total	C	O	0
			288	252	36	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	13	1	Total	C	O	0
			384	336	48	
41	14	1	Total	C	O	0
			192	168	24	
41	14	1	Total	C	O	0
			192	168	24	

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Mol	Chain	Residues	Atoms			AltConf
41	14	1	Total 192	C 168	O 24	0
41	14	1	Total 192	C 168	O 24	0
41	15	1	Total 336	C 294	O 42	0
41	15	1	Total 336	C 294	O 42	0
41	15	1	Total 336	C 294	O 42	0
41	15	1	Total 336	C 294	O 42	0
41	15	1	Total 336	C 294	O 42	0
41	15	1	Total 336	C 294	O 42	0
41	15	1	Total 336	C 294	O 42	0
41	16	1	Total 192	C 168	O 24	0
41	16	1	Total 192	C 168	O 24	0
41	16	1	Total 192	C 168	O 24	0
41	16	1	Total 192	C 168	O 24	0
41	17	1	Total 336	C 294	O 42	0
41	17	1	Total 336	C 294	O 42	0
41	17	1	Total 336	C 294	O 42	0
41	17	1	Total 336	C 294	O 42	0
41	17	1	Total 336	C 294	O 42	0
41	17	1	Total 336	C 294	O 42	0
41	17	1	Total 336	C 294	O 42	0
41	18	1	Total 192	C 168	O 24	0

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Mol	Chain	Residues	Atoms			AltConf
41	18	1	Total	C	O	0
			192	168	24	
41	18	1	Total	C	O	0
			192	168	24	
41	18	1	Total	C	O	0
			192	168	24	
41	19	1	Total	C	O	0
			144	126	18	
41	19	1	Total	C	O	0
			144	126	18	
41	19	1	Total	C	O	0
			144	126	18	
41	20	1	Total	C	O	0
			240	210	30	
41	20	1	Total	C	O	0
			240	210	30	
41	20	1	Total	C	O	0
			240	210	30	
41	20	1	Total	C	O	0
			240	210	30	
41	20	1	Total	C	O	0
			240	210	30	
41	21	1	Total	C	O	0
			240	210	30	
41	21	1	Total	C	O	0
			240	210	30	
41	21	1	Total	C	O	0
			240	210	30	
41	21	1	Total	C	O	0
			240	210	30	
41	21	1	Total	C	O	0
			240	210	30	
41	31	1	Total	C	O	0
			288	252	36	
41	31	1	Total	C	O	0
			288	252	36	
41	31	1	Total	C	O	0
			288	252	36	
41	31	1	Total	C	O	0
			288	252	36	
41	31	1	Total	C	O	0
			288	252	36	

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Mol	Chain	Residues	Atoms			AltConf
41	31	1	Total	C	O	0
			288	252	36	
41	32	1	Total	C	O	0
			336	294	42	
41	32	1	Total	C	O	0
			336	294	42	
41	32	1	Total	C	O	0
			336	294	42	
41	32	1	Total	C	O	0
			336	294	42	
41	32	1	Total	C	O	0
			336	294	42	
41	32	1	Total	C	O	0
			336	294	42	
41	32	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	33	1	Total	C	O	0
			336	294	42	
41	34	1	Total	C	O	0
			192	168	24	
41	34	1	Total	C	O	0
			192	168	24	
41	34	1	Total	C	O	0
			192	168	24	
41	34	1	Total	C	O	0
			192	168	24	
41	35	1	Total	C	O	0
			336	294	42	
41	35	1	Total	C	O	0
			336	294	42	

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Mol	Chain	Residues	Atoms			AltConf
41	35	1	Total 336	C 294	O 42	0
41	35	1	Total 336	C 294	O 42	0
41	35	1	Total 336	C 294	O 42	0
41	35	1	Total 336	C 294	O 42	0
41	35	1	Total 336	C 294	O 42	0
41	36	1	Total 192	C 168	O 24	0
41	36	1	Total 192	C 168	O 24	0
41	36	1	Total 192	C 168	O 24	0
41	36	1	Total 192	C 168	O 24	0
41	37	1	Total 336	C 294	O 42	0
41	37	1	Total 336	C 294	O 42	0
41	37	1	Total 336	C 294	O 42	0
41	37	1	Total 336	C 294	O 42	0
41	37	1	Total 336	C 294	O 42	0
41	37	1	Total 336	C 294	O 42	0
41	37	1	Total 336	C 294	O 42	0
41	38	1	Total 192	C 168	O 24	0
41	38	1	Total 192	C 168	O 24	0
41	38	1	Total 192	C 168	O 24	0
41	38	1	Total 192	C 168	O 24	0
41	39	1	Total 144	C 126	O 18	0

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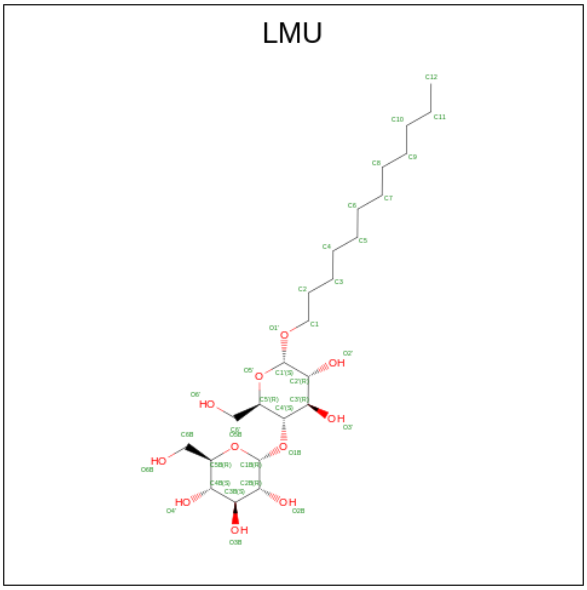
Mol	Chain	Residues	Atoms			AltConf
41	39	1	Total	C	O	0
			144	126	18	
41	39	1	Total	C	O	0
			144	126	18	
41	40	1	Total	C	O	0
			240	210	30	
41	40	1	Total	C	O	0
			240	210	30	
41	40	1	Total	C	O	0
			240	210	30	
41	40	1	Total	C	O	0
			240	210	30	
41	40	1	Total	C	O	0
			240	210	30	
41	41	1	Total	C	O	0
			240	210	30	
41	41	1	Total	C	O	0
			240	210	30	
41	41	1	Total	C	O	0
			240	210	30	
41	41	1	Total	C	O	0
			240	210	30	
41	41	1	Total	C	O	0
			240	210	30	

- Molecule 42 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



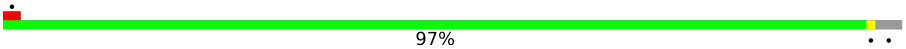
Mol	Chain	Residues	Atoms			AltConf
42	12	1	Total	C	O	0
			32	21	11	
42	32	1	Total	C	O	0
			32	21	11	

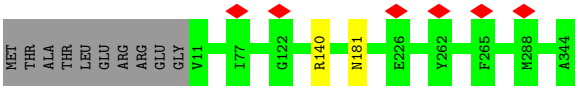
3 Residue-property plots (i)

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 II reaction center protein D1

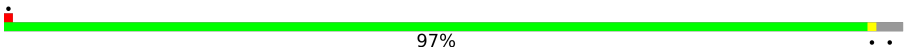
Chain A:

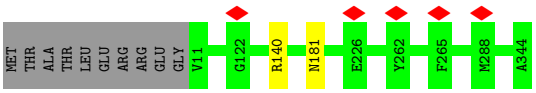




• Molecule 1: Photosystem II reaction center protein D1

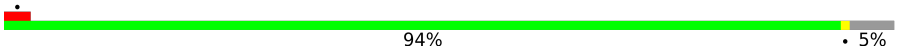
Chain a:

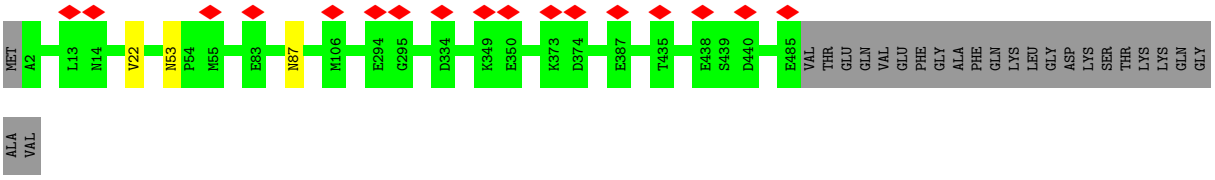




• Molecule 2: Photosystem II chlorophyll protein CP47

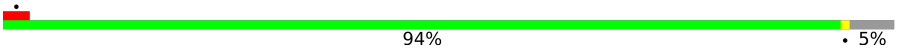
Chain B:

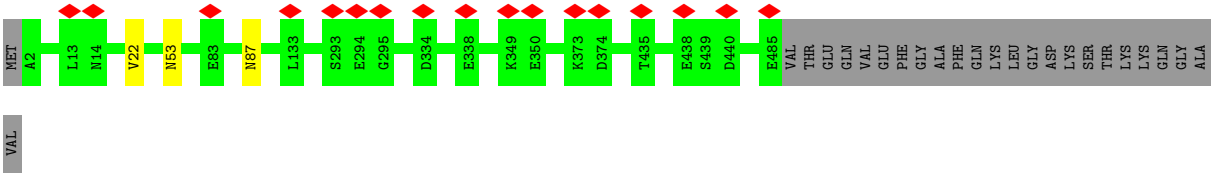




• Molecule 2: Photosystem II chlorophyll protein CP47

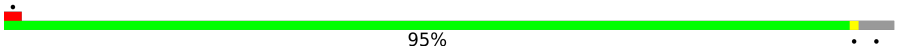
Chain b:

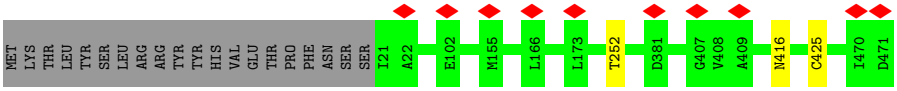




• Molecule 3: Photosystem II chlorophyll protein CP43

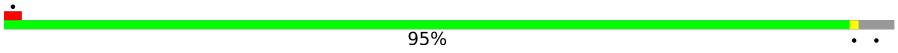
Chain C:

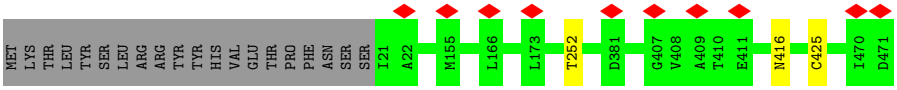




• Molecule 3: Photosystem II chlorophyll protein CP43

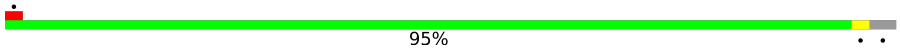
Chain c:

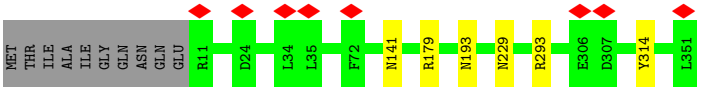




• Molecule 4: Photosystem II reaction center protein D2

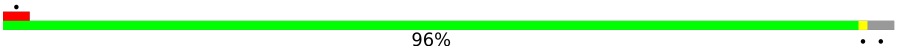
Chain D:

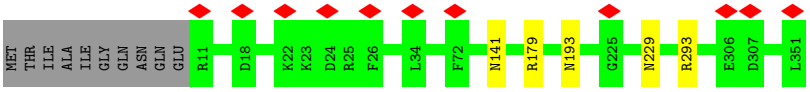




• Molecule 4: Photosystem II reaction center protein D2

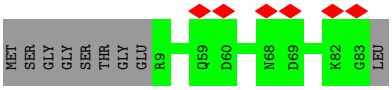
Chain d:





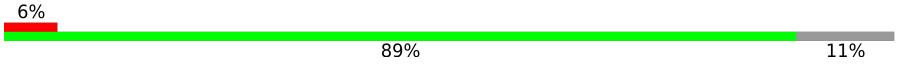
• Molecule 5: Cytochrome b559 subunit alpha

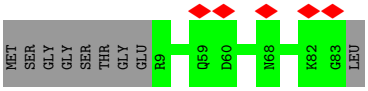
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

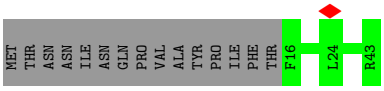
Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

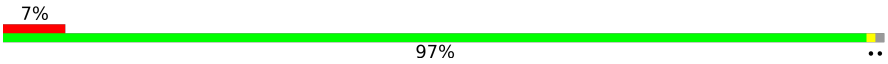


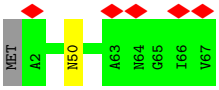
• Molecule 6: Cytochrome b559 subunit beta

Chain f:

• Molecule 7: Photosystem II reaction center protein H

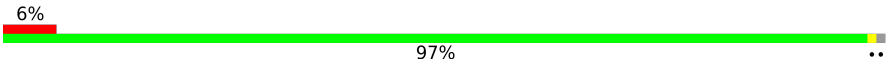
Chain H:

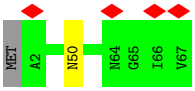




• Molecule 7: Photosystem II reaction center protein H

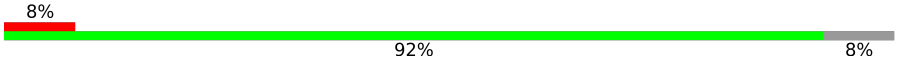
Chain h:

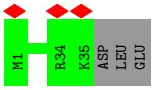




• Molecule 8: Photosystem II reaction center protein I

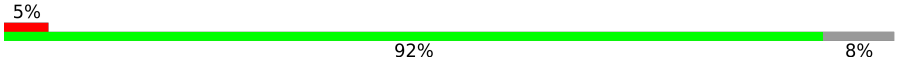
Chain I:

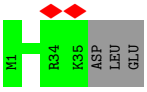




• Molecule 8: Photosystem II reaction center protein I

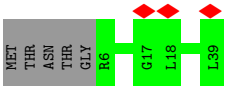
Chain i:





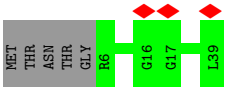
• Molecule 9: Photosystem II reaction center protein J

Chain J:



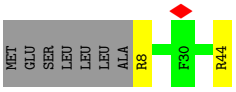
• Molecule 9: Photosystem II reaction center protein J

Chain j:



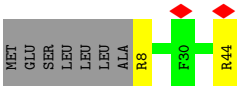
• Molecule 10: Photosystem II reaction center protein K

Chain K:



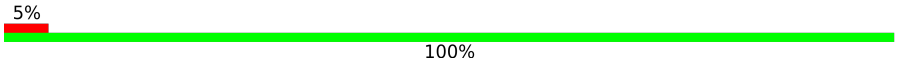
• Molecule 10: Photosystem II reaction center protein K

Chain k:



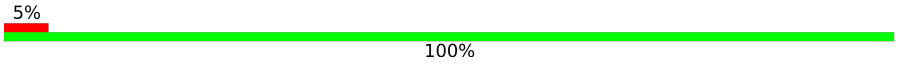
• Molecule 11: Photosystem II reaction center protein L

Chain L:



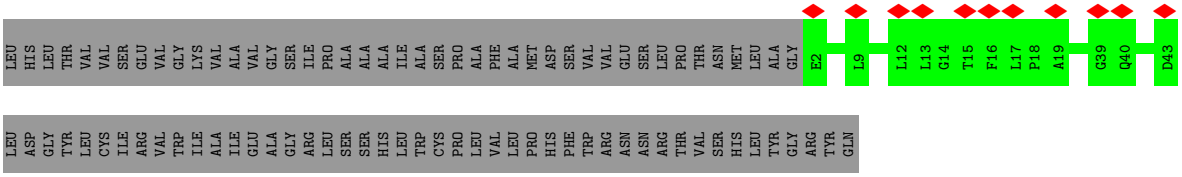
• Molecule 11: Photosystem II reaction center protein L

Chain l:



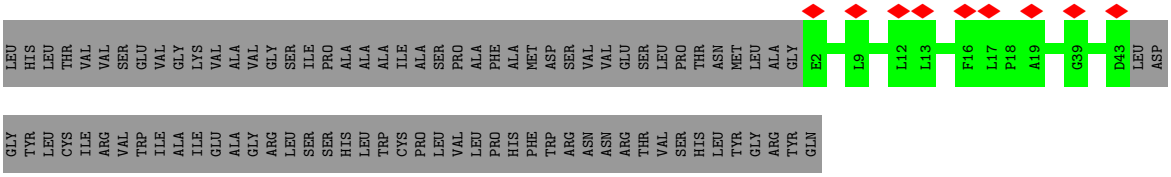
• Molecule 12: Photosystem II reaction center protein M

Chain M:

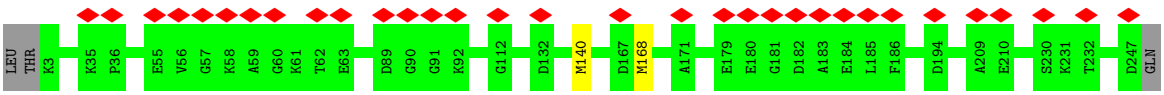


• Molecule 12: Photosystem II reaction center protein M

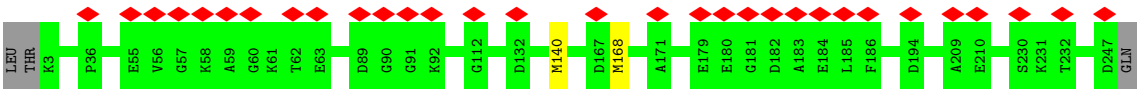
Chain m:



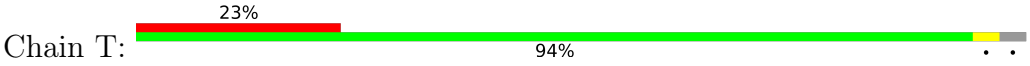
• Molecule 13: Extrinsic protein in photosystem II

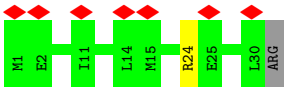


• Molecule 13: Extrinsic protein in photosystem II

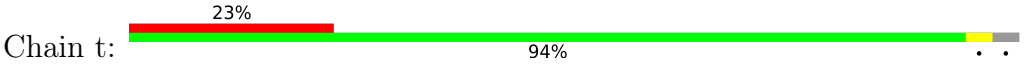


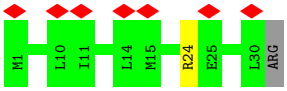
• Molecule 14: Photosystem II reaction center protein T



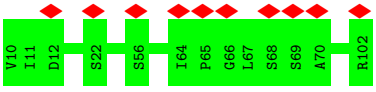


• Molecule 14: Photosystem II reaction center protein T

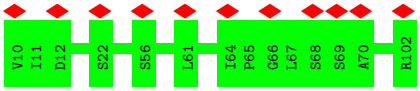




• Molecule 15: Extrinsic protein in photosystem II

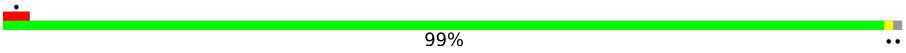


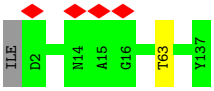
• Molecule 15: Extrinsic protein in photosystem II



• Molecule 16: Cytochrome c-550

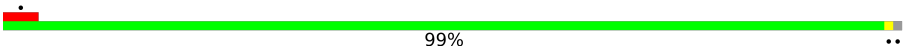
Chain V:

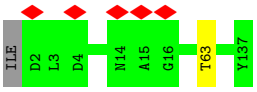




• Molecule 16: Cytochrome c-550

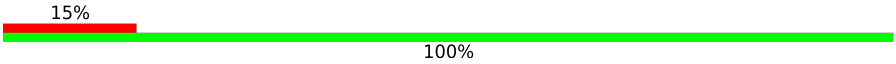
Chain v:

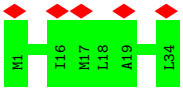




• Molecule 17: Photosystem II reaction center protein Ycf12

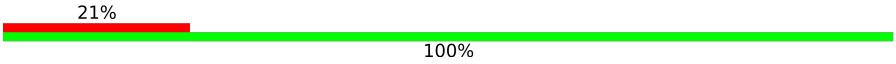
Chain Y:

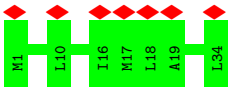




• Molecule 17: Photosystem II reaction center protein Ycf12

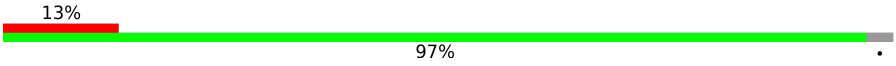
Chain y:

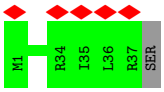




• Molecule 18: Photosystem II reaction center X protein

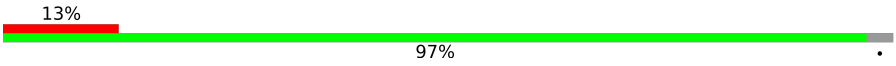
Chain X:

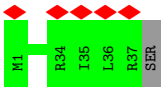




• Molecule 18: Photosystem II reaction center X protein

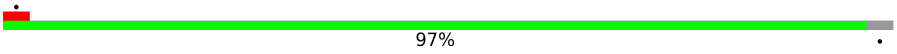
Chain x:

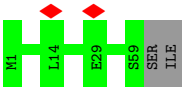




• Molecule 19: Photosystem II reaction center protein Z

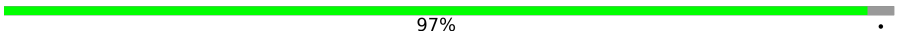
Chain Z:





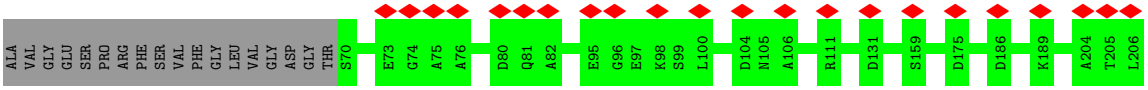
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



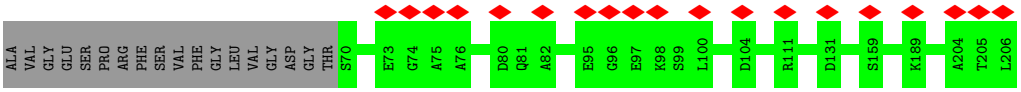
• Molecule 20: Extrinsic protein in photosystem II

Chain Q:



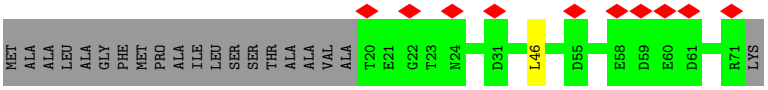
• Molecule 20: Extrinsic protein in photosystem II

Chain q:



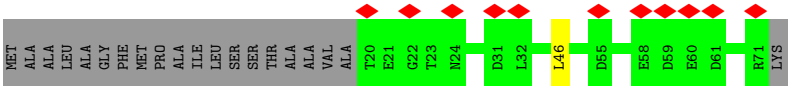
• Molecule 21: Photosystem II reaction center protein W

Chain W:



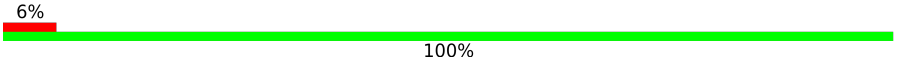
• Molecule 21: Photosystem II reaction center protein W

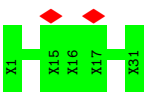
Chain w:



• Molecule 22: Unknown protein 0

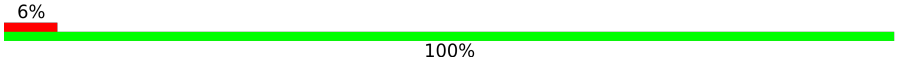
Chain 0:

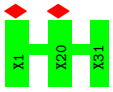




• Molecule 22: Unknown protein 0

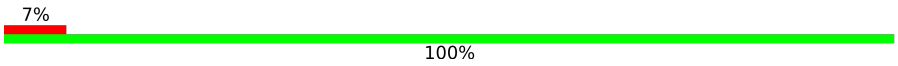
Chain 5:





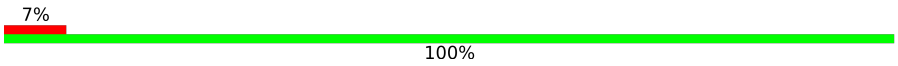
• Molecule 23: Unknown protein 1

Chain 1:



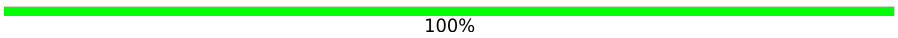
• Molecule 23: Unknown protein 1

Chain 6:



• Molecule 24: Unknown protein 2

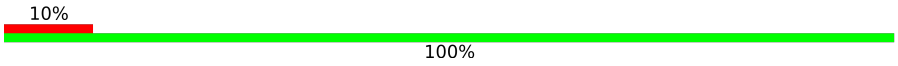
Chain 2:



There are no outlier residues recorded for this chain.

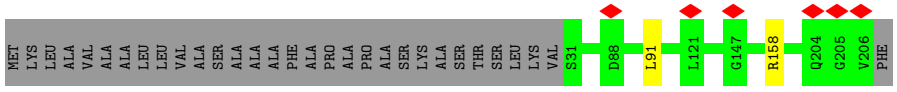
• Molecule 24: Unknown protein 2

Chain 7:



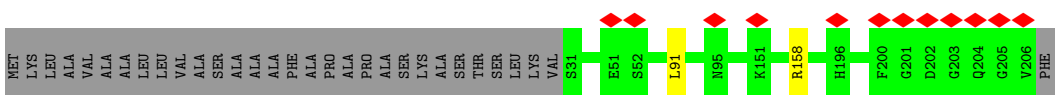
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:



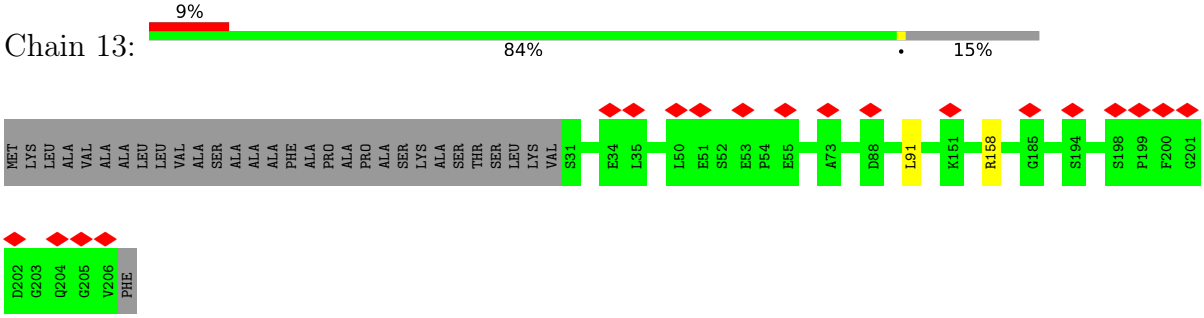
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:



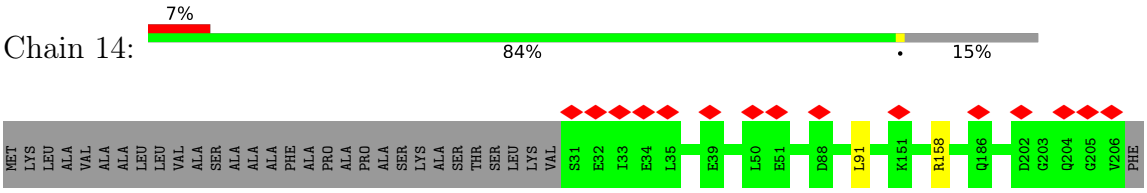
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13:



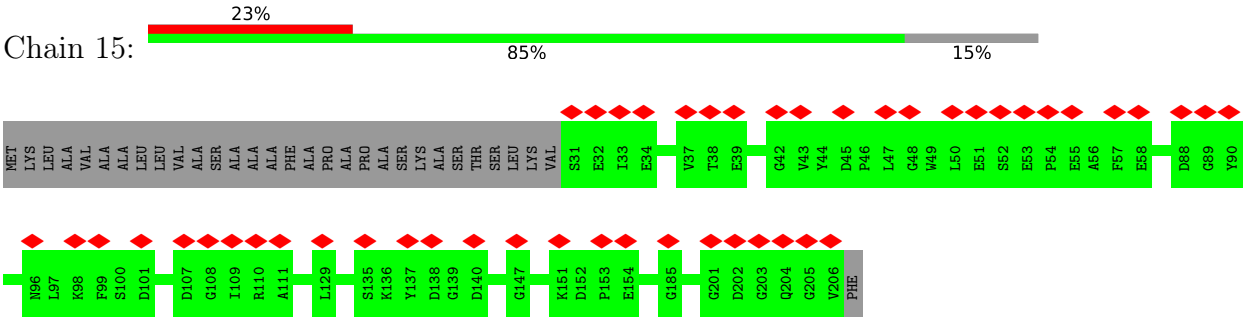
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 14:



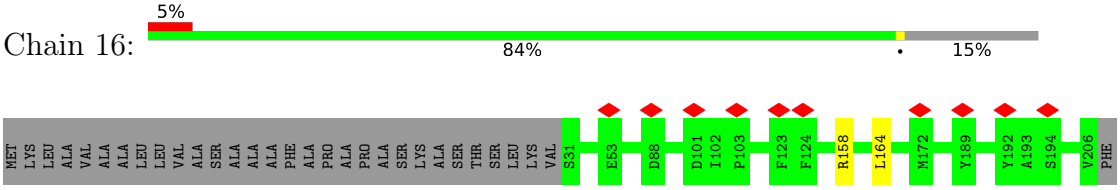
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 15:



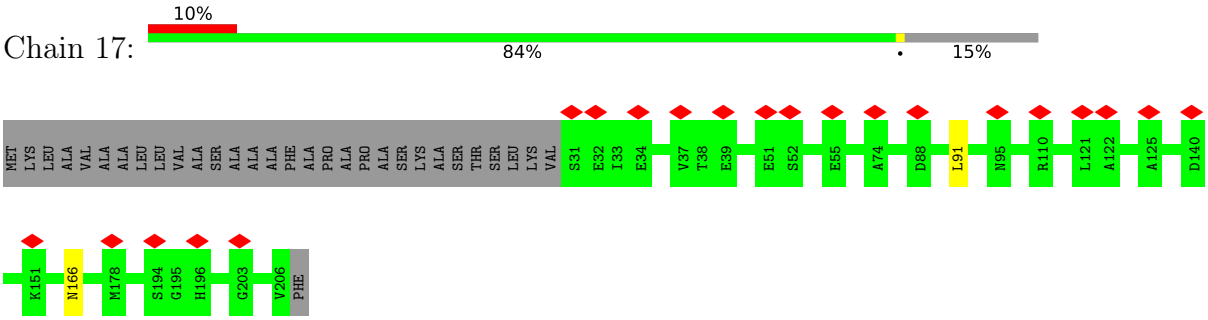
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 16:



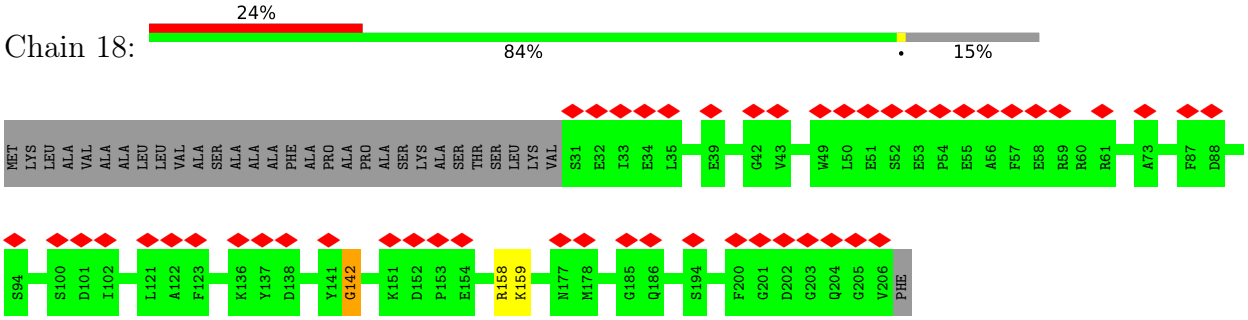
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 17:



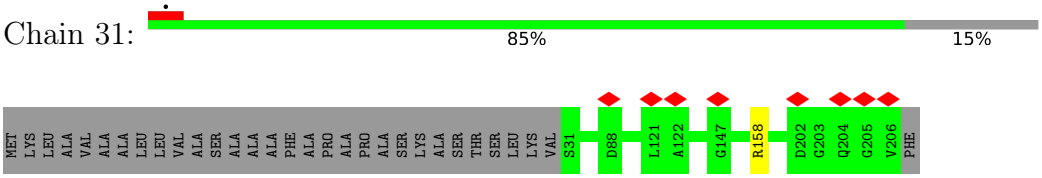
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 18:



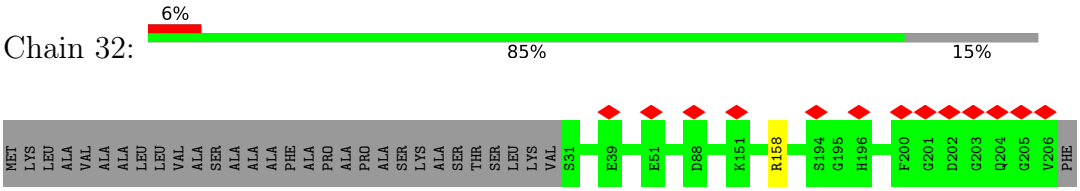
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 31:



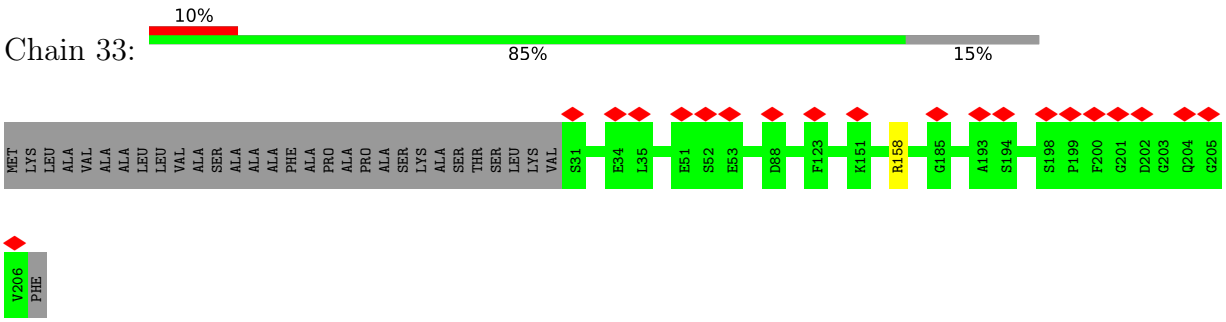
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 32:



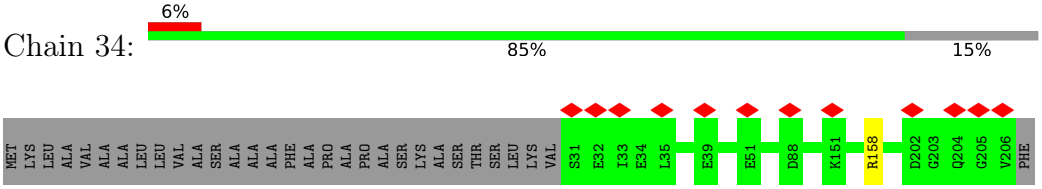
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 33:



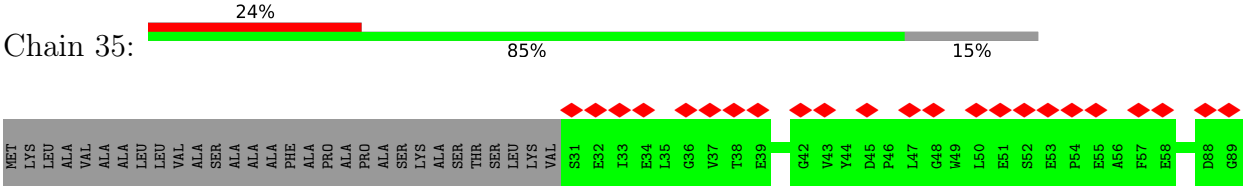
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

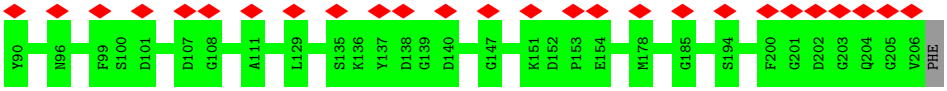
Chain 34:



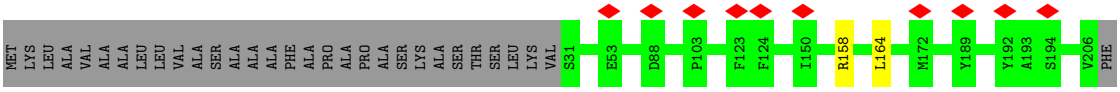
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 35:

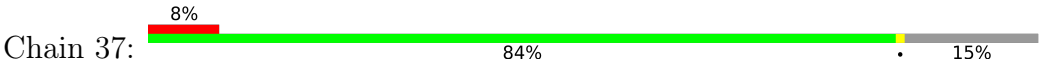


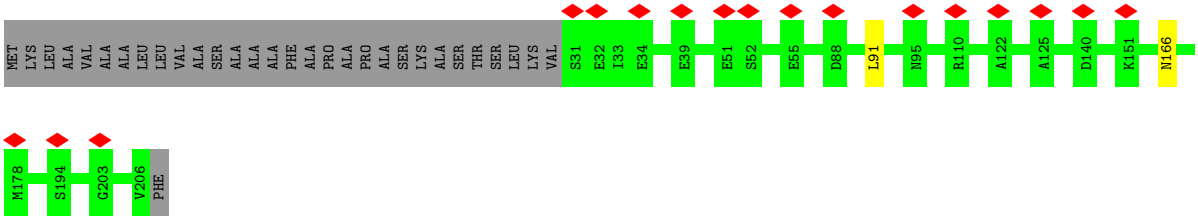


• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

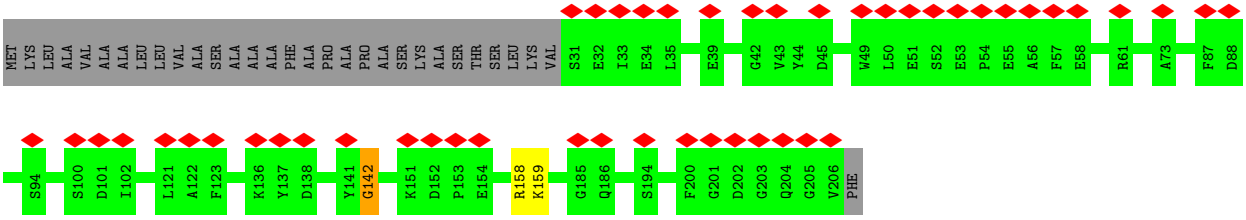


• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

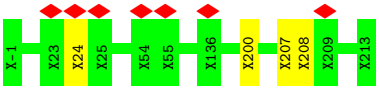




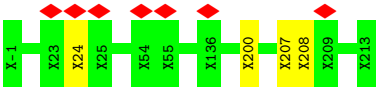
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



• Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1

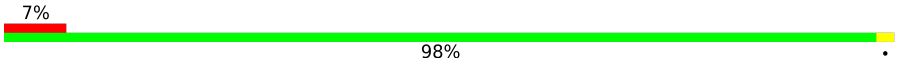


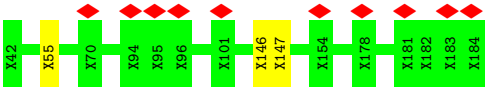
• Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1



• Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2

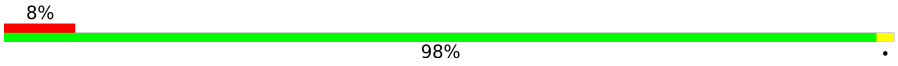
Chain 20:

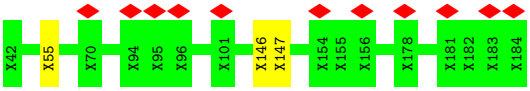




• Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2

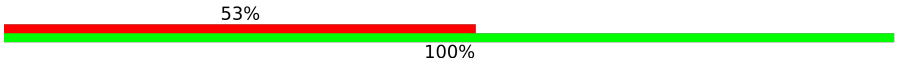
Chain 40:

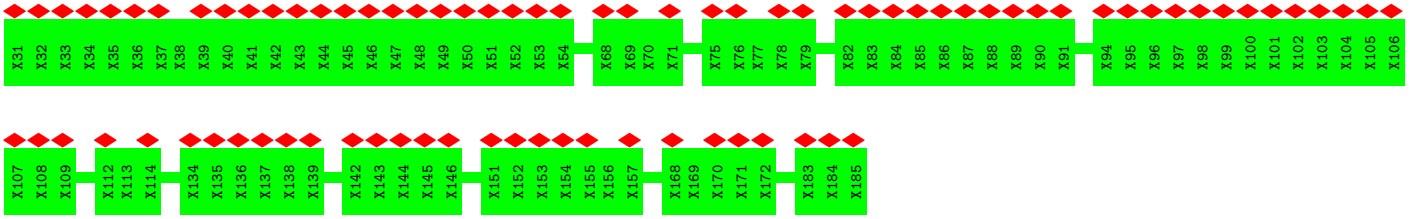




• Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3

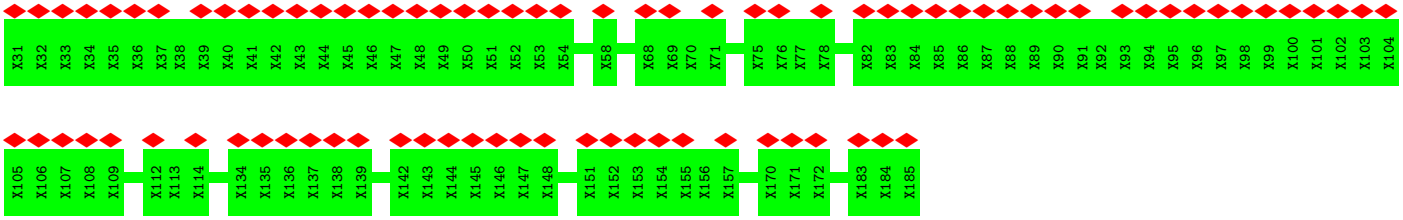
Chain 21:





• Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3

Chain 41:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	98936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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, FE2, BCT, LMG, HEM, A86, SQD, DGD, PHO, PL9, BCR, LHG, OEX, LMU

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	0.58	0/2701	0.60	0/3682
1	a	0.58	0/2701	0.60	0/3682
2	B	0.58	1/3942 (0.0%)	0.57	0/5362
2	b	0.58	1/3942 (0.0%)	0.57	0/5362
3	C	0.58	1/3620 (0.0%)	0.60	1/4933 (0.0%)
3	c	0.58	1/3620 (0.0%)	0.60	1/4933 (0.0%)
4	D	0.58	1/2789 (0.0%)	0.60	0/3803
4	d	0.58	0/2789	0.60	0/3803
5	E	0.44	0/634	0.53	0/864
5	e	0.44	0/634	0.53	0/864
6	F	0.46	0/235	0.70	0/316
6	f	0.45	0/235	0.70	0/316
7	H	0.49	0/523	0.61	0/714
7	h	0.49	0/523	0.61	0/714
8	I	0.62	0/294	0.70	0/397
8	i	0.63	0/294	0.70	0/397
9	J	0.43	0/260	0.59	0/351
9	j	0.43	0/260	0.59	0/351
10	K	0.57	0/313	0.69	0/429
10	k	0.57	0/313	0.68	0/429
11	L	0.61	0/319	0.55	0/433
11	l	0.61	0/319	0.55	0/433
12	M	0.47	0/321	0.61	0/433
12	m	0.47	0/321	0.61	0/433
13	O	0.42	0/1875	0.58	0/2528
13	o	0.41	0/1875	0.58	0/2528
14	T	0.45	0/256	0.52	0/346
14	t	0.45	0/256	0.52	0/346
15	U	0.40	0/728	0.58	0/989
15	u	0.41	0/728	0.58	0/989
16	V	0.42	0/1056	0.56	0/1435
16	v	0.42	0/1056	0.56	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.32	0/252	0.52	0/341
17	y	0.32	0/252	0.52	0/341
18	X	0.31	0/263	0.54	0/355
18	x	0.31	0/263	0.54	0/355
19	Z	0.41	0/456	0.58	0/624
19	z	0.41	0/456	0.58	0/624
20	Q	0.39	0/1099	0.56	0/1482
20	q	0.39	0/1099	0.56	0/1482
21	W	0.53	0/434	0.67	1/590 (0.2%)
21	w	0.53	0/434	0.67	1/590 (0.2%)
25	11	0.43	0/1373	0.55	1/1861 (0.1%)
25	12	0.43	0/1373	0.55	1/1861 (0.1%)
25	13	0.43	0/1373	0.55	1/1861 (0.1%)
25	14	0.43	0/1373	0.55	1/1861 (0.1%)
25	15	0.33	0/1373	0.52	0/1861
25	16	0.42	0/1373	0.64	1/1861 (0.1%)
25	17	0.41	0/1373	0.58	1/1861 (0.1%)
25	18	0.35	0/1373	0.54	0/1861
25	31	0.46	0/1373	0.56	0/1861
25	32	0.46	0/1373	0.56	0/1861
25	33	0.46	0/1373	0.56	0/1861
25	34	0.46	0/1373	0.56	0/1861
25	35	0.33	0/1373	0.52	0/1861
25	36	0.42	0/1373	0.64	1/1861 (0.1%)
25	37	0.41	0/1373	0.58	1/1861 (0.1%)
25	38	0.35	0/1373	0.54	0/1861
All	All	0.49	5/66708 (0.0%)	0.58	12/90590 (0.0%)

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
1	A	0	1
1	a	0	1
16	V	0	1
16	v	0	1
25	18	0	1
25	38	0	1
26	19	0	4
26	39	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	20	0	3
27	40	0	3
All	All	0	20

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	22	VAL	CB-CG1	-7.25	1.37	1.52
2	B	22	VAL	CB-CG1	-7.19	1.37	1.52
3	c	425	CYS	CB-SG	-5.08	1.73	1.81
4	D	314	TYR	CD1-CE1	-5.05	1.31	1.39
3	C	425	CYS	CB-SG	-5.01	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	252	THR	C-N-CA	6.18	137.15	121.70
3	c	252	THR	C-N-CA	6.15	137.08	121.70
21	W	46	LEU	CB-CG-CD1	-5.34	101.92	111.00
21	w	46	LEU	CB-CG-CD1	-5.34	101.93	111.00
25	16	164	LEU	CA-CB-CG	5.16	127.17	115.30
25	36	164	LEU	CA-CB-CG	5.16	127.17	115.30
25	17	91	LEU	CA-CB-CG	5.11	127.06	115.30
25	37	91	LEU	CA-CB-CG	5.10	127.03	115.30
25	14	91	LEU	CA-CB-CG	5.06	126.93	115.30
25	11	91	LEU	CA-CB-CG	5.05	126.91	115.30
25	13	91	LEU	CA-CB-CG	5.03	126.86	115.30
25	12	91	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	18	142	GLY	Peptide
26	19	200	UNK	Peptide
26	19	207	UNK	Peptide
26	19	208	UNK	Peptide
26	19	24	UNK	Peptide
27	20	146	UNK	Peptide
27	20	147	UNK	Peptide
27	20	55	UNK	Peptide

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Continued from previous page...

Mol	Chain	Res	Type	Group
25	38	142	GLY	Peptide
26	39	200	UNK	Peptide
26	39	207	UNK	Peptide
26	39	208	UNK	Peptide
26	39	24	UNK	Peptide
27	40	146	UNK	Peptide
27	40	147	UNK	Peptide
27	40	55	UNK	Peptide
1	A	140	ARG	Peptide
16	V	63	THR	Peptide
1	a	140	ARG	Peptide
16	v	63	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
2	B	482/509 (95%)	467 (97%)	15 (3%)	0	100	100
2	b	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
3	C	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
3	c	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
13	o	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
14	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
14	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
15	U	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
15	u	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
16	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
16	v	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
17	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
17	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
18	X	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
18	x	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	15	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	16	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	17	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	18	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	25	62
25	31	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	32	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	33	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	34	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	35	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	36	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	37	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	38	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	25	62
All	All	8276/9368 (88%)	7903 (96%)	371 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	18	142	GLY
25	38	142	GLY

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	272/280 (97%)	271 (100%)	1 (0%)	91	95
1	a	272/280 (97%)	271 (100%)	1 (0%)	91	95
2	B	385/405 (95%)	383 (100%)	2 (0%)	88	94
2	b	385/405 (95%)	383 (100%)	2 (0%)	88	94
3	C	356/376 (95%)	355 (100%)	1 (0%)	92	96
3	c	356/376 (95%)	355 (100%)	1 (0%)	92	96
4	D	273/281 (97%)	268 (98%)	5 (2%)	59	77
4	d	273/281 (97%)	268 (98%)	5 (2%)	59	77
5	E	69/75 (92%)	69 (100%)	0	100	100
5	e	69/75 (92%)	69 (100%)	0	100	100
6	F	22/36 (61%)	22 (100%)	0	100	100
6	f	22/36 (61%)	22 (100%)	0	100	100
7	H	55/56 (98%)	54 (98%)	1 (2%)	59	77
7	h	55/56 (98%)	54 (98%)	1 (2%)	59	77
8	I	34/37 (92%)	34 (100%)	0	100	100
8	i	34/37 (92%)	34 (100%)	0	100	100
9	J	27/31 (87%)	27 (100%)	0	100	100
9	j	27/31 (87%)	27 (100%)	0	100	100
10	K	32/38 (84%)	30 (94%)	2 (6%)	18	49
10	k	32/38 (84%)	30 (94%)	2 (6%)	18	49
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/104 (30%)	31 (100%)	0	100	100
12	m	31/104 (30%)	31 (100%)	0	100	100
13	O	196/201 (98%)	194 (99%)	2 (1%)	76	86
13	o	196/201 (98%)	194 (99%)	2 (1%)	76	86
14	T	27/28 (96%)	26 (96%)	1 (4%)	34	62
14	t	27/28 (96%)	26 (96%)	1 (4%)	34	62
15	U	77/77 (100%)	77 (100%)	0	100	100
15	u	77/77 (100%)	77 (100%)	0	100	100
16	V	114/115 (99%)	114 (100%)	0	100	100
16	v	114/115 (99%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/30 (97%)	29 (100%)	0	100	100
18	x	29/30 (97%)	29 (100%)	0	100	100
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	111 (100%)	0	100	100
20	q	111/124 (90%)	111 (100%)	0	100	100
21	W	43/55 (78%)	43 (100%)	0	100	100
21	w	43/55 (78%)	43 (100%)	0	100	100
25	11	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	12	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	13	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	14	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	15	138/158 (87%)	138 (100%)	0	100	100
25	16	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	17	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	18	138/158 (87%)	136 (99%)	2 (1%)	67	81
25	31	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	32	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	33	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	34	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	35	138/158 (87%)	138 (100%)	0	100	100
25	36	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	37	138/158 (87%)	137 (99%)	1 (1%)	84	91
25	38	138/158 (87%)	136 (99%)	2 (1%)	67	81
All	All	6732/7448 (90%)	6686 (99%)	46 (1%)	84	91

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	87	ASN
3	C	416	ASN
4	D	141	ASN
4	D	179	ARG
4	D	193	ASN
4	D	229	ASN
4	D	293	ARG
7	H	50	ASN
10	K	8	ARG
10	K	44	ARG
13	O	140	MET
13	O	168	MET
14	T	24	ARG
1	a	181	ASN
2	b	53	ASN
2	b	87	ASN
3	c	416	ASN
4	d	141	ASN
4	d	179	ARG
4	d	193	ASN
4	d	229	ASN
4	d	293	ARG
7	h	50	ASN
10	k	8	ARG
10	k	44	ARG
13	o	140	MET
13	o	168	MET
14	t	24	ARG
25	11	158	ARG
25	12	158	ARG
25	13	158	ARG
25	14	158	ARG
25	16	158	ARG
25	17	166	ASN
25	18	158	ARG
25	18	159	LYS
25	31	158	ARG
25	32	158	ARG
25	33	158	ARG
25	34	158	ARG
25	36	158	ARG
25	37	166	ASN

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Mol	Chain	Res	Type
25	38	158	ARG
25	38	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	303	ASN
2	B	87	ASN
2	B	179	GLN
2	B	457	ASN
3	C	325	ASN
3	C	416	ASN
4	D	193	ASN
4	D	229	ASN
4	D	291	ASN
5	E	62	GLN
11	L	9	GLN
13	O	7	ASN
13	O	109	GLN
13	O	222	GLN
16	V	25	GLN
16	V	68	ASN
20	Q	105	ASN
20	Q	162	GLN
1	a	303	ASN
2	b	87	ASN
2	b	179	GLN
2	b	457	ASN
3	c	325	ASN
3	c	416	ASN
4	d	193	ASN
4	d	219	ASN
4	d	229	ASN
4	d	349	ASN
5	e	62	GLN
13	o	7	ASN
13	o	109	GLN
13	o	222	GLN
16	v	25	GLN
16	v	68	ASN
17	y	33	ASN

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Mol	Chain	Res	Type
20	q	105	ASN
20	q	162	GLN
25	11	82	ASN
25	11	161	ASN
25	12	82	ASN
25	12	161	ASN
25	13	82	ASN
25	13	83	ASN
25	13	161	ASN
25	13	177	ASN
25	14	82	ASN
25	14	161	ASN
25	14	177	ASN
25	15	82	ASN
25	15	96	ASN
25	16	96	ASN
25	16	177	ASN
25	17	82	ASN
25	17	96	ASN
25	17	161	ASN
25	18	82	ASN
25	18	96	ASN
25	31	82	ASN
25	31	161	ASN
25	32	82	ASN
25	32	161	ASN
25	33	82	ASN
25	33	83	ASN
25	33	161	ASN
25	33	177	ASN
25	34	82	ASN
25	34	161	ASN
25	34	177	ASN
25	35	82	ASN
25	35	96	ASN
25	36	96	ASN
25	36	177	ASN
25	37	82	ASN
25	37	96	ASN
25	37	161	ASN
25	38	82	ASN
25	38	96	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 488 ligands modelled in this entry, 2 are monoatomic - leaving 486 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	$\#\|Z\| > 2$
30	CLA	b	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	32	303	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
41	A86	11	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	34	307	25	45,53,73	1.77	9 (20%)	52,89,113	1.84	9 (17%)
30	CLA	34	309	25	45,53,73	1.75	11 (24%)	52,89,113	1.77	9 (17%)
30	CLA	32	309	-	45,53,73	1.70	8 (17%)	52,89,113	1.69	7 (13%)
30	CLA	35	302	-	45,53,73	1.72	8 (17%)	52,89,113	1.88	9 (17%)
30	CLA	32	307	-	65,73,73	1.41	11 (16%)	76,113,113	1.60	10 (13%)
41	A86	40	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	a	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.60	8 (10%)
41	A86	16	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	A	404	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	10 (13%)
30	CLA	b	609	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	9 (11%)
41	A86	21	314	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LHG	a	407	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	8 (16%)
35	LHG	l	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
41	A86	38	315	-	44,50,50	4.03	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	36	307	25	45,53,73	1.76	10 (22%)	52,89,113	1.95	7 (13%)
30	CLA	12	310	25	45,53,73	1.76	8 (17%)	52,89,113	1.82	9 (17%)
41	A86	35	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.93	18 (35%)
41	A86	37	311	-	44,50,50	4.02	22 (50%)	51,76,76	8.33	19 (37%)
30	CLA	19	305	-	45,53,73	1.72	10 (22%)	52,89,113	1.69	6 (11%)
32	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
41	A86	21	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.41	21 (41%)
30	CLA	B	601	-	65,73,73	1.44	11 (16%)	76,113,113	1.49	8 (10%)
33	SQD	B	621	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
30	CLA	B	615	-	65,73,73	1.53	12 (18%)	76,113,113	1.44	11 (14%)
30	CLA	38	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	40	204	-	65,73,73	1.41	10 (15%)	76,113,113	1.52	9 (11%)
30	CLA	20	208	-	45,53,73	1.70	8 (17%)	52,89,113	1.78	9 (17%)
30	CLA	b	606	-	65,73,73	1.58	12 (18%)	76,113,113	1.61	13 (17%)
30	CLA	c	523	-	65,73,73	1.42	9 (13%)	76,113,113	1.68	11 (14%)
30	CLA	39	301	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	11 (14%)
41	A86	13	311	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	14	303	-	45,53,73	1.69	10 (22%)	52,89,113	1.81	9 (17%)
30	CLA	39	305	-	45,53,73	1.72	10 (22%)	52,89,113	1.69	6 (11%)
41	A86	35	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.59	20 (39%)
30	CLA	17	301	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	10 (13%)
30	CLA	d	406	-	65,73,73	1.48	9 (13%)	76,113,113	1.61	10 (13%)
32	BCR	B	617	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
32	BCR	H	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	7 (12%)
41	A86	33	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
35	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	35	305	-	45,53,73	1.76	6 (13%)	52,89,113	1.67	6 (11%)
30	CLA	37	310	-	45,53,73	1.74	9 (20%)	52,89,113	1.68	8 (15%)
41	A86	20	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.49	15 (29%)
41	A86	14	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
36	LMG	m	102	30	40,40,55	0.95	3 (7%)	48,48,63	1.34	7 (14%)
32	BCR	c	516	-	41,41,41	1.31	5 (12%)	56,56,56	1.40	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	15	308	25	45,53,73	1.75	10 (22%)	52,89,113	1.74	10 (19%)
30	CLA	13	310	-	45,53,73	1.75	9 (20%)	52,89,113	1.66	7 (13%)
41	A86	15	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	B	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.58	11 (14%)
30	CLA	13	309	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
40	HEM	v	201	16	41,50,50	1.60	5 (12%)	45,82,82	1.27	2 (4%)
30	CLA	c	507	-	65,73,73	1.52	11 (16%)	76,113,113	1.55	11 (14%)
41	A86	32	318	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
36	LMG	w	101	-	51,51,55	0.89	3 (5%)	59,59,63	1.40	7 (11%)
30	CLA	31	309	-	45,53,73	1.72	8 (17%)	52,89,113	1.67	7 (13%)
38	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
36	LMG	B	619	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)
34	BCT	A	407	29,1	2,3,3	1.26	0	2,3,3	3.93	2 (100%)
41	A86	33	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	c	502	-	65,73,73	1.40	11 (16%)	76,113,113	1.65	11 (14%)
38	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.41	8 (10%)
30	CLA	32	311	25	65,73,73	1.49	10 (15%)	76,113,113	1.56	10 (13%)
39	PL9	d	405	4	55,55,55	1.36	6 (10%)	68,69,69	1.50	14 (20%)
30	CLA	19	303	-	65,73,73	1.45	8 (12%)	76,113,113	1.55	9 (11%)
30	CLA	16	305	25	45,53,73	1.69	8 (17%)	52,89,113	1.92	10 (19%)
36	LMG	12	301	30	39,39,55	1.00	4 (10%)	47,47,63	1.21	4 (8%)
30	CLA	C	514	30	65,73,73	1.39	8 (12%)	76,113,113	1.63	9 (11%)
30	CLA	B	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	8 (10%)
36	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
30	CLA	16	306	25	45,53,73	1.73	9 (20%)	52,89,113	1.77	8 (15%)
41	A86	13	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	41	302	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	10 (19%)
30	CLA	14	306	-	45,53,73	1.72	8 (17%)	52,89,113	1.69	7 (13%)
41	A86	17	311	-	44,50,50	4.03	22 (50%)	51,76,76	8.33	19 (37%)
30	CLA	21	304	-	45,53,73	1.69	8 (17%)	52,89,113	1.64	6 (11%)
30	CLA	B	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.55	11 (14%)
36	LMG	M	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
41	A86	31	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	33	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	17	305	-	65,73,73	1.42	10 (15%)	76,113,113	1.53	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	A86	13	315	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
33	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
41	A86	40	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
30	CLA	16	304	-	65,73,73	1.42	10 (15%)	76,113,113	1.48	8 (10%)
41	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
30	CLA	B	606	-	65,73,73	1.59	12 (18%)	76,113,113	1.61	13 (17%)
30	CLA	14	304	-	65,73,73	1.41	10 (15%)	76,113,113	1.60	10 (13%)
30	CLA	B	614	-	65,73,73	1.39	10 (15%)	76,113,113	1.58	10 (13%)
30	CLA	37	305	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	9 (11%)
40	HEM	V	201	16	41,50,50	1.61	5 (12%)	45,82,82	1.28	4 (8%)
30	CLA	B	604	-	65,73,73	1.44	12 (18%)	76,113,113	1.67	15 (19%)
32	BCR	c	521	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	21	303	-	65,73,73	1.43	8 (12%)	76,113,113	1.41	7 (9%)
31	PHO	d	404	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	6 (12%)
30	CLA	38	310	25	65,73,73	1.47	8 (12%)	76,113,113	1.37	8 (10%)
30	CLA	41	305	28	45,53,73	1.76	6 (13%)	52,89,113	1.79	8 (15%)
30	CLA	19	306	-	45,53,73	1.72	11 (24%)	52,89,113	1.63	7 (13%)
30	CLA	37	306	25	45,53,73	1.71	7 (15%)	52,89,113	1.97	10 (19%)
41	A86	38	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
33	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
41	A86	14	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	16	303	-	45,53,73	1.69	8 (17%)	52,89,113	2.02	11 (21%)
30	CLA	12	312	-	65,73,73	1.47	9 (13%)	76,113,113	1.48	8 (10%)
30	CLA	b	614	-	65,73,73	1.39	10 (15%)	76,113,113	1.59	10 (13%)
30	CLA	38	304	-	45,53,73	1.72	8 (17%)	52,89,113	1.84	8 (15%)
32	BCR	a	404	-	41,41,41	1.29	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	17	309	25	45,53,73	1.79	10 (22%)	52,89,113	2.10	13 (25%)
30	CLA	15	302	-	45,53,73	1.72	8 (17%)	52,89,113	1.88	8 (15%)
30	CLA	35	309	-	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
41	A86	19	310	-	44,50,50	4.09	21 (47%)	51,76,76	7.18	19 (37%)
42	LMU	12	302	30	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
39	PL9	D	404	4	55,55,55	1.36	6 (10%)	68,69,69	1.49	14 (20%)
30	CLA	b	605	-	65,73,73	1.48	10 (15%)	76,113,113	1.50	9 (11%)
30	CLA	33	306	25	45,53,73	1.72	9 (20%)	52,89,113	2.09	12 (23%)
41	A86	18	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	C	504	-	65,73,73	1.48	11 (16%)	76,113,113	1.53	10 (13%)
30	CLA	12	311	25	65,73,73	1.48	10 (15%)	76,113,113	1.53	10 (13%)
41	A86	33	317	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
42	LMU	32	302	-	33,33,36	1.28	3 (9%)	44,44,47	1.57	8 (18%)
30	CLA	32	306	-	45,53,73	1.68	11 (24%)	52,89,113	1.81	9 (17%)
30	CLA	38	301	-	65,73,73	1.47	11 (16%)	76,113,113	1.44	11 (14%)
38	DGD	J	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
39	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
30	CLA	D	402	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	8 (10%)
30	CLA	36	302	25	65,73,73	1.49	10 (15%)	76,113,113	1.87	16 (21%)
32	BCR	B	618	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	9 (16%)
41	A86	20	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
32	BCR	Z	101	-	41,41,41	1.31	3 (7%)	56,56,56	1.41	8 (14%)
33	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	b	601	-	65,73,73	1.44	11 (16%)	76,113,113	1.50	8 (10%)
31	PHO	D	403	-	51,69,69	1.13	8 (15%)	47,99,99	1.29	6 (12%)
30	CLA	13	308	25	65,73,73	1.46	10 (15%)	76,113,113	1.55	10 (13%)
30	CLA	37	309	25	45,53,73	1.79	10 (22%)	52,89,113	2.10	13 (25%)
30	CLA	12	308	36,25	45,53,73	1.71	8 (17%)	52,89,113	2.04	12 (23%)
30	CLA	38	312	-	45,53,73	1.74	9 (20%)	52,89,113	1.61	7 (13%)
30	CLA	B	607	-	65,73,73	1.42	11 (16%)	76,113,113	1.57	7 (9%)
30	CLA	34	308	25	65,73,73	1.48	10 (15%)	76,113,113	1.57	10 (13%)
30	CLA	21	309	-	45,53,73	1.82	7 (15%)	52,89,113	1.72	11 (21%)
30	CLA	33	308	25	45,53,73	1.76	8 (17%)	52,89,113	1.84	8 (15%)
36	LMG	c	519	-	51,51,55	0.97	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	C	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.67	11 (14%)
30	CLA	C	506	-	65,73,73	1.46	11 (16%)	76,113,113	1.56	12 (15%)
41	A86	20	212	-	44,50,50	4.18	23 (52%)	51,76,76	8.23	15 (29%)
30	CLA	b	607	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	7 (9%)
30	CLA	C	512	3	65,73,73	1.50	10 (15%)	76,113,113	1.62	12 (15%)
41	A86	37	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
30	CLA	31	304	25	45,53,73	1.72	7 (15%)	52,89,113	2.08	13 (25%)
30	CLA	33	307	-	45,53,73	1.70	9 (20%)	52,89,113	1.73	7 (13%)
41	A86	40	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
30	CLA	33	311	-	45,53,73	1.74	9 (20%)	52,89,113	1.68	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	19	308	-	45,53,73	1.70	7 (15%)	52,89,113	1.80	9 (17%)
30	CLA	37	308	25	65,73,73	1.47	10 (15%)	76,113,113	1.52	11 (14%)
30	CLA	11	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	10 (19%)
30	CLA	b	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.58	11 (14%)
30	CLA	36	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	8 (10%)
30	CLA	41	308	-	45,53,73	1.75	6 (13%)	52,89,113	1.64	7 (13%)
30	CLA	C	521	-	65,73,73	1.42	9 (13%)	76,113,113	1.69	11 (14%)
41	A86	40	212	-	44,50,50	4.18	23 (52%)	51,76,76	8.23	15 (29%)
30	CLA	19	301	-	65,73,73	1.49	10 (15%)	76,113,113	1.49	11 (14%)
30	CLA	35	301	25	65,73,73	1.48	9 (13%)	76,113,113	1.56	10 (13%)
40	HEM	E	101	6,5	41,50,50	1.51	4 (9%)	45,82,82	1.24	5 (11%)
41	A86	33	314	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
30	CLA	38	306	25	45,53,73	1.74	7 (15%)	52,89,113	1.85	8 (15%)
32	BCR	B	616	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	7 (12%)
30	CLA	c	506	-	65,73,73	1.46	11 (16%)	76,113,113	1.56	12 (15%)
30	CLA	31	301	25	65,73,73	1.46	10 (15%)	76,113,113	1.67	8 (10%)
30	CLA	40	208	-	45,53,73	1.70	7 (15%)	52,89,113	1.78	9 (17%)
41	A86	32	314	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
41	A86	15	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	18	309	25	65,73,73	1.52	8 (12%)	76,113,113	1.60	10 (13%)
30	CLA	31	303	-	65,73,73	1.40	11 (16%)	76,113,113	1.58	10 (13%)
30	CLA	11	306	25	45,53,73	1.76	8 (17%)	52,89,113	1.82	7 (13%)
32	BCR	c	515	-	41,41,41	1.34	3 (7%)	56,56,56	1.41	8 (14%)
41	A86	41	312	-	44,50,50	3.82	21 (47%)	51,76,76	7.17	21 (41%)
30	CLA	15	303	-	65,73,73	1.42	7 (10%)	76,113,113	1.54	10 (13%)
41	A86	36	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	41	309	-	45,53,73	1.81	6 (13%)	52,89,113	1.72	11 (21%)
30	CLA	31	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.56	10 (13%)
30	CLA	32	313	-	45,53,73	1.72	9 (20%)	52,89,113	1.67	7 (13%)
32	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
41	A86	31	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
41	A86	19	311	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
30	CLA	40	205	-	45,53,73	1.73	10 (22%)	52,89,113	1.79	9 (17%)
41	A86	41	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.41	21 (41%)
30	CLA	B	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	20	203	30	45,53,73	1.78	9 (20%)	52,89,113	1.72	8 (15%)
30	CLA	14	308	25	65,73,73	1.47	10 (15%)	76,113,113	1.55	10 (13%)
36	LMG	d	410	-	51,51,55	0.89	3 (5%)	59,59,63	1.43	7 (11%)
30	CLA	D	406	-	65,73,73	1.41	11 (16%)	76,113,113	1.61	7 (9%)
30	CLA	11	304	25	45,53,73	1.72	8 (17%)	52,89,113	2.03	11 (21%)
41	A86	17	313	-	44,50,50	4.06	23 (52%)	51,76,76	7.82	19 (37%)
30	CLA	11	305	-	45,53,73	1.72	8 (17%)	52,89,113	1.72	7 (13%)
30	CLA	20	202	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	8 (10%)
41	A86	37	313	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
32	BCR	B	624	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	7 (12%)
30	CLA	13	303	-	45,53,73	1.69	10 (22%)	52,89,113	1.80	9 (17%)
41	A86	41	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.52	22 (43%)
30	CLA	21	301	28	65,73,73	1.48	8 (12%)	76,113,113	1.43	7 (9%)
30	CLA	13	304	-	65,73,73	1.41	10 (15%)	76,113,113	1.58	10 (13%)
30	CLA	d	407	-	65,73,73	1.40	11 (16%)	76,113,113	1.60	7 (9%)
41	A86	35	312	-	44,50,50	4.04	24 (54%)	51,76,76	7.81	20 (39%)
30	CLA	C	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.57	11 (14%)
30	CLA	38	311	25	45,53,73	1.82	9 (20%)	52,89,113	1.80	11 (21%)
30	CLA	15	305	-	45,53,73	1.76	6 (13%)	52,89,113	1.67	6 (11%)
41	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	32	312	25	45,53,73	1.76	11 (24%)	52,89,113	1.75	9 (17%)
30	CLA	37	307	25	45,53,73	1.80	9 (20%)	52,89,113	1.77	13 (25%)
30	CLA	m	101	12,36	65,73,73	1.42	11 (16%)	76,113,113	1.41	6 (7%)
41	A86	17	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	16	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	8 (10%)
30	CLA	34	302	25	65,73,73	1.46	10 (15%)	76,113,113	1.68	8 (10%)
30	CLA	20	204	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	10 (13%)
30	CLA	35	304	25	45,53,73	1.79	7 (15%)	52,89,113	1.78	9 (17%)
30	CLA	18	304	-	45,53,73	1.71	8 (17%)	52,89,113	1.82	8 (15%)
30	CLA	C	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	12 (15%)
30	CLA	18	305	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	7 (9%)
38	DGD	C	517	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
35	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
41	A86	15	312	-	44,50,50	4.05	24 (54%)	51,76,76	7.82	19 (37%)
33	SQD	b	620	-	36,37,54	1.20	7 (19%)	45,48,65	1.64	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	A86	17	312	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
41	A86	37	312	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
41	A86	11	314	-	44,50,50	3.92	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	14	310	-	45,53,73	1.75	9 (20%)	52,89,113	1.67	8 (15%)
35	LHG	d	409	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	12	307	-	65,73,73	1.43	10 (15%)	76,113,113	1.59	10 (13%)
41	A86	18	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.34	17 (33%)
35	LHG	b	621	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
41	A86	15	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	c	513	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	8 (10%)
30	CLA	16	308	25	45,53,73	1.78	9 (20%)	52,89,113	1.72	11 (21%)
30	CLA	b	610	-	65,73,73	1.51	11 (16%)	76,113,113	1.50	8 (10%)
41	A86	34	311	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
32	BCR	Y	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.47	9 (16%)
41	A86	38	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
38	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
30	CLA	13	306	-	45,53,73	1.70	8 (17%)	52,89,113	1.70	7 (13%)
41	A86	14	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.96	18 (35%)
32	BCR	c	520	-	41,41,41	1.28	3 (7%)	56,56,56	1.46	10 (17%)
30	CLA	c	522	-	65,73,73	1.42	11 (16%)	76,113,113	1.48	8 (10%)
36	LMG	32	301	30	39,39,55	1.00	4 (10%)	47,47,63	1.18	4 (8%)
41	A86	12	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	18	307	-	45,53,73	1.75	6 (13%)	52,89,113	1.63	8 (15%)
32	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	4 (7%)
41	A86	14	311	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
41	A86	15	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
41	A86	39	310	-	44,50,50	4.09	22 (50%)	51,76,76	7.17	19 (37%)
30	CLA	17	307	25	45,53,73	1.80	9 (20%)	52,89,113	1.76	13 (25%)
30	CLA	31	302	-	45,53,73	1.67	11 (24%)	52,89,113	1.81	9 (17%)
33	SQD	a	405	-	53,54,54	0.96	5 (9%)	62,65,65	1.58	11 (17%)
35	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	C	502	-	65,73,73	1.39	11 (16%)	76,113,113	1.65	12 (15%)
30	CLA	c	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.66	12 (15%)
30	CLA	12	305	25	65,73,73	1.46	9 (13%)	76,113,113	1.68	8 (10%)
30	CLA	41	307	-	65,73,73	1.44	6 (9%)	76,113,113	1.40	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	B	613	-	65,73,73	1.43	11 (16%)	76,113,113	1.61	10 (13%)
40	HEM	e	101	6,5	41,50,50	1.49	5 (12%)	45,82,82	1.26	5 (11%)
30	CLA	12	309	-	45,53,73	1.69	7 (15%)	52,89,113	1.70	7 (13%)
41	A86	21	311	-	44,50,50	3.90	23 (52%)	51,76,76	7.51	15 (29%)
41	A86	32	317	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	c	524	30	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
30	CLA	36	308	25	45,53,73	1.78	9 (20%)	52,89,113	1.72	11 (21%)
30	CLA	20	209	30	65,73,73	1.47	8 (12%)	76,113,113	1.44	9 (11%)
30	CLA	w	102	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	10 (13%)
30	CLA	C	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.65	9 (11%)
30	CLA	34	304	-	65,73,73	1.42	11 (16%)	76,113,113	1.59	10 (13%)
32	BCR	A	405	-	41,41,41	1.28	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	c	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	12 (15%)
30	CLA	15	304	25	45,53,73	1.79	7 (15%)	52,89,113	1.80	9 (17%)
30	CLA	35	303	-	65,73,73	1.42	7 (10%)	76,113,113	1.54	10 (13%)
30	CLA	W	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	7 (9%)
32	BCR	C	518	-	41,41,41	1.28	2 (4%)	56,56,56	1.36	6 (10%)
41	A86	21	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.51	22 (43%)
36	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
30	CLA	20	206	27	45,53,73	1.71	9 (20%)	52,89,113	1.80	10 (19%)
30	CLA	35	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
30	CLA	19	304	26	45,53,73	1.71	8 (17%)	52,89,113	1.82	11 (21%)
30	CLA	37	304	-	45,53,73	1.70	11 (24%)	52,89,113	1.82	9 (17%)
30	CLA	39	308	-	45,53,73	1.69	7 (15%)	52,89,113	1.79	9 (17%)
41	A86	31	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
30	CLA	34	303	-	45,53,73	1.66	11 (24%)	52,89,113	1.81	9 (17%)
30	CLA	17	308	25	65,73,73	1.48	10 (15%)	76,113,113	1.53	11 (14%)
41	A86	16	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
32	BCR	m	103	-	41,41,41	1.30	2 (4%)	56,56,56	1.39	8 (14%)
41	A86	12	318	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	15	301	25	65,73,73	1.48	9 (13%)	76,113,113	1.57	10 (13%)
30	CLA	41	304	-	45,53,73	1.68	8 (17%)	52,89,113	1.65	6 (11%)
41	A86	20	213	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
41	A86	35	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
41	A86	13	301	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	A86	39	309	-	44,50,50	3.88	23 (52%)	51,76,76	7.69	16 (31%)
38	DGD	c	517	-	63,63,67	1.06	8 (12%)	77,77,81	1.60	15 (19%)
30	CLA	b	603	-	65,73,73	1.44	11 (16%)	76,113,113	1.64	12 (15%)
30	CLA	19	302	-	45,53,73	1.65	9 (20%)	52,89,113	1.89	10 (19%)
41	A86	41	311	-	44,50,50	3.89	23 (52%)	51,76,76	7.51	15 (29%)
30	CLA	15	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
41	A86	12	315	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	D	401	-	65,73,73	1.50	12 (18%)	76,113,113	1.53	10 (13%)
30	CLA	15	309	-	45,53,73	1.75	9 (20%)	52,89,113	1.60	7 (13%)
30	CLA	37	303	25	65,73,73	1.49	10 (15%)	76,113,113	1.58	8 (10%)
32	BCR	h	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	7 (12%)
30	CLA	11	303	-	65,73,73	1.41	10 (15%)	76,113,113	1.59	10 (13%)
37	OEX	C	501	3,1	0,15,15	-	-	-		
30	CLA	20	205	-	45,53,73	1.74	10 (22%)	52,89,113	1.80	9 (17%)
30	CLA	12	313	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	9 (17%)
30	CLA	18	310	25	65,73,73	1.46	10 (15%)	76,113,113	1.38	8 (10%)
30	CLA	39	302	-	45,53,73	1.67	9 (20%)	52,89,113	1.89	10 (19%)
32	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
30	CLA	13	302	25	65,73,73	1.46	10 (15%)	76,113,113	1.68	8 (10%)
41	A86	32	315	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
41	A86	21	312	-	44,50,50	3.82	22 (50%)	51,76,76	7.17	21 (41%)
38	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	7 (9%)
31	PHO	A	403	-	51,69,69	1.24	9 (17%)	47,99,99	1.31	8 (17%)
30	CLA	14	309	25	45,53,73	1.76	11 (24%)	52,89,113	1.75	9 (17%)
41	A86	17	314	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	37	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	b	615	-	65,73,73	1.52	12 (18%)	76,113,113	1.44	11 (14%)
30	CLA	z	101	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	35	306	25	45,53,73	1.77	7 (15%)	52,89,113	1.79	9 (17%)
30	CLA	40	202	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
30	CLA	C	520	-	65,73,73	1.41	11 (16%)	76,113,113	1.49	8 (10%)
30	CLA	c	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.58	12 (15%)
30	CLA	14	307	25	45,53,73	1.75	8 (17%)	52,89,113	1.81	8 (15%)
41	A86	13	317	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	18 (35%)
41	A86	17	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	A86	13	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	12	303	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
41	A86	12	317	-	44,50,50	4.04	22 (50%)	51,76,76	7.80	19 (37%)
32	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	11	309	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	7 (13%)
41	A86	34	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	31	306	25	45,53,73	1.74	10 (22%)	52,89,113	1.84	9 (17%)
30	CLA	18	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
32	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
30	CLA	W	102	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	10 (13%)
30	CLA	C	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.68	12 (15%)
30	CLA	Z	102	30,19	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
41	A86	15	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.93	18 (35%)
30	CLA	17	306	25	45,53,73	1.71	7 (15%)	52,89,113	1.96	10 (19%)
34	BCT	a	406	29,1	2,3,3	1.26	0	2,3,3	3.95	2 (100%)
30	CLA	16	302	25	65,73,73	1.48	9 (13%)	76,113,113	1.86	16 (21%)
30	CLA	b	613	-	65,73,73	1.42	11 (16%)	76,113,113	1.64	9 (11%)
30	CLA	41	303	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	7 (9%)
30	CLA	21	306	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
41	A86	18	314	-	44,50,50	3.98	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	40	203	30	45,53,73	1.78	9 (20%)	52,89,113	1.71	9 (17%)
30	CLA	C	519	-	65,73,73	1.46	11 (16%)	76,113,113	1.47	7 (9%)
30	CLA	C	513	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	8 (10%)
41	A86	11	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.83	20 (39%)
41	A86	35	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	19 (37%)
30	CLA	33	305	-	65,73,73	1.41	11 (16%)	76,113,113	1.61	10 (13%)
30	CLA	15	306	25	45,53,73	1.77	8 (17%)	52,89,113	1.79	9 (17%)
41	A86	13	313	-	44,50,50	4.05	24 (54%)	51,76,76	7.81	19 (37%)
30	CLA	16	307	25	45,53,73	1.76	10 (22%)	52,89,113	1.96	7 (13%)
41	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
41	A86	41	314	-	44,50,50	4.00	23 (52%)	51,76,76	7.82	18 (35%)
41	A86	13	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	40	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.74	10 (19%)
30	CLA	c	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.68	11 (14%)
41	A86	39	311	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	C	510	-	65,73,73	1.48	12 (18%)	76,113,113	1.72	10 (13%)
41	A86	32	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	21 (41%)
30	CLA	32	308	36,25	45,53,73	1.72	8 (17%)	52,89,113	2.06	14 (26%)
30	CLA	M	101	12,36	65,73,73	1.42	10 (15%)	76,113,113	1.41	6 (7%)
30	CLA	c	512	3	65,73,73	1.51	10 (15%)	76,113,113	1.60	12 (15%)
30	CLA	14	305	25	45,53,73	1.70	8 (17%)	52,89,113	2.06	11 (21%)
30	CLA	36	306	25	45,53,73	1.74	9 (20%)	52,89,113	1.78	8 (15%)
30	CLA	21	308	-	45,53,73	1.75	6 (13%)	52,89,113	1.64	7 (13%)
30	CLA	21	302	-	45,53,73	1.74	7 (15%)	52,89,113	1.73	10 (19%)
30	CLA	d	402	-	65,73,73	1.45	11 (16%)	76,113,113	1.50	8 (10%)
31	PHO	d	403	-	51,69,69	1.23	8 (15%)	47,99,99	1.31	8 (17%)
41	A86	18	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
37	OEX	c	501	3,1	0,15,15	-	-	-		
41	A86	38	314	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	40	209	30	65,73,73	1.47	10 (15%)	76,113,113	1.44	9 (11%)
30	CLA	21	307	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	7 (9%)
35	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	33	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.69	8 (10%)
30	CLA	41	306	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
30	CLA	39	304	26	45,53,73	1.70	8 (17%)	52,89,113	1.82	11 (21%)
30	CLA	14	302	25	65,73,73	1.44	8 (12%)	76,113,113	1.68	9 (11%)
30	CLA	36	304	-	65,73,73	1.43	10 (15%)	76,113,113	1.48	8 (10%)
30	CLA	c	504	-	65,73,73	1.47	11 (16%)	76,113,113	1.51	10 (13%)
30	CLA	36	305	25	45,53,73	1.69	9 (20%)	52,89,113	1.91	10 (19%)
30	CLA	38	308	25	45,53,73	1.78	7 (15%)	52,89,113	1.72	8 (15%)
41	A86	31	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	B	610	-	65,73,73	1.50	11 (16%)	76,113,113	1.51	8 (10%)
41	A86	37	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	34	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
30	CLA	11	315	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	B	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	10 (13%)
41	A86	16	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
41	A86	34	312	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
41	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
41	A86	34	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	18	301	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	11 (14%)
30	CLA	38	305	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	7 (9%)
41	A86	15	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	33	310	25	45,53,73	1.74	11 (24%)	52,89,113	1.77	9 (17%)
32	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.40	9 (16%)
30	CLA	39	307	-	45,53,73	1.68	9 (20%)	52,89,113	1.79	7 (13%)
30	CLA	36	303	-	45,53,73	1.68	8 (17%)	52,89,113	2.02	11 (21%)
38	DGD	C	516	-	63,63,67	1.06	7 (11%)	77,77,81	1.60	15 (19%)
30	CLA	17	304	-	45,53,73	1.70	11 (24%)	52,89,113	1.83	9 (17%)
30	CLA	37	301	-	65,73,73	1.44	10 (15%)	76,113,113	1.48	10 (13%)
41	A86	33	316	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	11	301	25	65,73,73	1.45	8 (12%)	76,113,113	1.67	9 (11%)
30	CLA	33	304	-	45,53,73	1.67	11 (24%)	52,89,113	1.81	9 (17%)
30	CLA	18	311	25	45,53,73	1.83	9 (20%)	52,89,113	1.81	11 (21%)
41	A86	37	302	-	44,50,50	3.95	23 (52%)	51,76,76	8.11	21 (41%)
30	CLA	41	301	28	65,73,73	1.48	8 (12%)	76,113,113	1.43	7 (9%)
41	A86	32	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	B	612	-	65,73,73	1.50	9 (13%)	76,113,113	1.78	10 (13%)
30	CLA	d	401	-	65,73,73	1.49	12 (18%)	76,113,113	1.52	9 (11%)
39	PL9	d	408	-	55,55,55	2.33	14 (25%)	68,69,69	1.49	15 (22%)
30	CLA	12	314	-	45,53,73	1.74	9 (20%)	52,89,113	1.66	8 (15%)
30	CLA	19	307	-	45,53,73	1.69	8 (17%)	52,89,113	1.79	7 (13%)
41	A86	35	313	-	44,50,50	4.03	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	11	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.55	10 (13%)
30	CLA	b	604	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	15 (19%)
30	CLA	34	306	-	45,53,73	1.70	9 (20%)	52,89,113	1.69	7 (13%)
30	CLA	31	315	-	65,73,73	1.47	9 (13%)	76,113,113	1.50	8 (10%)
36	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
30	CLA	39	303	-	65,73,73	1.45	10 (15%)	76,113,113	1.55	9 (11%)
30	CLA	13	307	25	45,53,73	1.75	7 (15%)	52,89,113	1.82	7 (13%)
30	CLA	b	612	-	65,73,73	1.50	10 (15%)	76,113,113	1.77	10 (13%)
30	CLA	21	305	28	45,53,73	1.75	6 (13%)	52,89,113	1.79	8 (15%)
30	CLA	33	309	25	65,73,73	1.48	10 (15%)	76,113,113	1.54	10 (13%)
30	CLA	35	308	25	45,53,73	1.77	10 (22%)	52,89,113	1.75	10 (19%)
36	LMG	B	620	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	31	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.77	9 (17%)
41	A86	31	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
41	A86	40	213	-	44,50,50	4.02	23 (52%)	51,76,76	7.83	18 (35%)
30	CLA	c	514	30	65,73,73	1.40	9 (13%)	76,113,113	1.62	8 (10%)
30	CLA	39	306	-	45,53,73	1.71	11 (24%)	52,89,113	1.61	7 (13%)
30	CLA	14	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	8 (10%)
30	CLA	34	305	25	45,53,73	1.72	9 (20%)	52,89,113	2.07	14 (26%)
30	CLA	17	310	-	45,53,73	1.75	8 (17%)	52,89,113	1.68	9 (17%)
36	LMG	Q	301	-	51,51,55	0.97	4 (7%)	59,59,63	1.46	9 (15%)
41	A86	33	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	c	510	-	65,73,73	1.49	12 (18%)	76,113,113	1.73	10 (13%)
41	A86	17	302	-	44,50,50	3.94	23 (52%)	51,76,76	8.11	21 (41%)
30	CLA	B	603	-	65,73,73	1.41	11 (16%)	76,113,113	1.64	12 (15%)
30	CLA	18	306	25	45,53,73	1.75	7 (15%)	52,89,113	1.85	8 (15%)
41	A86	32	316	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	36	309	-	45,53,73	1.76	10 (22%)	52,89,113	1.61	9 (17%)
30	CLA	c	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.64	9 (11%)
41	A86	16	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	16	309	-	45,53,73	1.75	10 (22%)	52,89,113	1.61	9 (17%)
41	A86	36	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
30	CLA	32	305	25	65,73,73	1.47	10 (15%)	76,113,113	1.68	8 (10%)
30	CLA	12	306	42	45,53,73	1.69	11 (24%)	52,89,113	1.79	9 (17%)
30	CLA	18	312	-	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
30	CLA	D	405	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	11 (14%)
30	CLA	34	310	-	45,53,73	1.74	8 (17%)	52,89,113	1.67	7 (13%)
32	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	9 (16%)
41	A86	35	315	-	44,50,50	4.00	23 (52%)	51,76,76	7.59	20 (39%)
30	CLA	17	303	25	65,73,73	1.48	10 (15%)	76,113,113	1.58	8 (10%)
41	A86	20	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.31	17 (33%)
30	CLA	31	305	-	45,53,73	1.69	8 (17%)	52,89,113	1.70	7 (13%)
30	CLA	A	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.62	9 (11%)
41	A86	36	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.95	17 (33%)
30	CLA	w	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
30	CLA	38	307	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	8 (15%)
30	CLA	38	309	25	65,73,73	1.52	8 (12%)	76,113,113	1.61	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	C	507	-	65,73,73	1.52	11 (16%)	76,113,113	1.55	11 (14%)
30	CLA	b	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.54	12 (15%)
30	CLA	b	622	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)
30	CLA	20	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.73	10 (19%)
30	CLA	40	206	27	45,53,73	1.71	9 (20%)	52,89,113	1.78	10 (19%)
41	A86	12	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
30	CLA	11	302	-	45,53,73	1.69	11 (24%)	52,89,113	1.80	9 (17%)
30	CLA	32	310	25	45,53,73	1.75	9 (20%)	52,89,113	1.84	9 (17%)
30	CLA	33	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.50	8 (10%)
41	A86	19	309	-	44,50,50	3.89	23 (52%)	51,76,76	7.70	16 (31%)
30	CLA	B	623	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	14 (18%)
41	A86	31	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	18	308	25	45,53,73	1.78	7 (15%)	52,89,113	1.72	8 (15%)
36	LMG	b	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)
30	CLA	13	305	25	45,53,73	1.72	8 (17%)	52,89,113	2.02	11 (21%)
41	A86	36	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	a	403	-	65,73,73	1.48	11 (16%)	76,113,113	1.52	10 (13%)

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
30	CLA	b	608	-	1/1/15/20	8/37/115/115	-
30	CLA	32	303	-	1/1/15/20	10/37/115/115	-
41	A86	11	311	-	-	3/34/90/90	0/3/3/3
30	CLA	34	307	25	1/1/11/20	8/13/91/115	-
30	CLA	34	309	25	-	6/13/91/115	-
30	CLA	32	309	-	1/1/11/20	8/13/91/115	-
30	CLA	35	302	-	1/1/11/20	8/13/91/115	-
30	CLA	32	307	-	1/1/15/20	13/37/115/115	-
41	A86	40	210	-	-	14/34/90/90	0/3/3/3
30	CLA	a	402	-	1/1/15/20	7/37/115/115	-
41	A86	16	313	-	-	7/34/90/90	0/3/3/3
30	CLA	A	404	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	609	-	1/1/15/20	8/37/115/115	-
41	A86	21	314	-	-	12/34/90/90	0/3/3/3
35	LHG	a	407	-	-	23/50/50/53	-
35	LHG	l	102	-	-	22/53/53/53	-
41	A86	38	315	-	-	10/34/90/90	0/3/3/3
30	CLA	36	307	25	1/1/11/20	9/13/91/115	-
30	CLA	12	310	25	1/1/11/20	8/13/91/115	-
41	A86	35	311	-	-	3/34/90/90	0/3/3/3
41	A86	37	311	-	-	13/34/90/90	0/3/3/3
30	CLA	19	305	-	1/1/11/20	7/13/91/115	-
32	BCR	a	408	-	-	9/29/63/63	0/2/2/2
41	A86	21	310	-	-	9/34/90/90	0/3/3/3
30	CLA	B	601	-	1/1/15/20	18/37/115/115	-
33	SQD	B	621	-	-	9/32/52/69	0/1/1/1
30	CLA	B	615	-	1/1/15/20	13/37/115/115	-
30	CLA	38	303	25	1/1/15/20	14/37/115/115	-
30	CLA	40	204	-	1/1/15/20	13/37/115/115	-
30	CLA	20	208	-	-	8/13/91/115	-
30	CLA	b	606	-	1/1/15/20	7/37/115/115	-
30	CLA	c	523	-	1/1/15/20	14/37/115/115	-
30	CLA	39	301	-	-	12/37/115/115	-
41	A86	13	311	-	-	8/34/90/90	0/3/3/3
30	CLA	14	303	-	1/1/11/20	5/13/91/115	-
30	CLA	39	305	-	1/1/11/20	7/13/91/115	-
41	A86	35	316	-	-	16/34/90/90	0/3/3/3
30	CLA	17	301	-	1/1/15/20	14/37/115/115	-
30	CLA	d	406	-	1/1/15/20	8/37/115/115	-
32	BCR	B	617	-	-	9/29/63/63	0/2/2/2
32	BCR	H	101	-	-	7/29/63/63	0/2/2/2
41	A86	33	302	-	-	15/34/90/90	0/3/3/3
35	LHG	L	102	-	-	22/53/53/53	-
30	CLA	35	305	-	1/1/11/20	8/13/91/115	-
30	CLA	37	310	-	1/1/11/20	7/13/91/115	-
41	A86	20	211	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	14	314	-	-	10/34/90/90	0/3/3/3
36	LMG	m	102	30	-	10/35/55/70	0/1/1/1
32	BCR	c	516	-	-	10/29/63/63	0/2/2/2
30	CLA	15	308	25	1/1/11/20	6/13/91/115	-
30	CLA	13	310	-	1/1/11/20	6/13/91/115	-
41	A86	15	316	-	-	16/34/90/90	0/3/3/3
30	CLA	B	611	-	1/1/15/20	12/37/115/115	-
30	CLA	13	309	25	-	6/13/91/115	-
40	HEM	v	201	16	-	0/12/54/54	-
30	CLA	c	507	-	1/1/15/20	17/37/115/115	-
41	A86	32	318	-	-	7/34/90/90	0/3/3/3
36	LMG	w	101	-	-	28/46/66/70	0/1/1/1
30	CLA	31	309	-	1/1/11/20	5/13/91/115	-
38	DGD	c	518	-	-	22/51/91/95	0/2/2/2
36	LMG	B	619	-	-	18/46/66/70	0/1/1/1
41	A86	33	313	-	-	3/34/90/90	0/3/3/3
30	CLA	c	502	-	1/1/15/20	14/37/115/115	-
38	DGD	H	102	-	-	24/51/91/95	0/2/2/2
30	CLA	32	311	25	1/1/15/20	14/37/115/115	-
39	PL9	d	405	4	-	17/53/73/73	0/1/1/1
30	CLA	19	303	-	1/1/15/20	15/37/115/115	-
30	CLA	16	305	25	-	8/13/91/115	-
36	LMG	12	301	30	-	17/34/54/70	0/1/1/1
30	CLA	C	514	30	1/1/15/20	13/37/115/115	-
30	CLA	B	608	-	1/1/15/20	8/37/115/115	-
36	LMG	b	619	-	-	20/46/66/70	0/1/1/1
30	CLA	16	306	25	1/1/11/20	7/13/91/115	-
41	A86	13	316	-	-	16/34/90/90	0/3/3/3
30	CLA	41	302	-	-	7/13/91/115	-
30	CLA	14	306	-	1/1/11/20	8/13/91/115	-
41	A86	17	311	-	-	13/34/90/90	0/3/3/3
30	CLA	21	304	-	1/1/11/20	8/13/91/115	-
30	CLA	B	602	-	1/1/15/20	13/37/115/115	-
36	LMG	M	102	30	-	10/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	31	313	-	-	10/34/90/90	0/3/3/3
41	A86	33	312	-	-	8/34/90/90	0/3/3/3
30	CLA	17	305	-	1/1/15/20	19/37/115/115	-
41	A86	13	315	-	-	7/34/90/90	0/3/3/3
33	SQD	L	103	-	-	21/49/69/69	0/1/1/1
41	A86	40	201	-	-	12/34/90/90	0/3/3/3
30	CLA	16	304	-	1/1/15/20	15/37/115/115	-
41	A86	11	316	-	-	15/34/90/90	0/3/3/3
30	CLA	B	606	-	1/1/15/20	7/37/115/115	-
30	CLA	14	304	-	1/1/15/20	13/37/115/115	-
30	CLA	B	614	-	1/1/15/20	8/37/115/115	-
30	CLA	37	305	-	1/1/15/20	19/37/115/115	-
40	HEM	V	201	16	-	0/12/54/54	-
30	CLA	B	604	-	1/1/15/20	14/37/115/115	-
32	BCR	c	521	-	-	8/29/63/63	0/2/2/2
30	CLA	21	303	-	1/1/15/20	17/37/115/115	-
31	PHO	d	404	-	-	8/37/103/103	0/5/6/6
30	CLA	38	310	25	1/1/15/20	10/37/115/115	-
30	CLA	41	305	28	1/1/11/20	9/13/91/115	-
30	CLA	19	306	-	1/1/11/20	8/13/91/115	-
30	CLA	37	306	25	-	8/13/91/115	-
41	A86	38	313	-	-	8/34/90/90	0/3/3/3
33	SQD	A	406	-	-	14/49/69/69	0/1/1/1
41	A86	14	313	-	-	8/34/90/90	0/3/3/3
30	CLA	16	303	-	1/1/11/20	6/13/91/115	-
30	CLA	12	312	-	1/1/15/20	11/37/115/115	-
30	CLA	b	614	-	1/1/15/20	8/37/115/115	-
30	CLA	38	304	-	1/1/11/20	5/13/91/115	-
32	BCR	a	404	-	-	12/29/63/63	0/2/2/2
30	CLA	17	309	25	1/1/11/20	4/13/91/115	-
30	CLA	15	302	-	1/1/11/20	8/13/91/115	-
30	CLA	35	309	-	1/1/11/20	4/13/91/115	-
41	A86	19	310	-	-	17/34/90/90	0/3/3/3
42	LMU	12	302	30	-	7/18/58/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PL9	D	404	4	-	17/53/73/73	0/1/1/1
30	CLA	b	605	-	1/1/15/20	17/37/115/115	-
30	CLA	33	306	25	1/1/11/20	10/13/91/115	-
41	A86	18	315	-	-	10/34/90/90	0/3/3/3
30	CLA	C	504	-	1/1/15/20	17/37/115/115	-
30	CLA	12	311	25	1/1/15/20	14/37/115/115	-
41	A86	33	317	-	-	7/34/90/90	0/3/3/3
42	LMU	32	302	-	-	7/18/58/61	0/2/2/2
30	CLA	32	306	-	1/1/11/20	4/13/91/115	-
30	CLA	38	301	-	1/1/15/20	11/37/115/115	-
38	DGD	J	101	-	-	15/51/91/95	0/2/2/2
39	PL9	D	407	-	-	13/53/73/73	0/1/1/1
30	CLA	D	402	-	1/1/15/20	13/37/115/115	-
30	CLA	36	302	25	1/1/15/20	15/37/115/115	-
32	BCR	B	618	-	-	9/29/63/63	0/2/2/2
41	A86	20	201	-	-	12/34/90/90	0/3/3/3
32	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
33	SQD	l	101	-	-	21/49/69/69	0/1/1/1
30	CLA	b	601	-	1/1/15/20	18/37/115/115	-
31	PHO	D	403	-	-	8/37/103/103	0/5/6/6
30	CLA	13	308	25	1/1/15/20	14/37/115/115	-
30	CLA	37	309	25	1/1/11/20	4/13/91/115	-
30	CLA	12	308	36,25	1/1/11/20	9/13/91/115	-
30	CLA	38	312	-	1/1/11/20	4/13/91/115	-
30	CLA	B	607	-	1/1/15/20	12/37/115/115	-
30	CLA	34	308	25	1/1/15/20	14/37/115/115	-
30	CLA	21	309	-	1/1/11/20	6/13/91/115	-
30	CLA	33	308	25	1/1/11/20	8/13/91/115	-
36	LMG	c	519	-	-	22/46/66/70	0/1/1/1
30	CLA	C	505	-	1/1/15/20	17/37/115/115	-
30	CLA	C	506	-	1/1/15/20	16/37/115/115	-
41	A86	20	212	-	-	11/34/90/90	0/3/3/3
30	CLA	b	607	-	1/1/15/20	12/37/115/115	-
30	CLA	C	512	3	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	37	315	-	-	13/34/90/90	0/3/3/3
30	CLA	31	304	25	1/1/11/20	10/13/91/115	-
30	CLA	33	307	-	1/1/11/20	8/13/91/115	-
41	A86	40	211	-	-	8/34/90/90	0/3/3/3
30	CLA	33	311	-	1/1/11/20	5/13/91/115	-
30	CLA	19	308	-	1/1/11/20	8/13/91/115	-
30	CLA	37	308	25	1/1/15/20	17/37/115/115	-
30	CLA	11	308	25	-	6/13/91/115	-
30	CLA	b	611	-	1/1/15/20	12/37/115/115	-
30	CLA	36	301	-	1/1/15/20	10/37/115/115	-
30	CLA	41	308	-	1/1/11/20	8/13/91/115	-
30	CLA	C	521	-	1/1/15/20	14/37/115/115	-
41	A86	40	212	-	-	11/34/90/90	0/3/3/3
30	CLA	35	301	25	1/1/15/20	10/37/115/115	-
30	CLA	19	301	-	-	12/37/115/115	-
40	HEM	E	101	6,5	-	7/12/54/54	-
41	A86	33	314	-	-	9/34/90/90	0/3/3/3
30	CLA	38	306	25	-	9/13/91/115	-
32	BCR	B	616	-	-	8/29/63/63	0/2/2/2
30	CLA	c	506	-	1/1/15/20	16/37/115/115	-
30	CLA	31	301	25	1/1/15/20	12/37/115/115	-
30	CLA	40	208	-	-	8/13/91/115	-
41	A86	32	314	-	-	8/34/90/90	0/3/3/3
41	A86	15	315	-	-	15/34/90/90	0/3/3/3
30	CLA	18	309	25	1/1/15/20	16/37/115/115	-
30	CLA	31	303	-	1/1/15/20	13/37/115/115	-
30	CLA	11	306	25	1/1/11/20	8/13/91/115	-
32	BCR	c	515	-	-	15/29/63/63	0/2/2/2
41	A86	41	312	-	-	7/34/90/90	0/3/3/3
30	CLA	15	303	-	1/1/15/20	15/37/115/115	-
41	A86	36	311	-	-	3/34/90/90	0/3/3/3
30	CLA	41	309	-	1/1/11/20	6/13/91/115	-
30	CLA	31	307	25	1/1/15/20	14/37/115/115	-
30	CLA	32	313	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	b	616	-	-	9/29/63/63	0/2/2/2
41	A86	31	314	-	-	7/34/90/90	0/3/3/3
41	A86	19	311	-	-	8/34/90/90	0/3/3/3
30	CLA	40	205	-	-	9/13/91/115	-
41	A86	41	310	-	-	9/34/90/90	0/3/3/3
30	CLA	B	605	-	1/1/15/20	17/37/115/115	-
30	CLA	20	203	30	1/1/11/20	5/13/91/115	-
30	CLA	14	308	25	1/1/15/20	14/37/115/115	-
36	LMG	d	410	-	-	14/46/66/70	0/1/1/1
30	CLA	D	406	-	1/1/15/20	4/37/115/115	-
30	CLA	11	304	25	1/1/11/20	9/13/91/115	-
41	A86	17	313	-	-	8/34/90/90	0/3/3/3
30	CLA	11	305	-	1/1/11/20	8/13/91/115	-
30	CLA	20	202	-	-	19/37/115/115	-
41	A86	37	313	-	-	9/34/90/90	0/3/3/3
32	BCR	B	624	-	-	18/29/63/63	0/2/2/2
30	CLA	13	303	-	1/1/11/20	5/13/91/115	-
41	A86	41	313	-	-	16/34/90/90	0/3/3/3
30	CLA	21	301	28	-	14/37/115/115	-
30	CLA	13	304	-	1/1/15/20	13/37/115/115	-
30	CLA	d	407	-	1/1/15/20	4/37/115/115	-
41	A86	35	312	-	-	9/34/90/90	0/3/3/3
30	CLA	C	511	-	1/1/15/20	12/37/115/115	-
30	CLA	38	311	25	1/1/11/20	8/13/91/115	-
30	CLA	15	305	-	1/1/11/20	8/13/91/115	-
41	A86	11	313	-	-	10/34/90/90	0/3/3/3
30	CLA	32	312	25	-	6/13/91/115	-
30	CLA	37	307	25	1/1/11/20	7/13/91/115	-
30	CLA	m	101	12,36	1/1/15/20	19/37/115/115	-
41	A86	17	316	-	-	7/34/90/90	0/3/3/3
30	CLA	16	301	-	1/1/15/20	10/37/115/115	-
30	CLA	34	302	25	1/1/15/20	12/37/115/115	-
30	CLA	20	204	-	1/1/15/20	13/37/115/115	-
30	CLA	35	304	25	-	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	18	304	-	1/1/11/20	5/13/91/115	-
30	CLA	C	503	-	1/1/15/20	11/37/115/115	-
30	CLA	18	305	-	1/1/15/20	19/37/115/115	-
38	DGD	C	517	-	-	22/51/91/95	0/2/2/2
35	LHG	A	408	-	-	23/50/50/53	-
41	A86	15	312	-	-	8/34/90/90	0/3/3/3
33	SQD	b	620	-	-	9/32/52/69	0/1/1/1
41	A86	17	312	-	-	3/34/90/90	0/3/3/3
41	A86	37	312	-	-	3/34/90/90	0/3/3/3
41	A86	11	314	-	-	7/34/90/90	0/3/3/3
30	CLA	14	310	-	1/1/11/20	6/13/91/115	-
35	LHG	d	409	-	-	29/53/53/53	-
30	CLA	12	307	-	1/1/15/20	13/37/115/115	-
41	A86	18	313	-	-	8/34/90/90	0/3/3/3
35	LHG	b	621	-	-	20/53/53/53	-
41	A86	15	310	-	-	8/34/90/90	0/3/3/3
30	CLA	c	513	-	1/1/15/20	16/37/115/115	-
30	CLA	16	308	25	-	7/13/91/115	-
30	CLA	b	610	-	1/1/15/20	14/37/115/115	-
41	A86	34	311	-	-	8/34/90/90	0/3/3/3
32	BCR	Y	101	-	-	16/29/63/63	0/2/2/2
41	A86	38	302	-	-	15/34/90/90	0/3/3/3
38	DGD	j	101	-	-	15/51/91/95	0/2/2/2
30	CLA	13	306	-	1/1/11/20	8/13/91/115	-
41	A86	14	312	-	-	3/34/90/90	0/3/3/3
32	BCR	c	520	-	-	16/29/63/63	0/2/2/2
30	CLA	c	522	-	1/1/15/20	15/37/115/115	-
36	LMG	32	301	30	-	14/34/54/70	0/1/1/1
41	A86	12	316	-	-	3/34/90/90	0/3/3/3
30	CLA	18	307	-	1/1/11/20	6/13/91/115	-
32	BCR	A	409	-	-	9/29/63/63	0/2/2/2
41	A86	14	311	-	-	8/34/90/90	0/3/3/3
41	A86	15	313	-	-	10/34/90/90	0/3/3/3
41	A86	39	310	-	-	17/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	17	307	25	1/1/11/20	8/13/91/115	-
30	CLA	31	302	-	1/1/11/20	4/13/91/115	-
33	SQD	a	405	-	-	14/49/69/69	0/1/1/1
35	LHG	B	622	-	-	20/53/53/53	-
30	CLA	C	502	-	1/1/15/20	14/37/115/115	-
30	CLA	c	508	-	1/1/15/20	18/37/115/115	-
30	CLA	12	305	25	1/1/15/20	11/37/115/115	-
30	CLA	41	307	-	1/1/15/20	11/37/115/115	-
30	CLA	B	613	-	1/1/15/20	8/37/115/115	-
40	HEM	e	101	6,5	-	7/12/54/54	-
30	CLA	12	309	-	1/1/11/20	8/13/91/115	-
41	A86	21	311	-	-	8/34/90/90	0/3/3/3
41	A86	32	317	-	-	10/34/90/90	0/3/3/3
30	CLA	c	524	30	1/1/15/20	15/37/115/115	-
30	CLA	36	308	25	-	7/13/91/115	-
30	CLA	20	209	30	1/1/15/20	11/37/115/115	-
30	CLA	w	102	-	1/1/15/20	14/37/115/115	-
30	CLA	C	509	-	1/1/15/20	12/37/115/115	-
30	CLA	34	304	-	1/1/15/20	13/37/115/115	-
32	BCR	A	405	-	-	12/29/63/63	0/2/2/2
30	CLA	c	503	-	1/1/15/20	11/37/115/115	-
30	CLA	15	304	25	-	7/13/91/115	-
30	CLA	35	303	-	1/1/15/20	15/37/115/115	-
30	CLA	W	103	-	-	19/37/115/115	-
32	BCR	C	518	-	-	8/29/63/63	0/2/2/2
41	A86	21	313	-	-	16/34/90/90	0/3/3/3
36	LMG	D	408	-	-	14/46/66/70	0/1/1/1
30	CLA	20	206	27	1/1/11/20	7/13/91/115	-
30	CLA	35	307	25	1/1/15/20	11/37/115/115	-
30	CLA	19	304	26	1/1/11/20	9/13/91/115	-
30	CLA	37	304	-	-	6/13/91/115	-
30	CLA	39	308	-	1/1/11/20	8/13/91/115	-
41	A86	31	312	-	-	8/34/90/90	0/3/3/3
30	CLA	34	303	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	17	308	25	1/1/15/20	17/37/115/115	-
41	A86	16	310	-	-	12/34/90/90	0/3/3/3
32	BCR	m	103	-	-	8/29/63/63	0/2/2/2
41	A86	12	318	-	-	10/34/90/90	0/3/3/3
30	CLA	15	301	25	1/1/15/20	10/37/115/115	-
30	CLA	41	304	-	1/1/11/20	8/13/91/115	-
41	A86	20	213	-	-	12/34/90/90	0/3/3/3
41	A86	35	310	-	-	8/34/90/90	0/3/3/3
41	A86	13	301	-	-	15/34/90/90	0/3/3/3
41	A86	39	309	-	-	11/34/90/90	0/3/3/3
38	DGD	c	517	-	-	19/51/91/95	0/2/2/2
30	CLA	b	603	-	1/1/15/20	10/37/115/115	-
30	CLA	19	302	-	1/1/11/20	4/13/91/115	-
41	A86	41	311	-	-	8/34/90/90	0/3/3/3
30	CLA	15	307	25	1/1/15/20	11/37/115/115	-
41	A86	12	315	-	-	8/34/90/90	0/3/3/3
30	CLA	D	401	-	1/1/15/20	12/37/115/115	-
30	CLA	15	309	-	1/1/11/20	4/13/91/115	-
30	CLA	37	303	25	1/1/15/20	13/37/115/115	-
32	BCR	h	101	-	-	7/29/63/63	0/2/2/2
30	CLA	11	303	-	1/1/15/20	13/37/115/115	-
30	CLA	20	205	-	-	9/13/91/115	-
30	CLA	12	313	25	-	6/13/91/115	-
30	CLA	18	310	25	1/1/15/20	10/37/115/115	-
30	CLA	39	302	-	1/1/11/20	4/13/91/115	-
32	BCR	F	101	-	-	15/29/63/63	0/2/2/2
30	CLA	13	302	25	1/1/15/20	11/37/115/115	-
41	A86	32	315	-	-	3/34/90/90	0/3/3/3
41	A86	21	312	-	-	7/34/90/90	0/3/3/3
38	DGD	h	102	-	-	24/51/91/95	0/2/2/2
31	PHO	A	403	-	-	12/37/103/103	0/5/6/6
30	CLA	14	309	25	-	6/13/91/115	-
41	A86	17	314	-	-	10/34/90/90	0/3/3/3
41	A86	37	314	-	-	10/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	615	-	1/1/15/20	13/37/115/115	-
30	CLA	z	101	-	-	21/37/115/115	-
30	CLA	35	306	25	1/1/11/20	8/13/91/115	-
30	CLA	40	202	-	-	19/37/115/115	-
30	CLA	C	520	-	1/1/15/20	15/37/115/115	-
30	CLA	c	511	-	1/1/15/20	12/37/115/115	-
30	CLA	14	307	25	1/1/11/20	8/13/91/115	-
41	A86	13	317	-	-	7/34/90/90	0/3/3/3
41	A86	17	315	-	-	13/34/90/90	0/3/3/3
41	A86	13	314	-	-	10/34/90/90	0/3/3/3
30	CLA	12	303	-	1/1/15/20	11/37/115/115	-
41	A86	12	317	-	-	9/34/90/90	0/3/3/3
32	BCR	b	617	-	-	9/29/63/63	0/2/2/2
30	CLA	11	309	-	1/1/11/20	6/13/91/115	-
41	A86	34	314	-	-	10/34/90/90	0/3/3/3
30	CLA	31	306	25	1/1/11/20	8/13/91/115	-
30	CLA	18	303	25	1/1/15/20	14/37/115/115	-
32	BCR	b	623	-	-	18/29/63/63	0/2/2/2
30	CLA	W	102	-	1/1/15/20	14/37/115/115	-
30	CLA	C	508	-	1/1/15/20	18/37/115/115	-
30	CLA	Z	102	30,19	1/1/15/20	16/37/115/115	-
41	A86	15	311	-	-	3/34/90/90	0/3/3/3
30	CLA	17	306	25	-	8/13/91/115	-
30	CLA	16	302	25	1/1/15/20	15/37/115/115	-
30	CLA	b	613	-	1/1/15/20	8/37/115/115	-
30	CLA	41	303	-	1/1/15/20	17/37/115/115	-
30	CLA	21	306	-	1/1/15/20	14/37/115/115	-
41	A86	18	314	-	-	3/34/90/90	0/3/3/3
30	CLA	40	203	30	1/1/11/20	5/13/91/115	-
30	CLA	C	519	-	-	21/37/115/115	-
30	CLA	C	513	-	1/1/15/20	16/37/115/115	-
41	A86	11	312	-	-	8/34/90/90	0/3/3/3
41	A86	35	314	-	-	7/34/90/90	0/3/3/3
30	CLA	33	305	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	15	306	25	1/1/11/20	8/13/91/115	-
41	A86	13	313	-	-	8/34/90/90	0/3/3/3
30	CLA	16	307	25	1/1/11/20	9/13/91/115	-
41	A86	12	304	-	-	16/34/90/90	0/3/3/3
41	A86	41	314	-	-	12/34/90/90	0/3/3/3
41	A86	13	312	-	-	3/34/90/90	0/3/3/3
30	CLA	40	207	-	1/1/11/20	7/13/91/115	-
30	CLA	c	505	-	1/1/15/20	17/37/115/115	-
41	A86	39	311	-	-	8/34/90/90	0/3/3/3
30	CLA	C	510	-	1/1/15/20	12/37/115/115	-
41	A86	32	304	-	-	16/34/90/90	0/3/3/3
30	CLA	32	308	36,25	1/1/11/20	10/13/91/115	-
30	CLA	M	101	12,36	1/1/15/20	19/37/115/115	-
30	CLA	c	512	3	1/1/15/20	8/37/115/115	-
30	CLA	14	305	25	1/1/11/20	9/13/91/115	-
30	CLA	36	306	25	1/1/11/20	7/13/91/115	-
30	CLA	21	308	-	1/1/11/20	8/13/91/115	-
30	CLA	21	302	-	-	7/13/91/115	-
30	CLA	d	402	-	1/1/15/20	13/37/115/115	-
31	PHO	d	403	-	-	12/37/103/103	0/5/6/6
41	A86	18	302	-	-	15/34/90/90	0/3/3/3
41	A86	38	314	-	-	3/34/90/90	0/3/3/3
30	CLA	40	209	30	1/1/15/20	11/37/115/115	-
30	CLA	21	307	-	1/1/15/20	11/37/115/115	-
35	LHG	L	101	-	-	29/53/53/53	-
30	CLA	33	303	25	1/1/15/20	12/37/115/115	-
30	CLA	41	306	-	1/1/15/20	14/37/115/115	-
30	CLA	39	304	26	1/1/11/20	9/13/91/115	-
30	CLA	14	302	25	1/1/15/20	11/37/115/115	-
30	CLA	36	304	-	1/1/15/20	15/37/115/115	-
30	CLA	c	504	-	1/1/15/20	17/37/115/115	-
30	CLA	36	305	25	-	8/13/91/115	-
30	CLA	38	308	25	1/1/11/20	8/13/91/115	-
41	A86	31	310	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	610	-	1/1/15/20	14/37/115/115	-
41	A86	37	316	-	-	7/34/90/90	0/3/3/3
30	CLA	34	301	-	1/1/15/20	10/37/115/115	-
30	CLA	11	315	-	1/1/15/20	11/37/115/115	-
30	CLA	B	609	-	1/1/15/20	8/37/115/115	-
41	A86	16	311	-	-	3/34/90/90	0/3/3/3
41	A86	34	312	-	-	3/34/90/90	0/3/3/3
41	A86	11	310	-	-	8/34/90/90	0/3/3/3
41	A86	34	313	-	-	9/34/90/90	0/3/3/3
30	CLA	18	301	-	1/1/15/20	11/37/115/115	-
30	CLA	38	305	-	1/1/15/20	19/37/115/115	-
41	A86	15	314	-	-	7/34/90/90	0/3/3/3
30	CLA	33	310	25	-	6/13/91/115	-
32	BCR	C	515	-	-	10/29/63/63	0/2/2/2
30	CLA	39	307	-	1/1/11/20	3/13/91/115	-
30	CLA	36	303	-	1/1/11/20	6/13/91/115	-
38	DGD	C	516	-	-	19/51/91/95	0/2/2/2
30	CLA	37	301	-	1/1/15/20	14/37/115/115	-
30	CLA	17	304	-	-	6/13/91/115	-
41	A86	33	316	-	-	16/34/90/90	0/3/3/3
30	CLA	11	301	25	1/1/15/20	11/37/115/115	-
30	CLA	33	304	-	1/1/11/20	4/13/91/115	-
30	CLA	18	311	25	1/1/11/20	8/13/91/115	-
41	A86	37	302	-	-	16/34/90/90	1/3/3/3
30	CLA	41	301	28	-	14/37/115/115	-
41	A86	32	319	-	-	7/34/90/90	0/3/3/3
30	CLA	B	612	-	1/1/15/20	13/37/115/115	-
30	CLA	d	401	-	1/1/15/20	12/37/115/115	-
39	PL9	d	408	-	-	13/53/73/73	0/1/1/1
30	CLA	12	314	-	1/1/11/20	6/13/91/115	-
30	CLA	19	307	-	1/1/11/20	3/13/91/115	-
41	A86	35	313	-	-	10/34/90/90	0/3/3/3
30	CLA	11	307	25	1/1/15/20	14/37/115/115	-
30	CLA	b	604	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	34	306	-	1/1/11/20	8/13/91/115	-
30	CLA	31	315	-	1/1/15/20	10/37/115/115	-
36	LMG	W	101	-	-	28/46/66/70	0/1/1/1
30	CLA	39	303	-	1/1/15/20	15/37/115/115	-
30	CLA	13	307	25	1/1/11/20	8/13/91/115	-
30	CLA	b	612	-	1/1/15/20	13/37/115/115	-
30	CLA	21	305	28	1/1/11/20	9/13/91/115	-
30	CLA	33	309	25	1/1/15/20	14/37/115/115	-
30	CLA	35	308	25	1/1/11/20	6/13/91/115	-
36	LMG	B	620	-	-	20/46/66/70	0/1/1/1
30	CLA	31	308	25	-	6/13/91/115	-
41	A86	31	316	-	-	16/34/90/90	0/3/3/3
41	A86	40	213	-	-	12/34/90/90	0/3/3/3
30	CLA	c	514	30	1/1/15/20	13/37/115/115	-
30	CLA	39	306	-	1/1/11/20	8/13/91/115	-
30	CLA	14	301	-	1/1/15/20	11/37/115/115	-
30	CLA	34	305	25	1/1/11/20	9/13/91/115	-
30	CLA	17	310	-	1/1/11/20	7/13/91/115	-
36	LMG	Q	301	-	-	22/46/66/70	0/1/1/1
41	A86	33	315	-	-	10/34/90/90	0/3/3/3
30	CLA	c	510	-	1/1/15/20	12/37/115/115	-
41	A86	17	302	-	-	16/34/90/90	1/3/3/3
30	CLA	B	603	-	1/1/15/20	10/37/115/115	-
30	CLA	18	306	25	-	9/13/91/115	-
41	A86	32	316	-	-	9/34/90/90	0/3/3/3
30	CLA	36	309	-	1/1/11/20	5/13/91/115	-
30	CLA	c	509	-	1/1/15/20	12/37/115/115	-
41	A86	16	312	-	-	8/34/90/90	0/3/3/3
30	CLA	16	309	-	1/1/11/20	5/13/91/115	-
41	A86	36	310	-	-	12/34/90/90	0/3/3/3
30	CLA	32	305	25	1/1/15/20	12/37/115/115	-
30	CLA	12	306	42	1/1/11/20	4/13/91/115	-
30	CLA	18	312	-	1/1/11/20	4/13/91/115	-
30	CLA	D	405	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	34	310	-	1/1/11/20	5/13/91/115	-
32	BCR	f	101	-	-	15/29/63/63	0/2/2/2
41	A86	35	315	-	-	15/34/90/90	0/3/3/3
30	CLA	17	303	25	1/1/15/20	13/37/115/115	-
41	A86	20	210	-	-	14/34/90/90	0/3/3/3
30	CLA	31	305	-	1/1/11/20	8/13/91/115	-
30	CLA	A	402	-	1/1/15/20	7/37/115/115	-
41	A86	36	313	-	-	7/34/90/90	0/3/3/3
30	CLA	w	103	-	-	19/37/115/115	-
30	CLA	38	307	-	1/1/11/20	6/13/91/115	-
30	CLA	38	309	25	1/1/15/20	16/37/115/115	-
30	CLA	C	507	-	1/1/15/20	17/37/115/115	-
30	CLA	b	602	-	1/1/15/20	13/37/115/115	-
30	CLA	b	622	-	1/1/15/20	15/37/115/115	-
30	CLA	20	207	-	1/1/11/20	7/13/91/115	-
30	CLA	40	206	27	1/1/11/20	7/13/91/115	-
41	A86	12	319	-	-	7/34/90/90	0/3/3/3
30	CLA	11	302	-	1/1/11/20	5/13/91/115	-
30	CLA	32	310	25	1/1/11/20	8/13/91/115	-
30	CLA	33	301	-	1/1/15/20	10/37/115/115	-
41	A86	19	309	-	-	11/34/90/90	0/3/3/3
30	CLA	B	623	-	1/1/15/20	15/37/115/115	-
41	A86	31	311	-	-	3/34/90/90	0/3/3/3
30	CLA	18	308	25	1/1/11/20	8/13/91/115	-
36	LMG	b	618	-	-	18/46/66/70	0/1/1/1
30	CLA	13	305	25	1/1/11/20	9/13/91/115	-
41	A86	36	312	-	-	8/34/90/90	0/3/3/3
30	CLA	a	403	-	1/1/15/20	10/37/115/115	-

All (5718) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	39	310	A86	C14-C13	14.36	1.68	1.51
41	19	310	A86	C14-C13	14.29	1.68	1.51
41	11	313	A86	C14-C13	14.11	1.68	1.51
41	12	318	A86	C14-C13	14.10	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	33	315	A86	C14-C13	14.10	1.68	1.51
41	32	317	A86	C14-C13	14.06	1.68	1.51
41	31	313	A86	C14-C13	14.05	1.68	1.51
41	13	314	A86	C14-C13	14.05	1.68	1.51
41	38	315	A86	C14-C13	14.05	1.68	1.51
41	35	313	A86	C14-C13	14.05	1.68	1.51
41	15	313	A86	C14-C13	14.01	1.68	1.51
41	14	314	A86	C14-C13	14.00	1.68	1.51
41	18	315	A86	C14-C13	13.98	1.68	1.51
41	17	314	A86	C14-C13	13.96	1.68	1.51
41	20	212	A86	C14-C13	13.96	1.68	1.51
41	36	312	A86	C14-C13	13.96	1.68	1.51
41	40	212	A86	C14-C13	13.95	1.68	1.51
41	13	313	A86	C14-C13	13.94	1.68	1.51
41	37	314	A86	C14-C13	13.94	1.68	1.51
41	34	314	A86	C14-C13	13.93	1.68	1.51
41	17	313	A86	C14-C13	13.93	1.68	1.51
41	37	313	A86	C14-C13	13.93	1.68	1.51
41	12	317	A86	C14-C13	13.93	1.68	1.51
41	35	314	A86	C14-C13	13.93	1.68	1.51
41	15	312	A86	C14-C13	13.92	1.68	1.51
41	33	314	A86	C14-C13	13.92	1.68	1.51
41	13	317	A86	C14-C13	13.92	1.68	1.51
41	16	312	A86	C14-C13	13.91	1.68	1.51
41	12	319	A86	C14-C13	13.90	1.68	1.51
41	34	313	A86	C14-C13	13.90	1.68	1.51
41	32	316	A86	C14-C13	13.90	1.68	1.51
41	14	313	A86	C14-C13	13.87	1.68	1.51
41	36	313	A86	C14-C13	13.87	1.68	1.51
41	13	315	A86	C14-C13	13.87	1.68	1.51
41	35	312	A86	C14-C13	13.87	1.68	1.51
41	16	313	A86	C14-C13	13.87	1.68	1.51
41	15	314	A86	C14-C13	13.86	1.68	1.51
41	37	316	A86	C14-C13	13.85	1.68	1.51
41	17	316	A86	C14-C13	13.85	1.68	1.51
41	31	314	A86	C14-C13	13.85	1.68	1.51
41	32	319	A86	C14-C13	13.84	1.68	1.51
41	11	312	A86	C14-C13	13.84	1.68	1.51
41	31	312	A86	C14-C13	13.83	1.67	1.51
41	14	311	A86	C14-C13	13.83	1.67	1.51
41	31	310	A86	C14-C13	13.80	1.67	1.51
41	32	318	A86	C14-C13	13.80	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	34	311	A86	C14-C13	13.79	1.67	1.51
41	35	310	A86	C14-C13	13.78	1.67	1.51
41	33	317	A86	C14-C13	13.78	1.67	1.51
41	33	316	A86	C14-C13	13.78	1.67	1.51
41	12	315	A86	C14-C13	13.78	1.67	1.51
41	33	312	A86	C14-C13	13.77	1.67	1.51
41	13	311	A86	C14-C13	13.77	1.67	1.51
41	32	315	A86	C14-C13	13.77	1.67	1.51
41	40	210	A86	C14-C13	13.77	1.67	1.51
41	18	302	A86	C14-C13	13.76	1.67	1.51
41	11	314	A86	C14-C13	13.76	1.67	1.51
41	11	310	A86	C14-C13	13.75	1.67	1.51
41	38	302	A86	C14-C13	13.75	1.67	1.51
41	18	313	A86	C14-C13	13.75	1.67	1.51
41	38	313	A86	C14-C13	13.75	1.67	1.51
41	32	314	A86	C14-C13	13.74	1.67	1.51
41	13	301	A86	C14-C13	13.72	1.67	1.51
41	15	310	A86	C14-C13	13.72	1.67	1.51
41	13	316	A86	C14-C13	13.72	1.67	1.51
41	15	315	A86	C14-C13	13.72	1.67	1.51
41	18	314	A86	C14-C13	13.72	1.67	1.51
41	38	314	A86	C14-C13	13.72	1.67	1.51
41	36	311	A86	C14-C13	13.71	1.67	1.51
41	12	304	A86	C14-C13	13.71	1.67	1.51
41	33	302	A86	C14-C13	13.70	1.67	1.51
41	31	316	A86	C14-C13	13.70	1.67	1.51
41	32	304	A86	C14-C13	13.70	1.67	1.51
41	11	316	A86	C14-C13	13.69	1.67	1.51
41	37	312	A86	C14-C13	13.68	1.67	1.51
41	15	316	A86	C14-C13	13.68	1.67	1.51
41	35	315	A86	C14-C13	13.68	1.67	1.51
41	17	312	A86	C14-C13	13.68	1.67	1.51
41	20	210	A86	C14-C13	13.67	1.67	1.51
41	13	312	A86	C14-C13	13.66	1.67	1.51
41	17	315	A86	C14-C13	13.66	1.67	1.51
41	37	315	A86	C14-C13	13.66	1.67	1.51
41	12	316	A86	C14-C13	13.65	1.67	1.51
41	16	311	A86	C14-C13	13.65	1.67	1.51
41	35	316	A86	C14-C13	13.65	1.67	1.51
41	14	312	A86	C14-C13	13.64	1.67	1.51
41	31	311	A86	C14-C13	13.63	1.67	1.51
41	35	311	A86	C14-C13	13.62	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	33	313	A86	C14-C13	13.62	1.67	1.51
41	40	213	A86	C14-C13	13.59	1.67	1.51
41	34	312	A86	C14-C13	13.58	1.67	1.51
41	21	314	A86	C14-C13	13.57	1.67	1.51
41	11	311	A86	C14-C13	13.56	1.67	1.51
41	15	311	A86	C14-C13	13.53	1.67	1.51
41	20	213	A86	C14-C13	13.53	1.67	1.51
41	41	314	A86	C14-C13	13.46	1.67	1.51
41	36	310	A86	C14-C13	13.44	1.67	1.51
41	16	310	A86	C14-C13	13.39	1.67	1.51
41	17	311	A86	C14-C13	13.34	1.67	1.51
41	37	311	A86	C14-C13	13.33	1.67	1.51
41	19	311	A86	C14-C13	13.20	1.67	1.51
41	39	311	A86	C14-C13	13.20	1.67	1.51
41	37	302	A86	C14-C13	13.09	1.67	1.51
41	21	311	A86	C14-C13	13.08	1.67	1.51
41	17	302	A86	C14-C13	13.03	1.67	1.51
41	41	311	A86	C14-C13	13.01	1.67	1.51
41	40	211	A86	C14-C13	12.97	1.66	1.51
41	41	312	A86	C14-C13	12.96	1.66	1.51
41	19	309	A86	C14-C13	12.96	1.66	1.51
41	21	313	A86	C14-C13	12.93	1.66	1.51
41	20	211	A86	C14-C13	12.91	1.66	1.51
41	21	312	A86	C14-C13	12.91	1.66	1.51
41	41	313	A86	C14-C13	12.89	1.66	1.51
41	39	309	A86	C14-C13	12.89	1.66	1.51
41	41	310	A86	C14-C13	12.80	1.66	1.51
41	21	310	A86	C14-C13	12.73	1.66	1.51
41	40	201	A86	C14-C13	11.41	1.65	1.51
41	20	201	A86	C14-C13	11.40	1.65	1.51
41	40	212	A86	C30-C29	9.27	1.47	1.32
41	39	310	A86	C30-C29	9.25	1.47	1.32
41	19	310	A86	C30-C29	9.22	1.47	1.32
41	20	212	A86	C30-C29	9.18	1.47	1.32
41	39	311	A86	C30-C29	8.93	1.46	1.32
41	35	315	A86	C30-C29	8.93	1.46	1.32
41	19	311	A86	C30-C29	8.92	1.46	1.32
41	11	316	A86	C30-C29	8.91	1.46	1.32
41	35	316	A86	C30-C29	8.90	1.46	1.32
41	15	315	A86	C30-C29	8.89	1.46	1.32
41	32	304	A86	C30-C29	8.88	1.46	1.32
41	15	316	A86	C30-C29	8.88	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	18	302	A86	C30-C29	8.88	1.46	1.32
41	13	301	A86	C30-C29	8.87	1.46	1.32
41	33	302	A86	C30-C29	8.87	1.46	1.32
41	31	316	A86	C30-C29	8.87	1.46	1.32
41	33	316	A86	C30-C29	8.87	1.46	1.32
41	12	304	A86	C30-C29	8.84	1.46	1.32
41	38	302	A86	C30-C29	8.81	1.46	1.32
41	41	310	A86	C30-C29	8.81	1.46	1.32
41	13	316	A86	C30-C29	8.81	1.46	1.32
41	40	201	A86	C30-C29	8.79	1.46	1.32
41	21	310	A86	C30-C29	8.79	1.46	1.32
41	17	315	A86	C30-C29	8.79	1.46	1.32
41	20	201	A86	C30-C29	8.79	1.46	1.32
41	17	311	A86	C30-C29	8.76	1.46	1.32
41	40	210	A86	C30-C29	8.75	1.46	1.32
41	37	312	A86	C30-C29	8.75	1.46	1.32
41	36	312	A86	C30-C29	8.75	1.46	1.32
41	20	210	A86	C30-C29	8.74	1.46	1.32
41	37	315	A86	C30-C29	8.73	1.46	1.32
41	15	312	A86	C30-C29	8.73	1.46	1.32
41	17	312	A86	C30-C29	8.72	1.46	1.32
41	17	302	A86	C30-C29	8.72	1.46	1.32
41	33	313	A86	C30-C29	8.72	1.46	1.32
41	21	313	A86	C30-C29	8.72	1.46	1.32
41	37	311	A86	C30-C29	8.72	1.46	1.32
41	41	313	A86	C30-C29	8.72	1.46	1.32
41	37	302	A86	C30-C29	8.71	1.46	1.32
41	14	313	A86	C30-C29	8.70	1.46	1.32
41	20	213	A86	C30-C29	8.70	1.46	1.32
41	40	213	A86	C30-C29	8.70	1.46	1.32
41	12	317	A86	C30-C29	8.70	1.46	1.32
41	16	312	A86	C30-C29	8.70	1.46	1.32
41	32	316	A86	C30-C29	8.69	1.46	1.32
41	37	313	A86	C30-C29	8.69	1.46	1.32
41	38	314	A86	C30-C29	8.68	1.46	1.32
41	11	312	A86	C30-C29	8.68	1.46	1.32
41	21	314	A86	C30-C29	8.68	1.46	1.32
41	13	312	A86	C30-C29	8.68	1.46	1.32
41	31	312	A86	C30-C29	8.68	1.46	1.32
41	15	311	A86	C30-C29	8.68	1.46	1.32
41	11	311	A86	C30-C29	8.68	1.46	1.32
41	18	314	A86	C30-C29	8.68	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	14	312	A86	C30-C29	8.67	1.46	1.32
41	35	311	A86	C30-C29	8.66	1.46	1.32
41	34	313	A86	C30-C29	8.66	1.46	1.32
41	31	311	A86	C30-C29	8.66	1.46	1.32
41	17	313	A86	C30-C29	8.66	1.46	1.32
41	40	211	A86	C30-C29	8.66	1.46	1.32
41	35	312	A86	C30-C29	8.65	1.46	1.32
41	20	211	A86	C30-C29	8.64	1.46	1.32
41	35	313	A86	C30-C29	8.63	1.46	1.32
41	32	315	A86	C30-C29	8.63	1.46	1.32
41	12	316	A86	C30-C29	8.62	1.46	1.32
41	13	313	A86	C30-C29	8.62	1.46	1.32
41	18	315	A86	C30-C29	8.62	1.46	1.32
41	41	314	A86	C30-C29	8.62	1.46	1.32
41	36	311	A86	C30-C29	8.61	1.46	1.32
41	33	314	A86	C30-C29	8.61	1.46	1.32
41	34	312	A86	C30-C29	8.60	1.46	1.32
41	32	317	A86	C30-C29	8.59	1.46	1.32
41	37	314	A86	C30-C29	8.59	1.46	1.32
41	33	315	A86	C30-C29	8.58	1.46	1.32
41	38	315	A86	C30-C29	8.58	1.46	1.32
41	16	310	A86	C30-C29	8.58	1.46	1.32
41	21	311	A86	C30-C29	8.57	1.46	1.32
41	17	314	A86	C30-C29	8.57	1.46	1.32
41	41	311	A86	C30-C29	8.57	1.46	1.32
41	36	310	A86	C30-C29	8.56	1.46	1.32
41	14	311	A86	C30-C29	8.56	1.46	1.32
41	15	313	A86	C30-C29	8.56	1.46	1.32
41	18	313	A86	C30-C29	8.55	1.46	1.32
41	16	311	A86	C30-C29	8.55	1.46	1.32
41	34	314	A86	C30-C29	8.55	1.46	1.32
41	12	318	A86	C30-C29	8.54	1.46	1.32
41	34	311	A86	C30-C29	8.53	1.46	1.32
41	38	313	A86	C30-C29	8.52	1.46	1.32
41	31	313	A86	C30-C29	8.52	1.46	1.32
41	39	309	A86	C30-C29	8.52	1.46	1.32
41	14	314	A86	C30-C29	8.51	1.46	1.32
41	13	314	A86	C30-C29	8.50	1.46	1.32
41	19	309	A86	C30-C29	8.50	1.46	1.32
41	11	310	A86	C30-C29	8.50	1.46	1.32
41	11	313	A86	C30-C29	8.50	1.46	1.32
41	12	315	A86	C30-C29	8.49	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	314	A86	C30-C29	8.48	1.46	1.32
41	31	310	A86	C30-C29	8.47	1.46	1.32
41	15	310	A86	C30-C29	8.47	1.46	1.32
41	33	312	A86	C30-C29	8.45	1.46	1.32
41	35	310	A86	C30-C29	8.45	1.46	1.32
41	13	311	A86	C30-C29	8.44	1.46	1.32
41	37	316	A86	C30-C29	8.41	1.46	1.32
41	17	316	A86	C30-C29	8.39	1.45	1.32
41	13	317	A86	C30-C29	8.36	1.45	1.32
41	31	314	A86	C30-C29	8.34	1.45	1.32
41	13	315	A86	C30-C29	8.34	1.45	1.32
41	32	318	A86	C30-C29	8.33	1.45	1.32
41	11	314	A86	C30-C29	8.31	1.45	1.32
41	41	312	A86	C30-C29	8.31	1.45	1.32
41	36	313	A86	C30-C29	8.31	1.45	1.32
41	15	314	A86	C30-C29	8.29	1.45	1.32
41	16	313	A86	C30-C29	8.29	1.45	1.32
41	32	319	A86	C30-C29	8.29	1.45	1.32
41	33	317	A86	C30-C29	8.29	1.45	1.32
41	35	314	A86	C30-C29	8.28	1.45	1.32
41	12	319	A86	C30-C29	8.28	1.45	1.32
41	21	312	A86	C30-C29	8.26	1.45	1.32
39	D	407	PL9	C7-C3	-7.78	1.43	1.51
41	40	201	A86	C4-C5	7.73	1.67	1.43
41	20	201	A86	C4-C5	7.72	1.67	1.43
30	18	311	CLA	C4B-NB	7.64	1.42	1.35
30	21	309	CLA	C4B-NB	7.63	1.42	1.35
41	40	201	A86	C8-C6	7.62	1.62	1.45
41	20	201	A86	C8-C6	7.62	1.62	1.45
41	20	212	A86	C4-C5	7.58	1.66	1.43
30	35	304	CLA	C4B-NB	7.58	1.42	1.35
30	38	311	CLA	C4B-NB	7.57	1.42	1.35
30	41	309	CLA	C4B-NB	7.56	1.42	1.35
39	d	408	PL9	C7-C3	-7.56	1.43	1.51
41	20	212	A86	C8-C6	7.55	1.62	1.45
41	39	310	A86	C4-C5	7.55	1.66	1.43
41	19	310	A86	C4-C5	7.55	1.66	1.43
41	40	212	A86	C4-C5	7.54	1.66	1.43
41	40	212	A86	C8-C6	7.54	1.62	1.45
41	20	210	A86	C4-C5	7.52	1.66	1.43
41	40	210	A86	C4-C5	7.52	1.66	1.43
41	13	301	A86	C4-C5	7.51	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	13	316	A86	C4-C5	7.51	1.66	1.43
30	15	304	CLA	C4B-NB	7.51	1.41	1.35
41	17	315	A86	C4-C5	7.50	1.66	1.43
41	37	315	A86	C4-C5	7.50	1.66	1.43
41	15	315	A86	C4-C5	7.50	1.66	1.43
41	15	316	A86	C4-C5	7.50	1.66	1.43
41	32	304	A86	C4-C5	7.49	1.66	1.43
41	39	311	A86	C4-C5	7.49	1.66	1.43
41	12	304	A86	C4-C5	7.49	1.66	1.43
41	33	316	A86	C4-C5	7.48	1.66	1.43
41	35	316	A86	C4-C5	7.48	1.66	1.43
41	35	315	A86	C4-C5	7.48	1.66	1.43
41	11	316	A86	C4-C5	7.47	1.66	1.43
41	33	302	A86	C4-C5	7.47	1.66	1.43
41	31	316	A86	C4-C5	7.47	1.66	1.43
41	38	302	A86	C4-C5	7.47	1.66	1.43
41	19	311	A86	C4-C5	7.46	1.66	1.43
41	12	304	A86	C8-C6	7.46	1.62	1.45
41	32	304	A86	C8-C6	7.45	1.62	1.45
41	18	302	A86	C4-C5	7.45	1.66	1.43
41	15	316	A86	C8-C6	7.44	1.61	1.45
41	36	312	A86	C4-C5	7.43	1.66	1.43
41	13	316	A86	C8-C6	7.43	1.61	1.45
41	11	316	A86	C8-C6	7.42	1.61	1.45
41	16	312	A86	C4-C5	7.42	1.66	1.43
41	17	302	A86	C4-C5	7.42	1.66	1.43
41	15	315	A86	C8-C6	7.42	1.61	1.45
41	13	313	A86	C4-C5	7.42	1.66	1.43
41	20	213	A86	C4-C5	7.42	1.66	1.43
41	38	302	A86	C8-C6	7.42	1.61	1.45
41	21	314	A86	C4-C5	7.41	1.66	1.43
41	41	314	A86	C4-C5	7.41	1.66	1.43
41	37	302	A86	C4-C5	7.40	1.66	1.43
41	35	316	A86	C8-C6	7.40	1.61	1.45
41	18	302	A86	C8-C6	7.40	1.61	1.45
41	33	316	A86	C8-C6	7.40	1.61	1.45
41	33	314	A86	C4-C5	7.40	1.66	1.43
41	34	313	A86	C4-C5	7.40	1.66	1.43
41	31	316	A86	C8-C6	7.39	1.61	1.45
41	35	312	A86	C4-C5	7.39	1.66	1.43
41	14	313	A86	C4-C5	7.39	1.66	1.43
41	35	315	A86	C8-C6	7.39	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	37	311	A86	C4-C5	7.39	1.66	1.43
41	15	312	A86	C4-C5	7.39	1.66	1.43
41	13	301	A86	C8-C6	7.39	1.61	1.45
41	17	313	A86	C4-C5	7.39	1.66	1.43
41	37	313	A86	C4-C5	7.39	1.66	1.43
41	40	213	A86	C4-C5	7.39	1.66	1.43
41	19	311	A86	C8-C6	7.38	1.61	1.45
41	32	316	A86	C4-C5	7.38	1.66	1.43
41	17	311	A86	C4-C5	7.37	1.66	1.43
41	33	302	A86	C8-C6	7.37	1.61	1.45
41	16	310	A86	C4-C5	7.37	1.66	1.43
41	39	311	A86	C8-C6	7.36	1.61	1.45
41	40	211	A86	C4-C5	7.36	1.66	1.43
41	11	312	A86	C4-C5	7.36	1.66	1.43
41	31	312	A86	C4-C5	7.36	1.66	1.43
30	w	103	CLA	C4B-NB	7.36	1.41	1.35
41	12	317	A86	C4-C5	7.36	1.66	1.43
41	37	315	A86	C8-C6	7.35	1.61	1.45
41	41	310	A86	C4-C5	7.35	1.66	1.43
41	12	319	A86	C4-C5	7.35	1.66	1.43
41	20	211	A86	C4-C5	7.35	1.66	1.43
41	36	310	A86	C4-C5	7.34	1.66	1.43
30	17	307	CLA	C4B-NB	7.34	1.41	1.35
41	41	311	A86	C4-C5	7.34	1.66	1.43
41	33	313	A86	C4-C5	7.34	1.66	1.43
41	17	315	A86	C8-C6	7.33	1.61	1.45
41	38	315	A86	C4-C5	7.33	1.66	1.43
41	21	311	A86	C4-C5	7.33	1.66	1.43
41	35	311	A86	C4-C5	7.33	1.66	1.43
41	15	311	A86	C4-C5	7.33	1.66	1.43
41	21	310	A86	C4-C5	7.32	1.66	1.43
41	37	314	A86	C4-C5	7.32	1.66	1.43
41	36	313	A86	C4-C5	7.32	1.66	1.43
41	17	302	A86	C8-C6	7.32	1.61	1.45
41	18	314	A86	C4-C5	7.32	1.66	1.43
41	19	309	A86	C4-C5	7.32	1.66	1.43
41	13	312	A86	C4-C5	7.31	1.66	1.43
30	34	307	CLA	C4B-NB	7.31	1.41	1.35
41	36	311	A86	C4-C5	7.31	1.66	1.43
41	16	313	A86	C4-C5	7.31	1.66	1.43
41	18	315	A86	C4-C5	7.31	1.66	1.43
41	37	302	A86	C8-C6	7.31	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	11	314	A86	C4-C5	7.31	1.66	1.43
41	32	319	A86	C4-C5	7.31	1.66	1.43
30	41	305	CLA	C4B-NB	7.31	1.41	1.35
41	33	315	A86	C4-C5	7.31	1.66	1.43
41	35	313	A86	C4-C5	7.31	1.66	1.43
41	31	311	A86	C4-C5	7.31	1.66	1.43
41	16	311	A86	C4-C5	7.31	1.66	1.43
41	17	314	A86	C4-C5	7.30	1.66	1.43
41	17	313	A86	C8-C6	7.30	1.61	1.45
41	32	318	A86	C4-C5	7.30	1.66	1.43
41	13	315	A86	C4-C5	7.30	1.66	1.43
41	31	314	A86	C4-C5	7.30	1.66	1.43
41	11	313	A86	C4-C5	7.30	1.66	1.43
41	31	313	A86	C4-C5	7.30	1.66	1.43
41	33	314	A86	C8-C6	7.30	1.61	1.45
41	34	314	A86	C4-C5	7.30	1.66	1.43
41	39	309	A86	C4-C5	7.30	1.66	1.43
41	15	314	A86	C4-C5	7.30	1.66	1.43
30	11	306	CLA	C4B-NB	7.29	1.41	1.35
41	14	314	A86	C4-C5	7.29	1.66	1.43
41	37	312	A86	C4-C5	7.29	1.66	1.43
41	18	313	A86	C4-C5	7.29	1.66	1.43
41	15	313	A86	C4-C5	7.29	1.66	1.43
41	38	314	A86	C4-C5	7.29	1.66	1.43
41	37	313	A86	C8-C6	7.29	1.61	1.45
41	13	314	A86	C4-C5	7.29	1.66	1.43
41	12	316	A86	C4-C5	7.29	1.66	1.43
41	35	314	A86	C4-C5	7.29	1.66	1.43
41	12	318	A86	C4-C5	7.29	1.66	1.43
41	21	313	A86	C4-C5	7.29	1.66	1.43
41	17	312	A86	C4-C5	7.28	1.66	1.43
41	34	313	A86	C8-C6	7.28	1.61	1.45
41	11	311	A86	C4-C5	7.28	1.66	1.43
30	35	305	CLA	C4B-NB	7.28	1.41	1.35
41	37	315	A86	C19-C20	7.28	1.62	1.52
41	37	311	A86	C8-C6	7.28	1.61	1.45
41	13	317	A86	C4-C5	7.28	1.66	1.43
41	32	316	A86	C8-C6	7.28	1.61	1.45
41	38	313	A86	C4-C5	7.27	1.66	1.43
41	15	312	A86	C8-C6	7.27	1.61	1.45
41	32	317	A86	C4-C5	7.27	1.66	1.43
41	32	315	A86	C4-C5	7.27	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	16	312	A86	C8-C6	7.27	1.61	1.45
41	14	312	A86	C4-C5	7.27	1.66	1.43
41	33	317	A86	C4-C5	7.27	1.66	1.43
41	11	312	A86	C8-C6	7.26	1.61	1.45
41	34	312	A86	C4-C5	7.26	1.65	1.43
41	11	310	A86	C4-C5	7.26	1.65	1.43
30	37	307	CLA	C4B-NB	7.26	1.41	1.35
41	15	310	A86	C4-C5	7.26	1.65	1.43
30	15	305	CLA	C4B-NB	7.26	1.41	1.35
30	12	310	CLA	C4B-NB	7.26	1.41	1.35
41	37	316	A86	C4-C5	7.25	1.65	1.43
41	17	311	A86	C8-C6	7.25	1.61	1.45
30	W	103	CLA	C4B-NB	7.25	1.41	1.35
30	14	307	CLA	C4B-NB	7.25	1.41	1.35
41	17	316	A86	C4-C5	7.25	1.65	1.43
41	41	313	A86	C4-C5	7.25	1.65	1.43
41	14	311	A86	C4-C5	7.25	1.65	1.43
30	21	305	CLA	C4B-NB	7.25	1.41	1.35
30	18	308	CLA	C4B-NB	7.25	1.41	1.35
30	21	301	CLA	C4B-NB	7.24	1.41	1.35
41	12	315	A86	C4-C5	7.24	1.65	1.43
30	35	306	CLA	C4B-NB	7.24	1.41	1.35
41	35	310	A86	C4-C5	7.24	1.65	1.43
41	35	312	A86	C8-C6	7.24	1.61	1.45
41	21	312	A86	C4-C5	7.24	1.65	1.43
41	31	310	A86	C4-C5	7.24	1.65	1.43
41	33	312	A86	C4-C5	7.24	1.65	1.43
41	34	311	A86	C4-C5	7.24	1.65	1.43
41	14	313	A86	C8-C6	7.24	1.61	1.45
41	17	315	A86	C19-C20	7.24	1.62	1.52
41	12	317	A86	C8-C6	7.24	1.61	1.45
41	39	310	A86	C8-C6	7.24	1.61	1.45
30	38	308	CLA	C4B-NB	7.23	1.41	1.35
41	13	313	A86	C8-C6	7.23	1.61	1.45
41	36	312	A86	C8-C6	7.23	1.61	1.45
41	20	210	A86	C8-C6	7.23	1.61	1.45
41	32	314	A86	C4-C5	7.22	1.65	1.43
41	13	311	A86	C4-C5	7.22	1.65	1.43
41	40	210	A86	C8-C6	7.22	1.61	1.45
41	41	312	A86	C4-C5	7.22	1.65	1.43
41	19	310	A86	C8-C6	7.21	1.61	1.45
30	B	606	CLA	C4B-NB	7.21	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	306	CLA	C4B-NB	7.21	1.41	1.35
30	13	307	CLA	C4B-NB	7.21	1.41	1.35
41	31	312	A86	C8-C6	7.21	1.61	1.45
30	20	203	CLA	C4B-NB	7.19	1.41	1.35
41	20	210	A86	C19-C20	7.19	1.62	1.52
30	18	306	CLA	C4B-NB	7.19	1.41	1.35
41	41	314	A86	C8-C6	7.18	1.61	1.45
41	18	315	A86	C19-C20	7.17	1.62	1.52
41	40	210	A86	C19-C20	7.17	1.62	1.52
41	15	313	A86	C8-C6	7.17	1.61	1.45
41	21	314	A86	C8-C6	7.17	1.61	1.45
30	41	301	CLA	C4B-NB	7.17	1.41	1.35
41	38	315	A86	C19-C20	7.17	1.62	1.52
41	40	213	A86	C8-C6	7.16	1.61	1.45
30	40	203	CLA	C4B-NB	7.16	1.41	1.35
41	34	314	A86	C8-C6	7.16	1.61	1.45
30	38	309	CLA	C4B-NB	7.16	1.41	1.35
41	38	315	A86	C8-C6	7.16	1.61	1.45
30	37	309	CLA	C4B-NB	7.15	1.41	1.35
30	18	309	CLA	C4B-NB	7.15	1.41	1.35
30	33	308	CLA	C4B-NB	7.14	1.41	1.35
41	33	315	A86	C19-C20	7.14	1.62	1.52
41	20	212	A86	C19-C20	7.14	1.62	1.52
41	14	314	A86	C8-C6	7.14	1.61	1.45
41	20	213	A86	C8-C6	7.13	1.61	1.45
30	21	307	CLA	C4B-NB	7.13	1.41	1.35
41	35	313	A86	C19-C20	7.13	1.62	1.52
41	40	212	A86	C19-C20	7.12	1.62	1.52
41	21	312	A86	C8-C6	7.12	1.61	1.45
41	18	315	A86	C8-C6	7.12	1.61	1.45
41	17	314	A86	C19-C20	7.12	1.62	1.52
41	12	318	A86	C19-C20	7.12	1.62	1.52
41	11	313	A86	C19-C20	7.11	1.62	1.52
30	35	301	CLA	C4B-NB	7.11	1.41	1.35
41	15	313	A86	C19-C20	7.11	1.62	1.52
41	17	314	A86	C8-C6	7.11	1.61	1.45
41	35	313	A86	C8-C6	7.11	1.61	1.45
41	13	314	A86	C19-C20	7.10	1.62	1.52
30	38	307	CLA	C4B-NB	7.10	1.41	1.35
41	33	315	A86	C8-C6	7.10	1.61	1.45
41	36	311	A86	C8-C6	7.09	1.61	1.45
41	17	311	A86	C19-C20	7.09	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	38	306	CLA	C4B-NB	7.09	1.41	1.35
41	37	314	A86	C8-C6	7.09	1.61	1.45
30	18	307	CLA	C4B-NB	7.09	1.41	1.35
41	31	313	A86	C8-C6	7.09	1.61	1.45
41	13	314	A86	C8-C6	7.09	1.61	1.45
41	14	314	A86	C19-C20	7.09	1.62	1.52
41	11	313	A86	C8-C6	7.09	1.61	1.45
41	41	312	A86	C8-C6	7.08	1.61	1.45
30	17	309	CLA	C4B-NB	7.08	1.41	1.35
30	41	307	CLA	C4B-NB	7.08	1.41	1.35
41	31	313	A86	C19-C20	7.08	1.62	1.52
41	12	318	A86	C8-C6	7.08	1.61	1.45
30	b	606	CLA	C4B-NB	7.08	1.41	1.35
41	41	313	A86	C8-C6	7.07	1.61	1.45
41	32	315	A86	C8-C6	7.07	1.61	1.45
41	16	311	A86	C8-C6	7.07	1.61	1.45
41	34	314	A86	C19-C20	7.06	1.62	1.52
41	37	311	A86	C19-C20	7.06	1.62	1.52
41	32	317	A86	C8-C6	7.06	1.61	1.45
41	32	317	A86	C19-C20	7.06	1.62	1.52
41	37	312	A86	C8-C6	7.05	1.61	1.45
30	41	308	CLA	C4B-NB	7.05	1.41	1.35
41	11	311	A86	C8-C6	7.05	1.61	1.45
41	13	312	A86	C8-C6	7.05	1.61	1.45
41	31	311	A86	C8-C6	7.05	1.61	1.45
30	21	308	CLA	C4B-NB	7.05	1.41	1.35
30	32	310	CLA	C4B-NB	7.04	1.41	1.35
41	17	312	A86	C8-C6	7.04	1.61	1.45
41	37	314	A86	C19-C20	7.04	1.62	1.52
39	d	408	PL9	C3-C4	-7.04	1.37	1.49
41	21	313	A86	C8-C6	7.04	1.61	1.45
41	33	313	A86	C8-C6	7.03	1.61	1.45
41	21	310	A86	C8-C6	7.03	1.61	1.45
30	15	302	CLA	C4B-NB	7.03	1.41	1.35
41	14	312	A86	C8-C6	7.03	1.61	1.45
41	34	312	A86	C8-C6	7.03	1.61	1.45
30	16	308	CLA	C4B-NB	7.03	1.41	1.35
41	16	310	A86	C8-C6	7.02	1.61	1.45
41	15	311	A86	C8-C6	7.02	1.61	1.45
41	12	316	A86	C8-C6	7.02	1.61	1.45
30	36	308	CLA	C4B-NB	7.02	1.41	1.35
41	36	310	A86	C8-C6	7.01	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	31	306	CLA	C4B-NB	7.01	1.41	1.35
41	36	313	A86	C8-C6	7.00	1.61	1.45
41	41	310	A86	C8-C6	7.00	1.61	1.45
41	35	311	A86	C8-C6	7.00	1.61	1.45
30	15	301	CLA	C4B-NB	7.00	1.41	1.35
30	13	310	CLA	C4B-NB	7.00	1.41	1.35
41	16	313	A86	C8-C6	7.00	1.61	1.45
30	35	302	CLA	C4B-NB	6.99	1.41	1.35
41	33	317	A86	C8-C6	6.99	1.61	1.45
30	35	308	CLA	C4B-NB	6.99	1.41	1.35
41	35	314	A86	C8-C6	6.99	1.61	1.45
30	Z	102	CLA	C4B-NB	6.99	1.41	1.35
41	13	317	A86	C8-C6	6.98	1.60	1.45
41	12	319	A86	C8-C6	6.98	1.60	1.45
41	11	314	A86	C8-C6	6.98	1.60	1.45
41	15	314	A86	C8-C6	6.98	1.60	1.45
30	38	305	CLA	C4B-NB	6.98	1.41	1.35
41	20	211	A86	C8-C6	6.97	1.60	1.45
41	18	314	A86	C8-C6	6.97	1.60	1.45
30	B	608	CLA	C4B-NB	6.97	1.41	1.35
30	b	608	CLA	C4B-NB	6.97	1.41	1.35
30	c	524	CLA	C4B-NB	6.97	1.41	1.35
41	11	310	A86	C8-C6	6.97	1.60	1.45
41	40	211	A86	C8-C6	6.97	1.60	1.45
41	37	316	A86	C8-C6	6.97	1.60	1.45
41	32	318	A86	C8-C6	6.96	1.60	1.45
41	35	310	A86	C8-C6	6.96	1.60	1.45
39	D	407	PL9	C3-C4	-6.96	1.38	1.49
41	15	311	A86	C19-C20	6.96	1.62	1.52
41	31	310	A86	C8-C6	6.96	1.60	1.45
41	33	312	A86	C8-C6	6.95	1.60	1.45
30	17	310	CLA	C4B-NB	6.95	1.41	1.35
41	38	314	A86	C8-C6	6.94	1.60	1.45
41	13	315	A86	C8-C6	6.94	1.60	1.45
41	17	316	A86	C8-C6	6.94	1.60	1.45
41	32	319	A86	C8-C6	6.94	1.60	1.45
41	31	314	A86	C8-C6	6.94	1.60	1.45
41	40	201	A86	C19-C20	6.94	1.61	1.52
41	35	311	A86	C19-C20	6.93	1.61	1.52
41	21	311	A86	C8-C6	6.93	1.60	1.45
41	41	311	A86	C8-C6	6.93	1.60	1.45
41	20	201	A86	C19-C20	6.92	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	13	311	A86	C8-C6	6.92	1.60	1.45
41	15	310	A86	C8-C6	6.92	1.60	1.45
30	21	302	CLA	C4B-NB	6.92	1.41	1.35
41	15	310	A86	C19-C20	6.92	1.61	1.52
41	18	313	A86	C19-C20	6.92	1.61	1.52
41	39	309	A86	C8-C6	6.91	1.60	1.45
41	19	309	A86	C8-C6	6.91	1.60	1.45
30	37	310	CLA	C4B-NB	6.91	1.41	1.35
30	38	304	CLA	C4B-NB	6.91	1.41	1.35
30	40	209	CLA	C4B-NB	6.91	1.41	1.35
41	38	313	A86	C19-C20	6.91	1.61	1.52
30	18	304	CLA	C4B-NB	6.90	1.41	1.35
41	12	316	A86	C19-C20	6.90	1.61	1.52
30	12	314	CLA	C4B-NB	6.90	1.41	1.35
30	15	309	CLA	C4B-NB	6.90	1.41	1.35
41	40	201	A86	C25-C26	6.89	1.64	1.43
41	12	315	A86	C8-C6	6.89	1.60	1.45
30	21	306	CLA	C4B-NB	6.89	1.41	1.35
41	35	310	A86	C19-C20	6.89	1.61	1.52
41	20	201	A86	C25-C26	6.89	1.64	1.43
30	14	310	CLA	C4B-NB	6.89	1.41	1.35
41	40	212	A86	C25-C26	6.88	1.64	1.43
30	34	310	CLA	C4B-NB	6.88	1.41	1.35
41	20	212	A86	C25-C26	6.88	1.64	1.43
30	18	305	CLA	C4B-NB	6.88	1.41	1.35
41	17	312	A86	C19-C20	6.87	1.61	1.52
30	41	302	CLA	C4B-NB	6.87	1.41	1.35
30	41	306	CLA	C4B-NB	6.87	1.41	1.35
41	32	315	A86	C19-C20	6.87	1.61	1.52
41	11	311	A86	C19-C20	6.86	1.61	1.52
30	35	309	CLA	C4B-NB	6.86	1.41	1.35
41	31	311	A86	C19-C20	6.86	1.61	1.52
41	32	314	A86	C8-C6	6.86	1.60	1.45
41	18	313	A86	C8-C6	6.85	1.60	1.45
30	20	209	CLA	C4B-NB	6.85	1.41	1.35
41	14	311	A86	C8-C6	6.85	1.60	1.45
30	18	312	CLA	C4B-NB	6.85	1.41	1.35
30	11	309	CLA	C4B-NB	6.85	1.41	1.35
30	18	301	CLA	C4B-NB	6.85	1.41	1.35
41	14	311	A86	C19-C20	6.85	1.61	1.52
30	33	311	CLA	C4B-NB	6.84	1.41	1.35
30	39	303	CLA	C4B-NB	6.84	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	34	311	A86	C8-C6	6.84	1.60	1.45
41	17	312	A86	C25-C26	6.84	1.64	1.43
41	11	310	A86	C19-C20	6.84	1.61	1.52
41	36	311	A86	C19-C20	6.83	1.61	1.52
41	37	312	A86	C25-C26	6.83	1.64	1.43
30	16	301	CLA	C4B-NB	6.83	1.41	1.35
41	33	312	A86	C19-C20	6.83	1.61	1.52
30	15	303	CLA	C4B-NB	6.83	1.41	1.35
41	36	310	A86	C19-C20	6.83	1.61	1.52
30	40	202	CLA	C4B-NB	6.83	1.41	1.35
30	19	303	CLA	C4B-NB	6.83	1.41	1.35
41	13	312	A86	C25-C26	6.82	1.64	1.43
30	15	308	CLA	C4B-NB	6.82	1.41	1.35
30	38	301	CLA	C4B-NB	6.82	1.41	1.35
41	32	314	A86	C19-C20	6.82	1.61	1.52
41	41	314	A86	C19-C20	6.82	1.61	1.52
41	13	311	A86	C19-C20	6.82	1.61	1.52
41	39	310	A86	C19-C20	6.82	1.61	1.52
41	14	312	A86	C25-C26	6.82	1.64	1.43
41	37	312	A86	C19-C20	6.82	1.61	1.52
41	33	313	A86	C19-C20	6.81	1.61	1.52
41	38	313	A86	C8-C6	6.81	1.60	1.45
41	13	312	A86	C19-C20	6.81	1.61	1.52
41	11	311	A86	C25-C26	6.81	1.64	1.43
41	16	310	A86	C19-C20	6.81	1.61	1.52
41	33	313	A86	C25-C26	6.81	1.64	1.43
41	34	311	A86	C19-C20	6.81	1.61	1.52
30	20	202	CLA	C4B-NB	6.80	1.41	1.35
41	34	312	A86	C25-C26	6.80	1.64	1.43
41	31	311	A86	C25-C26	6.80	1.64	1.43
41	31	310	A86	C19-C20	6.80	1.61	1.52
41	35	311	A86	C25-C26	6.80	1.64	1.43
41	32	315	A86	C25-C26	6.80	1.64	1.43
41	17	313	A86	C25-C26	6.79	1.64	1.43
41	18	314	A86	C25-C26	6.79	1.64	1.43
41	19	311	A86	C25-C26	6.79	1.64	1.43
41	39	311	A86	C19-C20	6.79	1.61	1.52
41	38	314	A86	C25-C26	6.79	1.64	1.43
41	16	311	A86	C25-C26	6.78	1.64	1.43
30	36	301	CLA	C4B-NB	6.78	1.41	1.35
41	16	311	A86	C19-C20	6.78	1.61	1.52
41	36	311	A86	C25-C26	6.78	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	41	310	A86	C25-C26	6.78	1.64	1.43
41	19	310	A86	C19-C20	6.78	1.61	1.52
41	15	311	A86	C25-C26	6.77	1.64	1.43
41	21	310	A86	C25-C26	6.77	1.64	1.43
41	39	311	A86	C25-C26	6.77	1.64	1.43
41	12	316	A86	C25-C26	6.77	1.64	1.43
41	37	311	A86	C25-C26	6.77	1.64	1.43
41	15	315	A86	C25-C26	6.77	1.64	1.43
41	37	313	A86	C25-C26	6.77	1.64	1.43
41	17	311	A86	C25-C26	6.76	1.64	1.43
30	17	303	CLA	C4B-NB	6.76	1.41	1.35
30	38	310	CLA	C4B-NB	6.76	1.41	1.35
41	12	315	A86	C19-C20	6.76	1.61	1.52
41	20	213	A86	C19-C20	6.76	1.61	1.52
41	21	314	A86	C19-C20	6.76	1.61	1.52
41	35	315	A86	C25-C26	6.76	1.64	1.43
41	33	314	A86	C25-C26	6.76	1.64	1.43
41	35	316	A86	C25-C26	6.76	1.64	1.43
41	32	304	A86	C25-C26	6.76	1.64	1.43
41	14	312	A86	C19-C20	6.75	1.61	1.52
41	13	313	A86	C25-C26	6.75	1.64	1.43
41	20	210	A86	C25-C26	6.75	1.64	1.43
41	14	313	A86	C25-C26	6.75	1.64	1.43
41	12	304	A86	C25-C26	6.75	1.64	1.43
30	35	303	CLA	C4B-NB	6.75	1.41	1.35
30	37	303	CLA	C4B-NB	6.75	1.41	1.35
41	12	317	A86	C25-C26	6.75	1.64	1.43
41	34	313	A86	C25-C26	6.75	1.64	1.43
41	15	316	A86	C25-C26	6.74	1.64	1.43
41	11	316	A86	C25-C26	6.74	1.64	1.43
41	40	210	A86	C25-C26	6.74	1.64	1.43
41	19	310	A86	C25-C26	6.74	1.64	1.43
30	15	307	CLA	C4B-NB	6.74	1.41	1.35
41	38	302	A86	C25-C26	6.73	1.64	1.43
41	40	213	A86	C19-C20	6.73	1.61	1.52
41	31	316	A86	C25-C26	6.73	1.64	1.43
41	36	312	A86	C25-C26	6.73	1.64	1.43
30	35	307	CLA	C4B-NB	6.73	1.41	1.35
41	32	316	A86	C25-C26	6.73	1.64	1.43
41	33	316	A86	C25-C26	6.73	1.64	1.43
41	13	316	A86	C25-C26	6.73	1.64	1.43
30	40	208	CLA	C4B-NB	6.73	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	18	314	A86	C19-C20	6.73	1.61	1.52
41	18	302	A86	C25-C26	6.73	1.64	1.43
41	16	312	A86	C25-C26	6.73	1.64	1.43
41	34	312	A86	C19-C20	6.73	1.61	1.52
41	17	302	A86	C19-C20	6.73	1.61	1.52
30	20	208	CLA	C4B-NB	6.72	1.41	1.35
41	11	312	A86	C25-C26	6.71	1.64	1.43
30	19	304	CLA	C4B-NB	6.71	1.41	1.35
41	13	301	A86	C25-C26	6.71	1.64	1.43
30	20	205	CLA	C4B-NB	6.71	1.41	1.35
41	19	311	A86	C19-C20	6.71	1.61	1.52
41	15	312	A86	C25-C26	6.71	1.64	1.43
41	41	311	A86	C25-C26	6.71	1.64	1.43
41	31	312	A86	C25-C26	6.71	1.64	1.43
41	21	311	A86	C25-C26	6.71	1.64	1.43
41	39	310	A86	C25-C26	6.71	1.64	1.43
41	33	302	A86	C25-C26	6.70	1.64	1.43
41	35	312	A86	C25-C26	6.70	1.64	1.43
41	20	211	A86	C25-C26	6.70	1.64	1.43
30	14	301	CLA	C4B-NB	6.70	1.41	1.35
30	18	310	CLA	C4B-NB	6.70	1.41	1.35
41	38	314	A86	C19-C20	6.70	1.61	1.52
41	37	315	A86	C25-C26	6.69	1.64	1.43
41	40	211	A86	C25-C26	6.69	1.64	1.43
30	38	312	CLA	C4B-NB	6.68	1.41	1.35
30	14	306	CLA	C4B-NB	6.67	1.41	1.35
30	41	303	CLA	C4B-NB	6.67	1.41	1.35
41	17	315	A86	C25-C26	6.67	1.64	1.43
30	12	312	CLA	C4B-NB	6.67	1.41	1.35
30	B	609	CLA	C4B-NB	6.67	1.41	1.35
30	11	305	CLA	C4B-NB	6.67	1.41	1.35
30	12	309	CLA	C4B-NB	6.67	1.41	1.35
41	17	302	A86	C25-C26	6.67	1.64	1.43
30	18	303	CLA	C4B-NB	6.67	1.41	1.35
41	37	302	A86	C25-C26	6.66	1.64	1.43
30	40	207	CLA	C4B-NB	6.66	1.41	1.35
41	39	309	A86	C25-C26	6.66	1.64	1.43
30	38	303	CLA	C4B-NB	6.66	1.41	1.35
30	13	306	CLA	C4B-NB	6.65	1.41	1.35
41	19	309	A86	C25-C26	6.65	1.64	1.43
41	37	302	A86	C19-C20	6.65	1.61	1.52
41	40	213	A86	C25-C26	6.64	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	507	CLA	C4B-NB	6.64	1.41	1.35
30	32	313	CLA	C4B-NB	6.64	1.41	1.35
30	21	303	CLA	C4B-NB	6.64	1.41	1.35
41	20	213	A86	C25-C26	6.64	1.64	1.43
41	16	310	A86	C25-C26	6.63	1.64	1.43
41	36	310	A86	C25-C26	6.63	1.64	1.43
41	15	312	A86	C19-C20	6.63	1.61	1.52
30	31	309	CLA	C4B-NB	6.63	1.41	1.35
30	39	304	CLA	C4B-NB	6.62	1.41	1.35
41	21	314	A86	C25-C26	6.62	1.64	1.43
41	36	313	A86	C25-C26	6.62	1.64	1.43
41	35	312	A86	C19-C20	6.62	1.61	1.52
41	17	316	A86	C25-C26	6.62	1.63	1.43
41	41	314	A86	C25-C26	6.61	1.63	1.43
30	40	205	CLA	C4B-NB	6.61	1.41	1.35
41	21	312	A86	C25-C26	6.61	1.63	1.43
41	13	317	A86	C25-C26	6.61	1.63	1.43
41	36	312	A86	C19-C20	6.61	1.61	1.52
41	11	314	A86	C25-C26	6.61	1.63	1.43
41	31	314	A86	C25-C26	6.61	1.63	1.43
41	37	316	A86	C25-C26	6.60	1.63	1.43
41	13	315	A86	C25-C26	6.60	1.63	1.43
41	32	319	A86	C25-C26	6.60	1.63	1.43
30	31	315	CLA	C4B-NB	6.60	1.41	1.35
41	16	312	A86	C19-C20	6.60	1.61	1.52
41	33	317	A86	C25-C26	6.60	1.63	1.43
41	41	312	A86	C25-C26	6.60	1.63	1.43
30	20	207	CLA	C4B-NB	6.60	1.41	1.35
41	16	313	A86	C25-C26	6.59	1.63	1.43
41	41	313	A86	C25-C26	6.59	1.63	1.43
41	21	313	A86	C25-C26	6.58	1.63	1.43
41	14	313	A86	C19-C20	6.58	1.61	1.52
41	41	313	A86	C19-C20	6.58	1.61	1.52
30	11	315	CLA	C4B-NB	6.58	1.41	1.35
41	11	310	A86	C25-C26	6.58	1.63	1.43
41	31	313	A86	C25-C26	6.58	1.63	1.43
41	15	314	A86	C25-C26	6.58	1.63	1.43
41	32	318	A86	C25-C26	6.58	1.63	1.43
41	12	319	A86	C25-C26	6.58	1.63	1.43
41	35	314	A86	C25-C26	6.58	1.63	1.43
41	35	313	A86	C25-C26	6.58	1.63	1.43
41	12	318	A86	C25-C26	6.58	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	d	408	PL9	C6-C1	-6.57	1.36	1.48
41	11	313	A86	C25-C26	6.57	1.63	1.43
41	37	314	A86	C25-C26	6.57	1.63	1.43
41	11	312	A86	C19-C20	6.57	1.61	1.52
41	15	313	A86	C25-C26	6.57	1.63	1.43
41	17	314	A86	C25-C26	6.57	1.63	1.43
41	33	314	A86	C19-C20	6.57	1.61	1.52
41	21	313	A86	C19-C20	6.57	1.61	1.52
41	17	313	A86	C19-C20	6.57	1.61	1.52
30	33	301	CLA	C4B-NB	6.57	1.41	1.35
41	31	312	A86	C19-C20	6.57	1.61	1.52
30	32	309	CLA	C4B-NB	6.56	1.41	1.35
41	31	310	A86	C25-C26	6.56	1.63	1.43
41	18	315	A86	C25-C26	6.56	1.63	1.43
41	32	317	A86	C25-C26	6.56	1.63	1.43
41	18	313	A86	C25-C26	6.56	1.63	1.43
41	32	316	A86	C19-C20	6.56	1.61	1.52
41	15	310	A86	C25-C26	6.55	1.63	1.43
30	34	306	CLA	C4B-NB	6.55	1.41	1.35
41	38	315	A86	C25-C26	6.55	1.63	1.43
41	35	310	A86	C25-C26	6.55	1.63	1.43
30	C	519	CLA	C4B-NB	6.55	1.41	1.35
41	34	314	A86	C25-C26	6.55	1.63	1.43
41	13	313	A86	C19-C20	6.55	1.61	1.52
41	14	314	A86	C25-C26	6.54	1.63	1.43
41	32	314	A86	C25-C26	6.54	1.63	1.43
41	34	311	A86	C25-C26	6.54	1.63	1.43
30	21	304	CLA	C4B-NB	6.54	1.41	1.35
41	12	317	A86	C19-C20	6.54	1.61	1.52
41	34	313	A86	C19-C20	6.54	1.61	1.52
41	12	315	A86	C25-C26	6.54	1.63	1.43
41	37	313	A86	C19-C20	6.54	1.61	1.52
30	12	303	CLA	C4B-NB	6.54	1.41	1.35
41	14	311	A86	C25-C26	6.53	1.63	1.43
41	13	311	A86	C25-C26	6.53	1.63	1.43
41	33	315	A86	C25-C26	6.53	1.63	1.43
41	38	313	A86	C25-C26	6.53	1.63	1.43
41	33	312	A86	C25-C26	6.53	1.63	1.43
30	16	307	CLA	C4B-NB	6.52	1.41	1.35
30	36	307	CLA	C4B-NB	6.52	1.41	1.35
30	41	304	CLA	C4B-NB	6.52	1.41	1.35
41	13	314	A86	C25-C26	6.51	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	507	CLA	C4B-NB	6.51	1.41	1.35
30	36	309	CLA	C4B-NB	6.50	1.41	1.35
30	31	305	CLA	C4B-NB	6.48	1.41	1.35
30	W	102	CLA	C4B-NB	6.46	1.41	1.35
30	33	307	CLA	C4B-NB	6.45	1.41	1.35
30	19	308	CLA	C4B-NB	6.45	1.41	1.35
30	32	303	CLA	C4B-NB	6.45	1.41	1.35
30	34	301	CLA	C4B-NB	6.44	1.41	1.35
41	36	313	A86	C19-C20	6.44	1.61	1.52
30	16	309	CLA	C4B-NB	6.44	1.41	1.35
30	b	622	CLA	C4B-NB	6.43	1.40	1.35
39	D	407	PL9	C6-C1	-6.43	1.37	1.48
41	37	316	A86	C19-C20	6.43	1.61	1.52
30	36	306	CLA	C4B-NB	6.43	1.40	1.35
30	39	305	CLA	C4B-NB	6.42	1.40	1.35
41	19	309	A86	C19-C20	6.42	1.61	1.52
41	16	313	A86	C19-C20	6.41	1.61	1.52
30	11	308	CLA	C4B-NB	6.41	1.40	1.35
30	b	609	CLA	C4B-NB	6.41	1.40	1.35
41	33	317	A86	C19-C20	6.41	1.61	1.52
30	17	305	CLA	C4B-NB	6.41	1.40	1.35
30	c	513	CLA	C4B-NB	6.40	1.40	1.35
30	13	305	CLA	C4B-NB	6.40	1.40	1.35
30	36	305	CLA	C4B-NB	6.40	1.40	1.35
30	16	303	CLA	C4B-NB	6.40	1.40	1.35
30	14	303	CLA	C4B-NB	6.40	1.40	1.35
30	12	313	CLA	C4B-NB	6.40	1.40	1.35
30	19	305	CLA	C4B-NB	6.40	1.40	1.35
30	11	307	CLA	C4B-NB	6.40	1.40	1.35
41	13	315	A86	C19-C20	6.39	1.61	1.52
30	32	311	CLA	C4B-NB	6.39	1.40	1.35
30	36	304	CLA	C4B-NB	6.39	1.40	1.35
30	16	305	CLA	C4B-NB	6.39	1.40	1.35
41	20	211	A86	C19-C20	6.39	1.61	1.52
41	32	319	A86	C19-C20	6.39	1.61	1.52
30	40	206	CLA	C4B-NB	6.39	1.40	1.35
30	12	311	CLA	C4B-NB	6.38	1.40	1.35
30	16	304	CLA	C4B-NB	6.38	1.40	1.35
41	13	317	A86	C19-C20	6.37	1.61	1.52
30	w	102	CLA	C4B-NB	6.36	1.40	1.35
41	39	309	A86	C19-C20	6.35	1.61	1.52
30	13	304	CLA	C4B-NB	6.35	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	307	CLA	C4B-NB	6.35	1.40	1.35
30	13	302	CLA	C4B-NB	6.35	1.40	1.35
41	17	316	A86	C19-C20	6.35	1.61	1.52
30	37	304	CLA	C4B-NB	6.35	1.40	1.35
30	13	309	CLA	C4B-NB	6.34	1.40	1.35
30	40	204	CLA	C4B-NB	6.34	1.40	1.35
30	z	101	CLA	C4B-NB	6.34	1.40	1.35
30	16	306	CLA	C4B-NB	6.34	1.40	1.35
30	12	305	CLA	C4B-NB	6.33	1.40	1.35
41	40	211	A86	C19-C20	6.33	1.61	1.52
30	20	204	CLA	C4B-NB	6.32	1.40	1.35
30	20	206	CLA	C4B-NB	6.32	1.40	1.35
30	B	602	CLA	C4B-NB	6.32	1.40	1.35
30	39	308	CLA	C4B-NB	6.32	1.40	1.35
30	33	303	CLA	C4B-NB	6.32	1.40	1.35
41	41	311	A86	C19-C20	6.32	1.61	1.52
30	11	303	CLA	C4B-NB	6.32	1.40	1.35
30	14	309	CLA	C4B-NB	6.32	1.40	1.35
41	15	314	A86	C19-C20	6.31	1.61	1.52
41	12	319	A86	C19-C20	6.31	1.61	1.52
30	37	306	CLA	C4B-NB	6.31	1.40	1.35
30	11	301	CLA	C4B-NB	6.31	1.40	1.35
30	12	308	CLA	C4B-NB	6.30	1.40	1.35
41	35	314	A86	C19-C20	6.30	1.61	1.52
30	11	304	CLA	C4B-NB	6.30	1.40	1.35
30	37	305	CLA	C4B-NB	6.30	1.40	1.35
30	14	308	CLA	C4B-NB	6.29	1.40	1.35
30	B	623	CLA	C4B-NB	6.29	1.40	1.35
30	17	306	CLA	C4B-NB	6.28	1.40	1.35
41	11	314	A86	C19-C20	6.28	1.61	1.52
30	B	605	CLA	C4B-NB	6.28	1.40	1.35
30	c	512	CLA	C4B-NB	6.28	1.40	1.35
30	13	308	CLA	C4B-NB	6.27	1.40	1.35
30	36	302	CLA	C4B-NB	6.27	1.40	1.35
30	17	304	CLA	C4B-NB	6.27	1.40	1.35
30	36	303	CLA	C4B-NB	6.27	1.40	1.35
30	31	301	CLA	C4B-NB	6.27	1.40	1.35
30	C	513	CLA	C4B-NB	6.27	1.40	1.35
30	C	504	CLA	C4B-NB	6.27	1.40	1.35
30	32	305	CLA	C4B-NB	6.26	1.40	1.35
30	34	308	CLA	C4B-NB	6.26	1.40	1.35
30	32	312	CLA	C4B-NB	6.26	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	19	307	CLA	C4B-NB	6.26	1.40	1.35
30	14	304	CLA	C4B-NB	6.26	1.40	1.35
30	12	306	CLA	C4B-NB	6.25	1.40	1.35
41	31	314	A86	C19-C20	6.25	1.61	1.52
30	11	302	CLA	C4B-NB	6.25	1.40	1.35
30	b	605	CLA	C4B-NB	6.24	1.40	1.35
30	19	301	CLA	C4B-NB	6.24	1.40	1.35
30	33	309	CLA	C4B-NB	6.24	1.40	1.35
41	21	311	A86	C19-C20	6.24	1.60	1.52
41	21	310	A86	C19-C20	6.23	1.60	1.52
30	31	307	CLA	C4B-NB	6.23	1.40	1.35
41	32	318	A86	C19-C20	6.23	1.60	1.52
30	16	302	CLA	C4B-NB	6.22	1.40	1.35
30	c	504	CLA	C4B-NB	6.21	1.40	1.35
30	31	304	CLA	C4B-NB	6.21	1.40	1.35
30	b	602	CLA	C4B-NB	6.21	1.40	1.35
30	14	302	CLA	C4B-NB	6.20	1.40	1.35
30	39	301	CLA	C4B-NB	6.20	1.40	1.35
30	33	306	CLA	C4B-NB	6.20	1.40	1.35
30	d	406	CLA	C4B-NB	6.19	1.40	1.35
30	31	308	CLA	C4B-NB	6.19	1.40	1.35
30	39	307	CLA	C4B-NB	6.19	1.40	1.35
30	14	305	CLA	C4B-NB	6.18	1.40	1.35
30	34	302	CLA	C4B-NB	6.18	1.40	1.35
30	13	303	CLA	C4B-NB	6.17	1.40	1.35
30	32	307	CLA	C4B-NB	6.16	1.40	1.35
41	41	310	A86	C19-C20	6.16	1.60	1.52
41	13	316	A86	C19-C20	6.16	1.60	1.52
30	32	308	CLA	C4B-NB	6.13	1.40	1.35
30	B	615	CLA	C4B-NB	6.12	1.40	1.35
30	34	304	CLA	C4B-NB	6.11	1.40	1.35
41	13	301	A86	C19-C20	6.11	1.60	1.52
30	34	305	CLA	C4B-NB	6.11	1.40	1.35
30	34	309	CLA	C4B-NB	6.10	1.40	1.35
30	C	521	CLA	C4B-NB	6.10	1.40	1.35
41	33	316	A86	C19-C20	6.09	1.60	1.52
30	C	512	CLA	C4B-NB	6.09	1.40	1.35
30	19	306	CLA	C4B-NB	6.09	1.40	1.35
40	V	201	HEM	C3C-C2C	-6.08	1.31	1.40
41	15	315	A86	C19-C20	6.06	1.60	1.52
30	32	306	CLA	C4B-NB	6.06	1.40	1.35
41	33	302	A86	C19-C20	6.05	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	601	CLA	C4B-NB	6.05	1.40	1.35
30	c	522	CLA	C4B-NB	6.05	1.40	1.35
30	b	615	CLA	C4B-NB	6.04	1.40	1.35
41	32	304	A86	C19-C20	6.04	1.60	1.52
30	D	405	CLA	C4B-NB	6.04	1.40	1.35
41	35	315	A86	C19-C20	6.04	1.60	1.52
30	c	523	CLA	C4B-NB	6.03	1.40	1.35
41	18	302	A86	C19-C20	6.03	1.60	1.52
30	33	310	CLA	C4B-NB	6.03	1.40	1.35
30	31	303	CLA	C4B-NB	6.03	1.40	1.35
40	v	201	HEM	C3C-C2C	-6.02	1.32	1.40
41	38	302	A86	C19-C20	6.01	1.60	1.52
30	33	305	CLA	C4B-NB	6.01	1.40	1.35
30	39	306	CLA	C4B-NB	6.01	1.40	1.35
30	31	302	CLA	C4B-NB	6.00	1.40	1.35
30	b	610	CLA	C4B-NB	6.00	1.40	1.35
41	35	316	A86	C19-C20	6.00	1.60	1.52
41	15	316	A86	C19-C20	5.99	1.60	1.52
30	33	304	CLA	C4B-NB	5.99	1.40	1.35
41	12	304	A86	C19-C20	5.99	1.60	1.52
30	C	506	CLA	C4B-NB	5.98	1.40	1.35
41	31	316	A86	C19-C20	5.97	1.60	1.52
30	B	601	CLA	C4B-NB	5.96	1.40	1.35
30	17	301	CLA	C4B-NB	5.96	1.40	1.35
30	37	301	CLA	C4B-NB	5.96	1.40	1.35
41	11	316	A86	C19-C20	5.96	1.60	1.52
30	m	101	CLA	C4B-NB	5.94	1.40	1.35
30	C	520	CLA	C4B-NB	5.94	1.40	1.35
30	A	402	CLA	C4B-NB	5.93	1.40	1.35
30	34	303	CLA	C4B-NB	5.93	1.40	1.35
30	a	402	CLA	C4B-NB	5.90	1.40	1.35
30	d	407	CLA	C4B-NB	5.89	1.40	1.35
30	39	302	CLA	C4B-NB	5.88	1.40	1.35
30	c	506	CLA	C4B-NB	5.86	1.40	1.35
41	21	312	A86	C19-C20	5.85	1.60	1.52
30	D	406	CLA	C4B-NB	5.84	1.40	1.35
30	M	101	CLA	C4B-NB	5.84	1.40	1.35
30	B	610	CLA	C4B-NB	5.82	1.40	1.35
41	41	312	A86	C19-C20	5.79	1.60	1.52
30	A	404	CLA	C4B-NB	5.79	1.40	1.35
39	D	404	PL9	C7-C3	-5.77	1.45	1.51
30	a	403	CLA	C4B-NB	5.76	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	19	302	CLA	C4B-NB	5.75	1.40	1.35
39	d	405	PL9	C7-C3	-5.75	1.45	1.51
30	b	603	CLA	C4B-NB	5.70	1.40	1.35
30	B	611	CLA	C4B-NB	5.70	1.40	1.35
30	c	514	CLA	C4B-NB	5.70	1.40	1.35
30	B	607	CLA	C4B-NB	5.69	1.40	1.35
30	b	611	CLA	C4B-NB	5.68	1.40	1.35
30	d	402	CLA	C4B-NB	5.67	1.40	1.35
30	B	614	CLA	C4B-NB	5.67	1.40	1.35
30	b	607	CLA	C4B-NB	5.66	1.40	1.35
30	b	614	CLA	C4B-NB	5.65	1.40	1.35
30	D	402	CLA	C4B-NB	5.63	1.40	1.35
30	C	514	CLA	C4B-NB	5.56	1.40	1.35
30	c	502	CLA	C4B-NB	5.51	1.40	1.35
30	B	603	CLA	C4B-NB	5.50	1.40	1.35
30	c	505	CLA	C4B-NB	5.50	1.40	1.35
30	C	509	CLA	C4B-NB	5.49	1.40	1.35
30	C	505	CLA	C4B-NB	5.46	1.40	1.35
30	D	401	CLA	C4B-NB	5.46	1.40	1.35
30	C	502	CLA	C4B-NB	5.43	1.40	1.35
30	c	510	CLA	C4B-NB	5.39	1.40	1.35
30	b	612	CLA	C4B-NB	5.38	1.40	1.35
30	37	308	CLA	C4B-NB	5.38	1.40	1.35
30	c	508	CLA	C4B-NB	5.37	1.40	1.35
30	C	508	CLA	C4B-NB	5.36	1.40	1.35
30	d	401	CLA	C4B-NB	5.34	1.40	1.35
30	C	510	CLA	C4B-NB	5.34	1.40	1.35
30	c	509	CLA	C4B-NB	5.34	1.40	1.35
30	B	612	CLA	C4B-NB	5.33	1.40	1.35
30	17	308	CLA	C4B-NB	5.32	1.40	1.35
41	20	201	A86	C9-C8	5.21	1.48	1.34
41	40	201	A86	C9-C8	5.17	1.47	1.34
30	C	503	CLA	C4B-NB	5.05	1.39	1.35
41	12	317	A86	C9-C8	4.99	1.47	1.34
41	32	316	A86	C9-C8	4.97	1.47	1.34
41	39	310	A86	C9-C8	4.97	1.47	1.34
41	37	313	A86	C9-C8	4.96	1.47	1.34
41	17	311	A86	C9-C8	4.96	1.47	1.34
41	20	212	A86	C9-C8	4.96	1.47	1.34
41	31	312	A86	C9-C8	4.96	1.47	1.34
41	17	313	A86	C9-C8	4.95	1.47	1.34
41	19	310	A86	C9-C8	4.95	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	13	313	A86	C9-C8	4.95	1.47	1.34
41	36	312	A86	C9-C8	4.95	1.47	1.34
41	40	212	A86	C9-C8	4.95	1.47	1.34
41	16	312	A86	C9-C8	4.94	1.47	1.34
41	33	302	A86	C9-C8	4.94	1.47	1.34
30	B	613	CLA	C4B-NB	4.94	1.39	1.35
41	11	312	A86	C9-C8	4.94	1.47	1.34
41	37	311	A86	C9-C8	4.94	1.47	1.34
41	14	313	A86	C9-C8	4.93	1.47	1.34
41	33	314	A86	C9-C8	4.92	1.47	1.34
41	34	313	A86	C9-C8	4.92	1.47	1.34
41	35	312	A86	C9-C8	4.92	1.47	1.34
41	15	312	A86	C9-C8	4.90	1.47	1.34
41	20	212	A86	C26-C27	4.90	1.42	1.35
41	40	212	A86	C26-C27	4.90	1.42	1.35
41	13	301	A86	C9-C8	4.89	1.47	1.34
41	35	315	A86	C9-C8	4.88	1.47	1.34
41	31	316	A86	C9-C8	4.88	1.47	1.34
41	13	316	A86	C9-C8	4.87	1.47	1.34
41	11	316	A86	C9-C8	4.87	1.47	1.34
41	38	302	A86	C9-C8	4.86	1.47	1.34
41	17	315	A86	C9-C8	4.86	1.47	1.34
41	32	304	A86	C9-C8	4.86	1.47	1.34
41	33	316	A86	C9-C8	4.86	1.47	1.34
41	18	302	A86	C9-C8	4.85	1.47	1.34
41	15	316	A86	C9-C8	4.85	1.47	1.34
41	35	316	A86	C9-C8	4.85	1.47	1.34
41	37	315	A86	C9-C8	4.85	1.47	1.34
41	19	310	A86	C26-C27	4.84	1.42	1.35
41	12	304	A86	C9-C8	4.84	1.47	1.34
41	15	315	A86	C9-C8	4.83	1.47	1.34
41	40	210	A86	C9-C8	4.83	1.47	1.34
41	20	210	A86	C9-C8	4.81	1.47	1.34
41	39	310	A86	C26-C27	4.81	1.42	1.35
41	39	311	A86	C9-C8	4.80	1.46	1.34
30	b	613	CLA	C4B-NB	4.79	1.39	1.35
41	19	311	A86	C9-C8	4.79	1.46	1.34
30	c	503	CLA	C4B-NB	4.79	1.39	1.35
41	38	314	A86	C9-C8	4.78	1.46	1.34
41	21	314	A86	C9-C8	4.77	1.46	1.34
41	40	213	A86	C9-C8	4.77	1.46	1.34
41	37	312	A86	C9-C8	4.76	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	511	CLA	C4B-NB	4.76	1.39	1.35
41	41	312	A86	C9-C8	4.76	1.46	1.34
41	20	213	A86	C9-C8	4.75	1.46	1.34
41	17	312	A86	C9-C8	4.75	1.46	1.34
41	17	302	A86	C9-C8	4.75	1.46	1.34
41	18	314	A86	C9-C8	4.75	1.46	1.34
41	37	302	A86	C9-C8	4.75	1.46	1.34
41	41	314	A86	C9-C8	4.75	1.46	1.34
30	c	511	CLA	C4B-NB	4.74	1.39	1.35
41	21	312	A86	C9-C8	4.74	1.46	1.34
41	13	313	A86	C26-C27	4.73	1.42	1.35
41	31	314	A86	C9-C8	4.72	1.46	1.34
41	15	311	A86	C9-C8	4.72	1.46	1.34
41	11	311	A86	C9-C8	4.72	1.46	1.34
41	35	311	A86	C9-C8	4.72	1.46	1.34
30	B	604	CLA	C4B-NB	4.71	1.39	1.35
41	11	314	A86	C9-C8	4.71	1.46	1.34
41	31	311	A86	C9-C8	4.71	1.46	1.34
30	c	510	CLA	C4D-ND	-4.71	1.31	1.37
41	34	312	A86	C9-C8	4.71	1.46	1.34
41	38	313	A86	C9-C8	4.71	1.46	1.34
41	13	312	A86	C9-C8	4.70	1.46	1.34
41	16	311	A86	C9-C8	4.70	1.46	1.34
41	14	313	A86	C26-C27	4.70	1.42	1.35
41	15	310	A86	C9-C8	4.70	1.46	1.34
41	33	313	A86	C9-C8	4.70	1.46	1.34
30	C	510	CLA	C4D-ND	-4.70	1.31	1.37
41	17	313	A86	C26-C27	4.70	1.42	1.35
41	32	317	A86	C9-C8	4.70	1.46	1.34
41	14	312	A86	C9-C8	4.70	1.46	1.34
41	35	310	A86	C9-C8	4.69	1.46	1.34
41	37	313	A86	C26-C27	4.69	1.42	1.35
41	12	316	A86	C9-C8	4.68	1.46	1.34
41	34	313	A86	C26-C27	4.68	1.42	1.35
41	15	314	A86	C9-C8	4.68	1.46	1.34
41	41	314	A86	C17-C18	-4.67	1.45	1.52
41	12	318	A86	C9-C8	4.67	1.46	1.34
41	32	315	A86	C9-C8	4.67	1.46	1.34
41	36	313	A86	C9-C8	4.67	1.46	1.34
41	39	309	A86	C17-C18	-4.67	1.45	1.52
41	39	311	A86	C26-C27	4.67	1.42	1.35
41	31	313	A86	C9-C8	4.66	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	36	311	A86	C9-C8	4.66	1.46	1.34
41	41	313	A86	C9-C8	4.66	1.46	1.34
41	18	313	A86	C9-C8	4.66	1.46	1.34
30	b	604	CLA	C4B-NB	4.66	1.39	1.35
41	16	313	A86	C9-C8	4.66	1.46	1.34
41	32	319	A86	C9-C8	4.66	1.46	1.34
41	13	315	A86	C9-C8	4.66	1.46	1.34
41	21	313	A86	C9-C8	4.66	1.46	1.34
41	17	311	A86	C26-C27	4.66	1.42	1.35
41	35	314	A86	C9-C8	4.66	1.46	1.34
41	19	309	A86	C17-C18	-4.66	1.45	1.52
41	21	310	A86	C17-C18	-4.65	1.45	1.52
41	41	310	A86	C17-C18	-4.65	1.45	1.52
41	32	318	A86	C9-C8	4.65	1.46	1.34
41	12	315	A86	C9-C8	4.65	1.46	1.34
41	34	311	A86	C9-C8	4.65	1.46	1.34
41	21	314	A86	C17-C18	-4.65	1.45	1.52
41	32	314	A86	C9-C8	4.65	1.46	1.34
41	33	314	A86	C26-C27	4.65	1.41	1.35
41	12	319	A86	C9-C8	4.65	1.46	1.34
41	12	317	A86	C26-C27	4.65	1.41	1.35
41	13	311	A86	C9-C8	4.65	1.46	1.34
41	11	313	A86	C9-C8	4.65	1.46	1.34
41	14	311	A86	C9-C8	4.64	1.46	1.34
41	14	314	A86	C9-C8	4.64	1.46	1.34
41	41	311	A86	C9-C8	4.64	1.46	1.34
41	31	310	A86	C9-C8	4.64	1.46	1.34
41	35	313	A86	C9-C8	4.64	1.46	1.34
30	b	612	CLA	C4D-ND	-4.63	1.31	1.37
41	15	313	A86	C9-C8	4.63	1.46	1.34
41	13	317	A86	C9-C8	4.63	1.46	1.34
41	33	317	A86	C9-C8	4.63	1.46	1.34
41	31	312	A86	C26-C27	4.63	1.41	1.35
41	35	312	A86	C26-C27	4.63	1.41	1.35
41	11	310	A86	C9-C8	4.63	1.46	1.34
41	34	314	A86	C9-C8	4.62	1.46	1.34
41	37	313	A86	O4-C38	4.62	1.45	1.35
41	17	313	A86	O4-C38	4.62	1.45	1.35
41	33	312	A86	C9-C8	4.62	1.46	1.34
41	38	315	A86	C9-C8	4.62	1.46	1.34
41	21	311	A86	C9-C8	4.62	1.46	1.34
41	33	315	A86	C9-C8	4.62	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	16	312	A86	C26-C27	4.62	1.41	1.35
41	36	312	A86	C26-C27	4.62	1.41	1.35
41	37	311	A86	C26-C27	4.62	1.41	1.35
41	20	213	A86	C17-C18	-4.62	1.45	1.52
41	20	211	A86	C9-C8	4.62	1.46	1.34
41	40	212	A86	C2-C1	4.62	1.41	1.35
30	B	612	CLA	C4D-ND	-4.61	1.31	1.37
41	13	314	A86	C9-C8	4.61	1.46	1.34
41	37	316	A86	C9-C8	4.61	1.46	1.34
41	21	310	A86	C9-C8	4.61	1.46	1.34
41	32	316	A86	C26-C27	4.61	1.41	1.35
41	40	213	A86	C17-C18	-4.61	1.45	1.52
41	17	316	A86	C9-C8	4.61	1.46	1.34
41	34	313	A86	O4-C38	4.61	1.45	1.35
41	40	211	A86	C9-C8	4.61	1.46	1.34
41	37	314	A86	C9-C8	4.60	1.46	1.34
41	15	312	A86	C26-C27	4.60	1.41	1.35
41	18	315	A86	C9-C8	4.60	1.46	1.34
41	36	310	A86	C9-C8	4.60	1.46	1.34
41	15	312	A86	O4-C38	4.60	1.45	1.35
41	16	312	A86	O4-C38	4.60	1.45	1.35
41	33	314	A86	O4-C38	4.59	1.45	1.35
41	14	313	A86	O4-C38	4.59	1.45	1.35
41	41	310	A86	C9-C8	4.59	1.46	1.34
41	32	316	A86	O4-C38	4.59	1.45	1.35
41	35	312	A86	O4-C38	4.58	1.45	1.35
41	31	312	A86	O4-C38	4.58	1.45	1.35
41	36	312	A86	O4-C38	4.58	1.45	1.35
41	16	310	A86	C9-C8	4.58	1.46	1.34
41	17	314	A86	C9-C8	4.58	1.46	1.34
41	20	212	A86	C2-C1	4.58	1.41	1.35
41	19	311	A86	C26-C27	4.57	1.41	1.35
41	13	313	A86	O4-C38	4.57	1.45	1.35
41	17	315	A86	C26-C27	4.57	1.41	1.35
41	19	311	A86	O4-C38	4.57	1.45	1.35
41	19	310	A86	O4-C38	4.56	1.45	1.35
41	11	312	A86	O4-C38	4.56	1.45	1.35
41	21	310	A86	C26-C27	4.56	1.41	1.35
41	36	310	A86	C2-C1	4.56	1.41	1.35
41	21	311	A86	C17-C18	-4.55	1.45	1.52
41	11	312	A86	C26-C27	4.55	1.41	1.35
41	41	311	A86	C17-C18	-4.55	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	39	311	A86	C17-C18	-4.55	1.45	1.52
41	19	309	A86	C9-C8	4.55	1.46	1.34
41	19	311	A86	C17-C18	-4.55	1.45	1.52
41	12	317	A86	O4-C38	4.54	1.45	1.35
41	20	211	A86	C17-C18	-4.54	1.45	1.52
41	40	210	A86	C26-C27	4.54	1.41	1.35
41	16	310	A86	C2-C1	4.54	1.41	1.35
40	E	101	HEM	C3C-C2C	-4.54	1.34	1.40
41	39	309	A86	C9-C8	4.53	1.46	1.34
41	39	311	A86	O4-C38	4.53	1.45	1.35
41	41	310	A86	C26-C27	4.53	1.41	1.35
41	39	310	A86	O4-C38	4.53	1.45	1.35
41	40	211	A86	C17-C18	-4.52	1.45	1.52
41	37	315	A86	C26-C27	4.52	1.41	1.35
41	17	311	A86	C17-C18	-4.52	1.45	1.52
41	36	311	A86	C17-C18	-4.51	1.45	1.52
41	19	310	A86	C19-C18	4.50	1.58	1.52
41	39	310	A86	C19-C18	4.50	1.58	1.52
41	38	314	A86	C17-C18	-4.50	1.45	1.52
41	20	210	A86	C26-C27	4.50	1.41	1.35
41	20	213	A86	C26-C27	4.49	1.41	1.35
41	33	313	A86	C17-C18	-4.49	1.45	1.52
41	37	311	A86	C17-C18	-4.48	1.45	1.52
41	21	314	A86	C26-C27	4.47	1.41	1.35
41	13	312	A86	C17-C18	-4.47	1.45	1.52
41	32	315	A86	C17-C18	-4.47	1.45	1.52
41	20	212	A86	O4-C38	4.47	1.45	1.35
41	40	212	A86	O4-C38	4.47	1.45	1.35
41	16	313	A86	C26-C27	4.46	1.41	1.35
41	17	313	A86	C17-C18	-4.46	1.45	1.52
41	34	312	A86	C17-C18	-4.46	1.45	1.52
41	41	313	A86	C17-C18	-4.46	1.45	1.52
41	41	314	A86	C26-C27	4.45	1.41	1.35
41	12	304	A86	C26-C27	4.44	1.41	1.35
41	18	314	A86	C17-C18	-4.44	1.45	1.52
41	41	314	A86	C2-C1	4.44	1.41	1.35
41	15	311	A86	C17-C18	-4.44	1.45	1.52
41	35	311	A86	C17-C18	-4.44	1.45	1.52
41	20	210	A86	C2-C1	4.43	1.41	1.35
41	40	213	A86	C26-C27	4.43	1.41	1.35
41	11	311	A86	C17-C18	-4.43	1.45	1.52
41	12	316	A86	C17-C18	-4.43	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	304	A86	C26-C27	4.43	1.41	1.35
41	32	315	A86	C26-C27	4.43	1.41	1.35
41	11	316	A86	C26-C27	4.42	1.41	1.35
41	31	311	A86	C17-C18	-4.42	1.46	1.52
41	37	312	A86	C17-C18	-4.42	1.46	1.52
41	36	313	A86	C26-C27	4.41	1.41	1.35
41	13	313	A86	C17-C18	-4.41	1.46	1.52
41	16	311	A86	C17-C18	-4.41	1.46	1.52
41	14	312	A86	C26-C27	4.41	1.41	1.35
40	e	101	HEM	C3C-C2C	-4.41	1.34	1.40
41	32	316	A86	C2-C1	4.41	1.41	1.35
41	39	309	A86	C26-C27	4.41	1.41	1.35
41	40	210	A86	C2-C1	4.41	1.41	1.35
41	19	309	A86	C26-C27	4.41	1.41	1.35
41	20	201	A86	C26-C27	4.41	1.41	1.35
41	15	311	A86	C26-C27	4.41	1.41	1.35
41	31	316	A86	C26-C27	4.40	1.41	1.35
41	37	302	A86	C26-C27	4.40	1.41	1.35
41	17	312	A86	C17-C18	-4.40	1.46	1.52
41	37	313	A86	C17-C18	-4.39	1.46	1.52
41	35	315	A86	C26-C27	4.39	1.41	1.35
41	33	314	A86	C17-C18	-4.39	1.46	1.52
41	16	310	A86	C17-C18	-4.39	1.46	1.52
41	12	316	A86	C26-C27	4.39	1.41	1.35
30	d	401	CLA	C4D-ND	-4.39	1.31	1.37
41	15	316	A86	C26-C27	4.39	1.41	1.35
41	34	312	A86	C26-C27	4.39	1.41	1.35
41	20	201	A86	C2-C1	4.39	1.41	1.35
41	40	213	A86	C2-C1	4.39	1.41	1.35
41	14	312	A86	C17-C18	-4.38	1.46	1.52
41	35	316	A86	C26-C27	4.38	1.41	1.35
41	15	315	A86	C26-C27	4.38	1.41	1.35
41	18	315	A86	C26-C27	4.38	1.41	1.35
41	35	311	A86	C26-C27	4.38	1.41	1.35
41	17	302	A86	C17-C18	-4.38	1.46	1.52
41	40	201	A86	C26-C27	4.38	1.41	1.35
41	40	201	A86	C2-C1	4.38	1.41	1.35
41	11	311	A86	C26-C27	4.37	1.41	1.35
41	18	314	A86	C26-C27	4.37	1.41	1.35
41	33	302	A86	C26-C27	4.37	1.41	1.35
41	13	312	A86	C26-C27	4.37	1.41	1.35
41	21	313	A86	C17-C18	-4.36	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	15	314	A86	C26-C27	4.36	1.41	1.35
41	17	302	A86	C26-C27	4.36	1.41	1.35
41	36	312	A86	C2-C1	4.36	1.41	1.35
41	13	301	A86	C26-C27	4.36	1.41	1.35
41	38	315	A86	C26-C27	4.36	1.41	1.35
41	38	314	A86	C26-C27	4.35	1.41	1.35
41	20	213	A86	C2-C1	4.35	1.41	1.35
41	41	311	A86	C26-C27	4.35	1.41	1.35
41	31	311	A86	C26-C27	4.35	1.41	1.35
41	21	314	A86	C2-C1	4.35	1.41	1.35
41	33	313	A86	C26-C27	4.35	1.41	1.35
41	36	310	A86	C17-C18	-4.35	1.46	1.52
41	35	312	A86	C17-C18	-4.34	1.46	1.52
41	32	318	A86	C26-C27	4.34	1.41	1.35
41	18	302	A86	C26-C27	4.34	1.41	1.35
41	33	316	A86	C26-C27	4.34	1.41	1.35
30	32	305	CLA	C4D-ND	-4.34	1.31	1.37
41	41	312	A86	C17-C18	-4.33	1.46	1.52
41	35	314	A86	C26-C27	4.33	1.41	1.35
41	33	317	A86	C26-C27	4.33	1.41	1.35
41	38	302	A86	C26-C27	4.33	1.41	1.35
41	31	314	A86	C26-C27	4.33	1.41	1.35
41	16	312	A86	C17-C18	-4.33	1.46	1.52
30	33	303	CLA	C4D-ND	-4.33	1.31	1.37
41	31	312	A86	C2-C1	4.33	1.41	1.35
41	13	315	A86	C17-C18	-4.32	1.46	1.52
41	11	312	A86	C17-C18	-4.32	1.46	1.52
30	D	401	CLA	C4D-ND	-4.32	1.31	1.37
41	12	317	A86	C2-C1	4.32	1.41	1.35
41	15	312	A86	C17-C18	-4.32	1.46	1.52
41	32	319	A86	C26-C27	4.32	1.41	1.35
41	18	302	A86	C17-C18	-4.32	1.46	1.52
41	37	302	A86	C17-C18	-4.32	1.46	1.52
41	13	316	A86	C26-C27	4.32	1.41	1.35
41	35	312	A86	C2-C1	4.32	1.41	1.35
30	C	509	CLA	C4D-ND	-4.32	1.31	1.37
41	15	312	A86	C2-C1	4.31	1.41	1.35
41	16	311	A86	C26-C27	4.31	1.41	1.35
41	31	312	A86	C17-C18	-4.31	1.46	1.52
41	32	316	A86	C17-C18	-4.31	1.46	1.52
41	14	314	A86	C26-C27	4.31	1.41	1.35
41	40	212	A86	C7-C6	4.30	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	34	313	A86	C17-C18	-4.30	1.46	1.52
41	14	313	A86	C2-C1	4.30	1.41	1.35
41	34	313	A86	C2-C1	4.30	1.41	1.35
41	13	317	A86	C26-C27	4.30	1.41	1.35
41	21	311	A86	C26-C27	4.30	1.41	1.35
41	12	319	A86	C26-C27	4.30	1.41	1.35
41	36	311	A86	C26-C27	4.30	1.41	1.35
41	11	312	A86	C2-C1	4.30	1.41	1.35
41	13	316	A86	C17-C18	-4.29	1.46	1.52
41	33	316	A86	C17-C18	-4.29	1.46	1.52
41	11	314	A86	C26-C27	4.29	1.41	1.35
41	20	201	A86	C19-C18	4.29	1.58	1.52
41	13	315	A86	C26-C27	4.29	1.41	1.35
41	37	312	A86	C26-C27	4.29	1.41	1.35
41	14	313	A86	C17-C18	-4.29	1.46	1.52
41	21	312	A86	C17-C18	-4.29	1.46	1.52
41	20	212	A86	C17-C18	-4.29	1.46	1.52
41	35	315	A86	C2-C1	4.29	1.41	1.35
41	34	314	A86	C26-C27	4.28	1.41	1.35
41	17	312	A86	C26-C27	4.28	1.41	1.35
41	36	312	A86	C17-C18	-4.28	1.46	1.52
41	16	312	A86	C2-C1	4.28	1.41	1.35
41	17	314	A86	C26-C27	4.28	1.41	1.35
41	37	313	A86	C2-C1	4.27	1.41	1.35
41	40	211	A86	C26-C27	4.27	1.41	1.35
41	20	212	A86	C7-C6	4.27	1.59	1.50
41	13	317	A86	C17-C18	-4.27	1.46	1.52
41	13	316	A86	O4-C38	4.27	1.44	1.35
41	12	304	A86	O4-C38	4.27	1.44	1.35
41	17	313	A86	C2-C1	4.27	1.41	1.35
41	21	311	A86	C2-C1	4.27	1.41	1.35
41	33	302	A86	O4-C38	4.27	1.44	1.35
41	33	316	A86	C2-C1	4.27	1.41	1.35
41	15	313	A86	C26-C27	4.27	1.41	1.35
41	17	316	A86	C17-C18	-4.27	1.46	1.52
41	37	311	A86	O4-C38	4.27	1.44	1.35
41	40	201	A86	C10-C11	4.27	1.46	1.34
41	41	311	A86	C2-C1	4.27	1.41	1.35
41	13	301	A86	O4-C38	4.26	1.44	1.35
41	36	313	A86	C17-C18	-4.26	1.46	1.52
30	B	611	CLA	C4D-ND	-4.26	1.31	1.37
30	b	613	CLA	C4D-ND	-4.26	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	15	313	A86	O4-C38	4.26	1.44	1.35
41	37	314	A86	O4-C38	4.26	1.44	1.35
30	d	406	CLA	C4D-ND	-4.26	1.31	1.37
41	40	210	A86	C7-C6	4.26	1.59	1.50
41	36	310	A86	C26-C27	4.26	1.41	1.35
41	17	311	A86	O4-C38	4.26	1.44	1.35
30	34	302	CLA	C4D-ND	-4.26	1.31	1.37
41	12	317	A86	C17-C18	-4.25	1.46	1.52
41	38	302	A86	C17-C18	-4.25	1.46	1.52
41	12	304	A86	C7-C6	4.25	1.59	1.50
41	32	304	A86	O4-C38	4.25	1.44	1.35
41	11	313	A86	C26-C27	4.25	1.41	1.35
41	11	316	A86	O4-C38	4.25	1.44	1.35
41	20	201	A86	C10-C11	4.25	1.46	1.34
41	31	316	A86	C7-C6	4.25	1.59	1.50
41	15	315	A86	C2-C1	4.25	1.41	1.35
41	20	210	A86	C7-C6	4.25	1.59	1.50
41	37	316	A86	C26-C27	4.25	1.41	1.35
41	32	317	A86	C26-C27	4.25	1.41	1.35
41	33	316	A86	O4-C38	4.25	1.44	1.35
41	32	318	A86	C17-C18	-4.25	1.46	1.52
41	38	315	A86	O4-C38	4.24	1.44	1.35
41	35	313	A86	C7-C6	4.24	1.59	1.50
41	19	309	A86	O4-C38	4.24	1.44	1.35
41	31	313	A86	C26-C27	4.24	1.41	1.35
41	16	310	A86	C26-C27	4.24	1.41	1.35
41	35	313	A86	C26-C27	4.24	1.41	1.35
41	11	316	A86	C7-C6	4.24	1.59	1.50
41	17	314	A86	O4-C38	4.24	1.44	1.35
41	39	309	A86	O4-C38	4.24	1.44	1.35
41	17	316	A86	C26-C27	4.24	1.41	1.35
41	32	317	A86	O4-C38	4.24	1.44	1.35
41	20	211	A86	C26-C27	4.24	1.41	1.35
41	11	316	A86	C17-C18	-4.24	1.46	1.52
41	32	319	A86	C17-C18	-4.24	1.46	1.52
41	33	316	A86	C7-C6	4.24	1.59	1.50
41	33	317	A86	C17-C18	-4.24	1.46	1.52
41	15	315	A86	O4-C38	4.23	1.44	1.35
41	13	314	A86	O4-C38	4.23	1.44	1.35
41	15	315	A86	C7-C6	4.23	1.59	1.50
41	32	317	A86	C7-C6	4.23	1.59	1.50
41	35	313	A86	O4-C38	4.23	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	31	313	A86	C7-C6	4.23	1.59	1.50
41	21	313	A86	O4-C38	4.23	1.44	1.35
41	20	210	A86	O4-C38	4.23	1.44	1.35
41	37	314	A86	C26-C27	4.23	1.41	1.35
41	12	318	A86	C26-C27	4.23	1.41	1.35
41	40	201	A86	C19-C18	4.23	1.58	1.52
41	40	213	A86	O4-C38	4.22	1.44	1.35
41	40	212	A86	C17-C18	-4.22	1.46	1.52
41	35	315	A86	C7-C6	4.22	1.59	1.50
41	32	304	A86	C7-C6	4.22	1.59	1.50
41	31	316	A86	O4-C38	4.22	1.44	1.35
41	13	301	A86	C17-C18	-4.22	1.46	1.52
30	13	302	CLA	C4D-ND	-4.22	1.31	1.37
41	21	313	A86	C26-C27	4.22	1.41	1.35
41	17	315	A86	C17-C18	-4.22	1.46	1.52
41	40	210	A86	O4-C38	4.22	1.44	1.35
41	13	316	A86	C2-C1	4.22	1.41	1.35
41	31	316	A86	C17-C18	-4.22	1.46	1.52
41	11	313	A86	C7-C6	4.22	1.59	1.50
41	35	315	A86	C17-C18	-4.22	1.46	1.52
41	11	313	A86	O4-C38	4.22	1.44	1.35
41	18	315	A86	O4-C38	4.22	1.44	1.35
41	35	316	A86	O4-C38	4.21	1.44	1.35
30	B	613	CLA	C4D-ND	-4.21	1.31	1.37
41	37	316	A86	C17-C18	-4.21	1.46	1.52
41	18	315	A86	C7-C6	4.21	1.59	1.50
41	38	302	A86	O4-C38	4.21	1.44	1.35
41	12	318	A86	O4-C38	4.21	1.44	1.35
41	21	312	A86	O4-C38	4.21	1.44	1.35
41	34	314	A86	C7-C6	4.21	1.59	1.50
41	34	314	A86	O4-C38	4.21	1.44	1.35
41	37	314	A86	C7-C6	4.21	1.59	1.50
41	13	313	A86	C2-C1	4.21	1.41	1.35
41	33	314	A86	C2-C1	4.21	1.41	1.35
41	41	313	A86	C26-C27	4.21	1.41	1.35
41	20	213	A86	O4-C38	4.21	1.44	1.35
41	20	211	A86	C2-C1	4.21	1.41	1.35
41	11	313	A86	C17-C18	-4.20	1.46	1.52
41	33	315	A86	O4-C38	4.20	1.44	1.35
41	19	310	A86	C7-C6	4.20	1.59	1.50
41	15	315	A86	C17-C18	-4.20	1.46	1.52
41	35	314	A86	C17-C18	-4.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	502	CLA	C4D-ND	-4.20	1.31	1.37
41	13	314	A86	C7-C6	4.20	1.59	1.50
41	12	318	A86	C7-C6	4.20	1.59	1.50
41	31	314	A86	C17-C18	-4.20	1.46	1.52
41	37	302	A86	C2-C1	4.20	1.41	1.35
41	16	313	A86	C17-C18	-4.20	1.46	1.52
41	38	302	A86	C7-C6	4.20	1.59	1.50
41	31	313	A86	O4-C38	4.20	1.44	1.35
30	31	301	CLA	C4D-ND	-4.20	1.31	1.37
41	35	316	A86	C7-C6	4.20	1.59	1.50
41	15	313	A86	C7-C6	4.20	1.59	1.50
41	33	302	A86	C17-C18	-4.19	1.46	1.52
41	19	311	A86	C2-C1	4.19	1.41	1.35
30	D	405	CLA	C4D-ND	-4.19	1.31	1.37
41	14	314	A86	O4-C38	4.19	1.44	1.35
41	33	302	A86	C7-C6	4.19	1.59	1.50
41	35	313	A86	C17-C18	-4.19	1.46	1.52
41	18	302	A86	O4-C38	4.19	1.44	1.35
41	15	316	A86	O4-C38	4.19	1.44	1.35
41	18	302	A86	C7-C6	4.19	1.59	1.50
41	12	304	A86	C2-C1	4.19	1.41	1.35
41	13	314	A86	C26-C27	4.19	1.41	1.35
41	15	316	A86	C7-C6	4.19	1.59	1.50
41	15	316	A86	C2-C1	4.19	1.41	1.35
41	13	312	A86	O4-C38	4.19	1.44	1.35
41	13	316	A86	C7-C6	4.18	1.59	1.50
41	17	312	A86	O4-C38	4.18	1.44	1.35
41	41	312	A86	O4-C38	4.18	1.44	1.35
41	32	304	A86	C2-C1	4.18	1.41	1.35
41	37	312	A86	O4-C38	4.18	1.44	1.35
41	17	316	A86	C7-C6	4.18	1.59	1.50
41	17	314	A86	C17-C18	-4.18	1.46	1.52
41	37	315	A86	C17-C18	-4.18	1.46	1.52
30	C	502	CLA	C4D-ND	-4.18	1.32	1.37
41	12	319	A86	C17-C18	-4.18	1.46	1.52
41	17	314	A86	C2-C1	4.18	1.41	1.35
41	37	314	A86	C2-C1	4.18	1.41	1.35
41	15	316	A86	C17-C18	-4.18	1.46	1.52
41	38	314	A86	O4-C38	4.17	1.44	1.35
41	12	304	A86	C17-C18	-4.17	1.46	1.52
30	a	402	CLA	C4D-ND	-4.17	1.32	1.37
41	13	301	A86	C2-C1	4.17	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	317	A86	C17-C18	-4.17	1.46	1.52
41	35	316	A86	C2-C1	4.17	1.41	1.35
41	14	314	A86	C7-C6	4.17	1.59	1.50
41	17	314	A86	C7-C6	4.17	1.59	1.50
41	38	315	A86	C7-C6	4.17	1.59	1.50
41	41	313	A86	O4-C38	4.17	1.44	1.35
41	31	313	A86	C17-C18	-4.17	1.46	1.52
41	36	310	A86	O4-C38	4.17	1.44	1.35
41	13	301	A86	C7-C6	4.17	1.59	1.50
41	37	316	A86	C7-C6	4.16	1.59	1.50
41	13	317	A86	C7-C6	4.16	1.59	1.50
41	35	315	A86	O4-C38	4.16	1.44	1.35
41	16	310	A86	O4-C38	4.16	1.44	1.35
41	33	317	A86	C7-C6	4.16	1.59	1.50
41	17	315	A86	O4-C38	4.16	1.44	1.35
41	20	201	A86	C7-C6	4.16	1.59	1.50
41	39	311	A86	C2-C1	4.16	1.41	1.35
30	12	305	CLA	C4D-ND	-4.16	1.32	1.37
41	38	315	A86	C17-C18	-4.16	1.46	1.52
41	31	316	A86	C2-C1	4.16	1.41	1.35
41	40	201	A86	C7-C6	4.16	1.59	1.50
41	37	302	A86	C7-C6	4.16	1.59	1.50
41	17	302	A86	C7-C6	4.16	1.59	1.50
41	21	313	A86	C7-C6	4.16	1.59	1.50
41	11	316	A86	C2-C1	4.15	1.41	1.35
41	11	312	A86	C7-C6	4.15	1.59	1.50
41	32	304	A86	C17-C18	-4.15	1.46	1.52
41	13	315	A86	C7-C6	4.15	1.59	1.50
41	33	315	A86	C7-C6	4.15	1.59	1.50
41	14	313	A86	C7-C6	4.15	1.59	1.50
41	31	312	A86	C7-C6	4.15	1.59	1.50
41	41	314	A86	O4-C38	4.15	1.44	1.35
41	41	312	A86	C26-C27	4.15	1.41	1.35
41	17	311	A86	C7-C6	4.15	1.59	1.50
41	20	213	A86	C7-C6	4.15	1.59	1.50
41	37	315	A86	O4-C38	4.15	1.44	1.35
41	33	315	A86	C26-C27	4.15	1.41	1.35
41	38	302	A86	C2-C1	4.14	1.41	1.35
41	15	314	A86	C21-C20	4.14	1.58	1.51
41	33	315	A86	C17-C18	-4.14	1.46	1.52
41	21	313	A86	C2-C1	4.14	1.41	1.35
41	35	316	A86	C17-C18	-4.14	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	318	A86	C21-C20	4.14	1.58	1.51
41	40	211	A86	O4-C38	4.14	1.44	1.35
30	A	402	CLA	C4D-ND	-4.14	1.32	1.37
41	31	314	A86	C21-C20	4.14	1.58	1.51
41	37	302	A86	O4-C38	4.14	1.44	1.35
30	b	611	CLA	C4D-ND	-4.14	1.32	1.37
41	32	319	A86	C7-C6	4.14	1.59	1.50
41	40	213	A86	C7-C6	4.14	1.59	1.50
41	35	312	A86	C7-C6	4.14	1.59	1.50
41	35	311	A86	O4-C38	4.14	1.44	1.35
41	15	312	A86	C7-C6	4.14	1.59	1.50
41	31	314	A86	C7-C6	4.14	1.59	1.50
41	41	311	A86	O4-C38	4.14	1.44	1.35
41	18	314	A86	O4-C38	4.13	1.44	1.35
30	c	509	CLA	C4D-ND	-4.13	1.32	1.37
41	14	312	A86	O4-C38	4.13	1.44	1.35
41	37	314	A86	C17-C18	-4.13	1.46	1.52
41	11	314	A86	C21-C20	4.13	1.58	1.51
41	32	318	A86	C7-C6	4.13	1.59	1.50
41	16	311	A86	O4-C38	4.13	1.44	1.35
41	37	311	A86	C7-C6	4.13	1.59	1.50
41	15	311	A86	O4-C38	4.13	1.44	1.35
41	21	314	A86	C7-C6	4.13	1.59	1.50
30	B	604	CLA	C4D-ND	-4.13	1.32	1.37
41	35	314	A86	C21-C20	4.13	1.58	1.51
41	11	314	A86	C7-C6	4.13	1.59	1.50
41	21	311	A86	O4-C38	4.13	1.44	1.35
41	18	313	A86	C17-C18	-4.13	1.46	1.52
41	18	315	A86	C17-C18	-4.13	1.46	1.52
41	12	318	A86	C17-C18	-4.13	1.46	1.52
30	14	302	CLA	C4D-ND	-4.13	1.32	1.37
41	33	313	A86	O4-C38	4.13	1.44	1.35
41	16	313	A86	C7-C6	4.12	1.59	1.50
41	17	302	A86	C2-C1	4.12	1.41	1.35
41	11	314	A86	C17-C18	-4.12	1.46	1.52
41	12	316	A86	O4-C38	4.12	1.44	1.35
41	21	314	A86	O4-C38	4.12	1.44	1.35
30	d	402	CLA	C4D-ND	-4.12	1.32	1.37
41	37	315	A86	C2-C1	4.12	1.41	1.35
41	40	211	A86	C2-C1	4.12	1.41	1.35
41	33	302	A86	C2-C1	4.12	1.41	1.35
41	16	312	A86	C7-C6	4.12	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	39	310	A86	C7-C6	4.12	1.59	1.50
41	41	314	A86	C7-C6	4.12	1.59	1.50
30	b	604	CLA	C4D-ND	-4.12	1.32	1.37
41	12	315	A86	C17-C18	-4.12	1.46	1.52
41	15	313	A86	C17-C18	-4.12	1.46	1.52
41	17	311	A86	C2-C1	4.12	1.41	1.35
41	34	311	A86	C17-C18	-4.12	1.46	1.52
41	36	313	A86	C7-C6	4.11	1.59	1.50
41	33	314	A86	C7-C6	4.11	1.59	1.50
41	41	313	A86	C2-C1	4.11	1.41	1.35
41	34	313	A86	C7-C6	4.11	1.59	1.50
41	38	313	A86	C17-C18	-4.11	1.46	1.52
41	20	211	A86	O4-C38	4.11	1.44	1.35
41	32	315	A86	O4-C38	4.11	1.44	1.35
41	21	310	A86	C2-C1	4.11	1.41	1.35
41	12	319	A86	C7-C6	4.11	1.59	1.50
41	15	314	A86	C17-C18	-4.11	1.46	1.52
41	21	312	A86	C26-C27	4.11	1.41	1.35
41	41	313	A86	C7-C6	4.11	1.59	1.50
41	36	311	A86	O4-C38	4.11	1.44	1.35
41	14	312	A86	C7-C6	4.11	1.59	1.50
41	11	316	A86	C21-C20	4.11	1.58	1.51
30	11	301	CLA	C4D-ND	-4.10	1.32	1.37
41	11	311	A86	O4-C38	4.10	1.44	1.35
41	17	302	A86	O4-C38	4.10	1.44	1.35
41	37	311	A86	C2-C1	4.10	1.41	1.35
41	31	311	A86	O4-C38	4.10	1.44	1.35
41	13	315	A86	C2-C1	4.10	1.41	1.35
41	34	312	A86	C7-C6	4.10	1.59	1.50
41	13	314	A86	C17-C18	-4.10	1.46	1.52
41	21	311	A86	C7-C6	4.10	1.59	1.50
30	B	610	CLA	C4D-ND	-4.09	1.32	1.37
41	34	314	A86	C17-C18	-4.09	1.46	1.52
41	17	316	A86	C21-C20	4.09	1.58	1.51
41	13	317	A86	C21-C20	4.09	1.58	1.51
30	A	404	CLA	C4D-ND	-4.09	1.32	1.37
41	14	314	A86	C17-C18	-4.09	1.46	1.52
41	13	313	A86	C7-C6	4.09	1.59	1.50
39	d	408	PL9	C7-C8	-4.09	1.44	1.50
41	12	319	A86	C21-C20	4.09	1.58	1.51
41	17	313	A86	C7-C6	4.09	1.59	1.50
41	33	315	A86	C2-C1	4.09	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	18	314	A86	C7-C6	4.09	1.59	1.50
30	a	403	CLA	C4D-ND	-4.09	1.32	1.37
41	32	317	A86	C21-C20	4.09	1.58	1.51
41	36	310	A86	C7-C6	4.09	1.59	1.50
41	20	201	A86	O4-C38	4.08	1.44	1.35
30	c	514	CLA	C4D-ND	-4.08	1.32	1.37
41	36	312	A86	C7-C6	4.08	1.59	1.50
41	18	302	A86	C2-C1	4.08	1.41	1.35
30	39	301	CLA	C4D-ND	-4.08	1.32	1.37
41	13	315	A86	C21-C20	4.08	1.58	1.51
41	32	319	A86	O4-C38	4.08	1.44	1.35
41	35	314	A86	O4-C38	4.08	1.44	1.35
41	16	313	A86	C2-C1	4.08	1.41	1.35
41	15	314	A86	C7-C6	4.08	1.59	1.50
41	33	317	A86	O4-C38	4.08	1.44	1.35
41	33	317	A86	C21-C20	4.08	1.58	1.51
41	16	311	A86	C7-C6	4.08	1.59	1.50
41	16	310	A86	C7-C6	4.08	1.59	1.50
41	31	313	A86	C21-C20	4.07	1.58	1.51
41	13	315	A86	O4-C38	4.07	1.44	1.35
30	c	508	CLA	C4D-ND	-4.07	1.32	1.37
41	37	316	A86	O4-C38	4.07	1.44	1.35
41	32	319	A86	C21-C20	4.07	1.58	1.51
30	B	623	CLA	C4D-ND	-4.07	1.32	1.37
41	33	312	A86	C26-C27	4.07	1.41	1.35
41	33	316	A86	C21-C20	4.07	1.58	1.51
41	40	201	A86	O4-C38	4.07	1.44	1.35
41	38	314	A86	C7-C6	4.07	1.59	1.50
41	32	314	A86	C7-C6	4.06	1.59	1.50
30	c	503	CLA	C4D-ND	-4.06	1.32	1.37
41	17	315	A86	C2-C1	4.06	1.41	1.35
41	19	311	A86	C7-C6	4.06	1.59	1.50
41	37	313	A86	C7-C6	4.06	1.59	1.50
41	36	313	A86	O4-C38	4.06	1.44	1.35
41	32	314	A86	C17-C18	-4.06	1.46	1.52
41	35	311	A86	C7-C6	4.06	1.59	1.50
41	34	312	A86	O4-C38	4.06	1.44	1.35
41	16	313	A86	O4-C38	4.06	1.44	1.35
41	15	314	A86	C2-C1	4.06	1.41	1.35
41	13	317	A86	O4-C38	4.06	1.44	1.35
30	C	508	CLA	C4D-ND	-4.06	1.32	1.37
41	36	313	A86	C2-C1	4.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	31	311	A86	C7-C6	4.06	1.59	1.50
41	15	311	A86	C7-C6	4.05	1.59	1.50
41	41	310	A86	C7-C6	4.05	1.59	1.50
41	32	316	A86	C7-C6	4.05	1.59	1.50
41	20	211	A86	C7-C6	4.05	1.59	1.50
41	17	312	A86	C7-C6	4.05	1.59	1.50
41	12	316	A86	C7-C6	4.05	1.59	1.50
41	31	314	A86	O4-C38	4.05	1.44	1.35
41	35	314	A86	C7-C6	4.05	1.59	1.50
41	12	318	A86	C21-C20	4.05	1.58	1.51
41	41	311	A86	C7-C6	4.05	1.59	1.50
41	37	316	A86	C21-C20	4.05	1.58	1.51
41	14	311	A86	C17-C18	-4.05	1.46	1.52
41	40	211	A86	C7-C6	4.05	1.59	1.50
41	36	311	A86	C7-C6	4.05	1.59	1.50
30	19	301	CLA	C4D-ND	-4.05	1.32	1.37
41	39	311	A86	C7-C6	4.05	1.59	1.50
41	33	312	A86	C17-C18	-4.04	1.46	1.52
41	15	316	A86	C21-C20	4.04	1.58	1.51
41	13	311	A86	C17-C18	-4.04	1.46	1.52
41	11	311	A86	C7-C6	4.04	1.59	1.50
30	c	505	CLA	C4D-ND	-4.04	1.32	1.37
41	31	310	A86	C17-C18	-4.04	1.46	1.52
41	34	311	A86	C21-C20	4.04	1.58	1.51
41	35	316	A86	C21-C20	4.04	1.58	1.51
30	D	402	CLA	C4D-ND	-4.04	1.32	1.37
41	13	311	A86	C26-C27	4.04	1.41	1.35
41	17	316	A86	O4-C38	4.04	1.44	1.35
41	15	314	A86	O4-C38	4.03	1.44	1.35
41	18	313	A86	C7-C6	4.03	1.59	1.50
41	39	309	A86	C7-C6	4.03	1.59	1.50
41	39	309	A86	C2-C1	4.03	1.41	1.35
41	31	316	A86	C21-C20	4.03	1.58	1.51
41	34	312	A86	C2-C1	4.03	1.41	1.35
41	35	310	A86	C7-C6	4.03	1.59	1.50
41	17	316	A86	C2-C1	4.03	1.41	1.35
41	14	311	A86	C7-C6	4.03	1.59	1.50
41	11	310	A86	C17-C18	-4.03	1.46	1.52
41	12	317	A86	C7-C6	4.03	1.59	1.50
41	33	313	A86	C7-C6	4.03	1.59	1.50
41	37	316	A86	C2-C1	4.03	1.41	1.35
41	34	311	A86	C7-C6	4.03	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	15	313	A86	C21-C20	4.03	1.58	1.51
41	19	309	A86	C7-C6	4.03	1.59	1.50
41	41	310	A86	C2-C1	4.03	1.41	1.35
41	31	310	A86	C7-C6	4.02	1.59	1.50
41	33	302	A86	C21-C20	4.02	1.58	1.51
41	40	210	A86	C21-C20	4.02	1.58	1.51
41	12	315	A86	C7-C6	4.02	1.59	1.50
41	13	316	A86	C21-C20	4.02	1.58	1.51
41	16	313	A86	C21-C20	4.02	1.58	1.51
41	12	319	A86	C2-C1	4.02	1.41	1.35
41	11	310	A86	C7-C6	4.02	1.59	1.50
41	21	310	A86	C7-C6	4.02	1.59	1.50
41	15	311	A86	C2-C1	4.02	1.41	1.35
41	12	315	A86	C21-C20	4.02	1.58	1.51
41	32	315	A86	C7-C6	4.02	1.59	1.50
41	20	210	A86	C21-C20	4.02	1.58	1.51
41	32	318	A86	O4-C38	4.01	1.44	1.35
41	38	313	A86	C7-C6	4.01	1.59	1.50
41	17	315	A86	C7-C6	4.01	1.59	1.50
41	35	310	A86	C17-C18	-4.01	1.46	1.52
41	37	312	A86	C7-C6	4.01	1.59	1.50
30	b	610	CLA	C4D-ND	-4.01	1.32	1.37
41	41	310	A86	O4-C38	4.01	1.44	1.35
41	38	302	A86	C21-C20	4.01	1.58	1.51
41	11	314	A86	O4-C38	4.01	1.44	1.35
41	35	314	A86	C2-C1	4.01	1.41	1.35
41	38	315	A86	C21-C20	4.01	1.58	1.51
41	37	315	A86	C9-C10	4.01	1.55	1.43
41	13	314	A86	C2-C1	4.01	1.41	1.35
41	36	311	A86	C2-C1	4.01	1.41	1.35
41	11	310	A86	C21-C20	4.01	1.58	1.51
41	15	310	A86	C7-C6	4.01	1.59	1.50
41	35	313	A86	C21-C20	4.01	1.58	1.51
30	b	622	CLA	C4D-ND	-4.00	1.32	1.37
41	17	311	A86	C21-C20	4.00	1.58	1.51
41	35	311	A86	C2-C1	4.00	1.41	1.35
41	36	313	A86	C21-C20	4.00	1.58	1.51
41	17	315	A86	C9-C10	4.00	1.55	1.43
30	16	307	CLA	C4D-ND	-4.00	1.32	1.37
41	16	311	A86	C2-C1	4.00	1.41	1.35
41	32	317	A86	C2-C1	4.00	1.41	1.35
41	38	313	A86	C26-C27	4.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	304	A86	C21-C20	4.00	1.58	1.51
30	C	514	CLA	C4D-ND	-4.00	1.32	1.37
41	13	301	A86	C21-C20	4.00	1.58	1.51
41	12	319	A86	O4-C38	4.00	1.44	1.35
41	31	310	A86	C21-C20	4.00	1.58	1.51
41	15	315	A86	C21-C20	3.99	1.58	1.51
41	11	313	A86	C21-C20	3.99	1.58	1.51
41	32	319	A86	C2-C1	3.99	1.41	1.35
41	14	314	A86	C21-C20	3.99	1.58	1.51
41	11	313	A86	C2-C1	3.99	1.41	1.35
41	41	312	A86	C7-C6	3.99	1.59	1.50
41	31	313	A86	C2-C1	3.99	1.41	1.35
30	C	507	CLA	CMB-C2B	-3.99	1.43	1.51
41	15	310	A86	C17-C18	-3.99	1.46	1.52
41	32	318	A86	C2-C1	3.99	1.41	1.35
41	37	311	A86	C21-C20	3.99	1.58	1.51
41	15	313	A86	C2-C1	3.99	1.41	1.35
41	35	310	A86	C21-C20	3.98	1.58	1.51
41	21	310	A86	O4-C38	3.98	1.44	1.35
41	35	315	A86	C21-C20	3.98	1.58	1.51
41	34	314	A86	C21-C20	3.98	1.58	1.51
41	14	311	A86	C21-C20	3.98	1.58	1.51
41	32	314	A86	C21-C20	3.98	1.58	1.51
30	b	607	CLA	C4D-ND	-3.98	1.32	1.37
41	18	313	A86	C26-C27	3.98	1.41	1.35
41	15	310	A86	C21-C20	3.98	1.58	1.51
30	36	306	CLA	C1D-ND	3.98	1.42	1.37
41	18	313	A86	O4-C38	3.97	1.44	1.35
41	12	304	A86	C21-C20	3.97	1.58	1.51
30	C	513	CLA	C4D-ND	-3.97	1.32	1.37
41	18	314	A86	C2-C1	3.97	1.41	1.35
41	38	314	A86	C2-C1	3.97	1.41	1.35
30	B	606	CLA	C4D-ND	-3.97	1.32	1.37
41	13	312	A86	C7-C6	3.97	1.59	1.50
41	17	312	A86	C2-C1	3.97	1.41	1.35
41	38	313	A86	C21-C20	3.97	1.58	1.51
41	37	312	A86	C2-C1	3.97	1.41	1.35
41	33	313	A86	C2-C1	3.97	1.41	1.35
41	33	317	A86	C2-C1	3.97	1.41	1.35
41	40	210	A86	C17-C18	-3.97	1.46	1.52
30	C	503	CLA	C4D-ND	-3.97	1.32	1.37
41	14	312	A86	C2-C1	3.97	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	38	315	A86	C2-C1	3.96	1.41	1.35
41	13	311	A86	C7-C6	3.96	1.59	1.50
41	21	312	A86	C7-C6	3.96	1.59	1.50
41	37	315	A86	C10-C11	3.96	1.46	1.34
41	37	315	A86	C7-C6	3.96	1.59	1.50
41	14	311	A86	C26-C27	3.96	1.41	1.35
41	33	312	A86	C21-C20	3.96	1.58	1.51
30	16	306	CLA	C1D-ND	3.96	1.42	1.37
30	c	507	CLA	CMB-C2B	-3.96	1.43	1.51
41	18	313	A86	C21-C20	3.96	1.58	1.51
41	20	210	A86	C17-C18	-3.96	1.46	1.52
41	18	315	A86	C21-C20	3.96	1.58	1.51
41	38	313	A86	O4-C38	3.96	1.44	1.35
41	31	314	A86	C2-C1	3.96	1.41	1.35
41	33	312	A86	C7-C6	3.95	1.59	1.50
41	34	311	A86	C26-C27	3.95	1.41	1.35
41	35	313	A86	C2-C1	3.95	1.41	1.35
41	11	310	A86	O4-C38	3.95	1.44	1.35
41	13	311	A86	O4-C38	3.95	1.44	1.35
41	13	312	A86	C2-C1	3.95	1.41	1.35
41	33	312	A86	C2-C1	3.95	1.41	1.35
30	17	301	CLA	C4D-ND	-3.95	1.32	1.37
41	41	312	A86	C2-C1	3.95	1.41	1.35
30	B	607	CLA	C4D-ND	-3.95	1.32	1.37
41	12	315	A86	O4-C38	3.95	1.44	1.35
41	35	310	A86	O4-C38	3.95	1.44	1.35
41	17	314	A86	C21-C20	3.94	1.58	1.51
41	15	310	A86	C26-C27	3.94	1.41	1.35
30	C	512	CLA	C4D-ND	-3.94	1.32	1.37
41	20	212	A86	C5-C6	3.94	1.41	1.35
41	17	315	A86	C10-C11	3.94	1.46	1.34
41	31	310	A86	O4-C38	3.94	1.44	1.35
41	14	314	A86	C2-C1	3.94	1.41	1.35
30	c	513	CLA	C4D-ND	-3.94	1.32	1.37
41	13	311	A86	C21-C20	3.94	1.58	1.51
41	31	310	A86	C2-C1	3.94	1.41	1.35
41	13	317	A86	C2-C1	3.94	1.41	1.35
41	15	310	A86	C2-C1	3.94	1.41	1.35
41	15	310	A86	O4-C38	3.94	1.44	1.35
30	36	307	CLA	C4D-ND	-3.94	1.32	1.37
41	32	315	A86	C2-C1	3.93	1.41	1.35
30	36	302	CLA	C4D-ND	-3.93	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	611	CLA	CMB-C2B	-3.93	1.43	1.51
30	35	304	CLA	C1D-ND	3.93	1.42	1.37
41	33	312	A86	O4-C38	3.93	1.44	1.35
41	14	311	A86	O4-C38	3.93	1.44	1.35
41	21	312	A86	C2-C1	3.93	1.41	1.35
30	c	509	CLA	CMB-C2B	-3.93	1.43	1.51
41	20	201	A86	C9-C10	3.93	1.55	1.43
41	35	310	A86	C26-C27	3.93	1.41	1.35
41	32	314	A86	O4-C38	3.93	1.44	1.35
30	b	606	CLA	C4D-ND	-3.93	1.32	1.37
41	40	201	A86	C9-C10	3.93	1.55	1.43
30	c	512	CLA	C4D-ND	-3.92	1.32	1.37
30	37	301	CLA	C4D-ND	-3.92	1.32	1.37
41	11	310	A86	C2-C1	3.92	1.41	1.35
41	19	309	A86	C2-C1	3.92	1.41	1.35
41	13	314	A86	C21-C20	3.92	1.58	1.51
30	15	304	CLA	C1D-ND	3.92	1.42	1.37
41	40	212	A86	C10-C11	3.92	1.45	1.34
41	12	318	A86	C2-C1	3.92	1.41	1.35
41	33	315	A86	C21-C20	3.92	1.58	1.51
30	c	511	CLA	C4D-ND	-3.92	1.32	1.37
30	34	304	CLA	C4D-ND	-3.92	1.32	1.37
41	34	314	A86	C2-C1	3.92	1.41	1.35
41	11	310	A86	C26-C27	3.92	1.41	1.35
41	11	314	A86	C2-C1	3.92	1.41	1.35
41	18	315	A86	C2-C1	3.92	1.41	1.35
30	C	505	CLA	C4D-ND	-3.91	1.32	1.37
41	12	316	A86	C2-C1	3.91	1.41	1.35
41	34	311	A86	O4-C38	3.91	1.44	1.35
41	31	310	A86	C26-C27	3.91	1.41	1.35
41	20	212	A86	C9-C10	3.91	1.55	1.43
30	D	406	CLA	C4D-ND	-3.91	1.32	1.37
41	40	212	A86	C5-C6	3.91	1.41	1.35
41	18	302	A86	C21-C20	3.91	1.58	1.51
41	40	212	A86	C9-C10	3.91	1.55	1.43
41	20	210	A86	C19-C18	3.91	1.58	1.52
41	34	311	A86	C2-C1	3.90	1.41	1.35
41	13	311	A86	C2-C1	3.90	1.41	1.35
41	31	311	A86	C2-C1	3.90	1.41	1.35
41	40	210	A86	C19-C18	3.90	1.57	1.52
30	16	302	CLA	C4D-ND	-3.90	1.32	1.37
41	20	212	A86	C10-C11	3.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	12	315	A86	C26-C27	3.89	1.40	1.35
30	W	103	CLA	C1D-ND	3.89	1.42	1.37
41	35	310	A86	C2-C1	3.89	1.40	1.35
41	20	212	A86	C21-C20	3.89	1.57	1.51
39	D	407	PL9	C7-C8	-3.89	1.45	1.50
41	32	315	A86	C21-C20	3.89	1.57	1.51
41	40	212	A86	C21-C20	3.88	1.57	1.51
41	11	311	A86	C2-C1	3.88	1.40	1.35
41	36	311	A86	C21-C20	3.88	1.57	1.51
30	C	504	CLA	C4D-ND	-3.88	1.32	1.37
30	d	407	CLA	C4D-ND	-3.88	1.32	1.37
41	37	311	A86	C9-C10	3.88	1.55	1.43
41	20	210	A86	C10-C11	3.88	1.45	1.34
30	33	305	CLA	C4D-ND	-3.87	1.32	1.37
41	37	312	A86	C21-C20	3.87	1.57	1.51
41	32	314	A86	C26-C27	3.87	1.40	1.35
41	34	313	A86	C9-C10	3.87	1.55	1.43
41	19	310	A86	C2-C1	3.86	1.40	1.35
41	14	311	A86	C2-C1	3.86	1.40	1.35
30	B	611	CLA	CMB-C2B	-3.86	1.43	1.51
41	19	311	A86	C9-C10	3.86	1.55	1.43
30	C	507	CLA	C4D-ND	-3.86	1.32	1.37
30	41	305	CLA	C1D-ND	3.86	1.42	1.37
30	37	303	CLA	C4D-ND	-3.86	1.32	1.37
41	12	316	A86	C21-C20	3.86	1.57	1.51
41	37	314	A86	C21-C20	3.85	1.57	1.51
30	21	309	CLA	C1D-ND	3.85	1.42	1.37
30	w	103	CLA	C1D-ND	3.85	1.42	1.37
41	15	312	A86	C9-C10	3.85	1.55	1.43
41	39	311	A86	C9-C10	3.85	1.55	1.43
41	17	313	A86	C9-C10	3.85	1.55	1.43
41	40	210	A86	C10-C11	3.85	1.45	1.34
41	13	313	A86	C9-C10	3.85	1.55	1.43
41	31	312	A86	C9-C10	3.85	1.55	1.43
41	17	311	A86	C9-C10	3.84	1.55	1.43
41	16	311	A86	C21-C20	3.84	1.57	1.51
30	17	303	CLA	C4D-ND	-3.84	1.32	1.37
41	40	212	A86	C19-C18	3.84	1.57	1.52
41	14	313	A86	C9-C10	3.84	1.55	1.43
41	35	312	A86	C9-C10	3.84	1.55	1.43
30	38	309	CLA	C4D-ND	-3.83	1.32	1.37
41	32	304	A86	C9-C10	3.83	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	18	309	CLA	C4D-ND	-3.83	1.32	1.37
30	z	101	CLA	C4D-ND	-3.83	1.32	1.37
41	11	312	A86	C9-C10	3.83	1.55	1.43
41	19	310	A86	C10-C11	3.83	1.45	1.34
41	37	313	A86	C9-C10	3.83	1.55	1.43
30	39	307	CLA	C4D-ND	-3.83	1.32	1.37
41	40	213	A86	C9-C10	3.83	1.55	1.43
39	D	407	PL9	C52-C5	-3.83	1.42	1.50
41	20	210	A86	C9-C10	3.83	1.55	1.43
41	33	314	A86	C9-C10	3.83	1.55	1.43
41	41	314	A86	C9-C10	3.82	1.55	1.43
30	b	603	CLA	C4D-ND	-3.82	1.32	1.37
41	32	314	A86	C2-C1	3.82	1.40	1.35
41	12	317	A86	C10-C11	3.82	1.45	1.34
30	39	302	CLA	C4D-ND	-3.82	1.32	1.37
41	20	213	A86	C9-C10	3.82	1.55	1.43
41	12	315	A86	C2-C1	3.82	1.40	1.35
41	11	316	A86	C9-C10	3.82	1.55	1.43
30	19	307	CLA	C4D-ND	-3.82	1.32	1.37
41	13	301	A86	C9-C10	3.82	1.55	1.43
41	33	316	A86	C9-C10	3.82	1.55	1.43
41	32	316	A86	C9-C10	3.82	1.55	1.43
41	37	311	A86	C19-C18	3.82	1.57	1.52
41	31	316	A86	C9-C10	3.81	1.55	1.43
41	18	313	A86	C2-C1	3.81	1.40	1.35
41	36	312	A86	C9-C10	3.81	1.55	1.43
41	21	314	A86	C9-C10	3.81	1.55	1.43
41	14	313	A86	C10-C11	3.81	1.45	1.34
30	C	511	CLA	C4D-ND	-3.81	1.32	1.37
41	20	212	A86	C19-C18	3.81	1.57	1.52
41	35	315	A86	C9-C10	3.81	1.55	1.43
41	16	312	A86	C9-C10	3.81	1.55	1.43
41	12	304	A86	C9-C10	3.81	1.55	1.43
41	13	316	A86	C9-C10	3.81	1.55	1.43
41	12	317	A86	C9-C10	3.81	1.55	1.43
41	39	310	A86	C9-C10	3.81	1.55	1.43
41	33	302	A86	C9-C10	3.80	1.55	1.43
41	17	312	A86	C21-C20	3.80	1.57	1.51
41	15	315	A86	C9-C10	3.80	1.55	1.43
41	16	312	A86	C10-C11	3.80	1.45	1.34
30	C	509	CLA	CMB-C2B	-3.80	1.43	1.51
41	40	201	A86	C21-C20	3.80	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	40	210	A86	C5-C6	3.80	1.40	1.35
41	39	310	A86	C10-C11	3.80	1.45	1.34
41	15	312	A86	C10-C11	3.80	1.45	1.34
41	35	312	A86	C10-C11	3.80	1.45	1.34
41	37	313	A86	C10-C11	3.80	1.45	1.34
41	19	310	A86	C9-C10	3.80	1.55	1.43
41	36	312	A86	C10-C11	3.80	1.45	1.34
41	20	210	A86	C5-C6	3.80	1.40	1.35
35	L	101	LHG	O7-C5	-3.79	1.37	1.46
30	34	308	CLA	C4D-ND	-3.79	1.32	1.37
41	35	316	A86	C9-C10	3.79	1.55	1.43
41	15	316	A86	C9-C10	3.79	1.55	1.43
41	19	311	A86	C21-C20	3.79	1.57	1.51
41	38	313	A86	C2-C1	3.79	1.40	1.35
41	32	316	A86	C10-C11	3.79	1.45	1.34
32	B	616	BCR	C30-C25	-3.79	1.48	1.53
30	B	615	CLA	C3B-C2B	-3.79	1.35	1.40
41	17	311	A86	C10-C11	3.79	1.45	1.34
41	33	313	A86	C21-C20	3.78	1.57	1.51
41	17	311	A86	C19-C18	3.78	1.57	1.52
41	32	316	A86	C5-C6	3.78	1.40	1.35
41	17	313	A86	C10-C11	3.78	1.45	1.34
41	20	213	A86	C10-C11	3.78	1.45	1.34
39	d	408	PL9	C52-C5	-3.78	1.42	1.50
41	34	313	A86	C10-C11	3.78	1.45	1.34
30	36	304	CLA	C4D-ND	-3.78	1.32	1.37
30	41	309	CLA	C1D-ND	3.78	1.42	1.37
30	c	507	CLA	C4D-ND	-3.78	1.32	1.37
41	40	210	A86	C9-C10	3.78	1.55	1.43
41	39	310	A86	C2-C1	3.78	1.40	1.35
41	11	311	A86	C21-C20	3.77	1.57	1.51
41	41	314	A86	C10-C11	3.77	1.45	1.34
41	36	313	A86	C9-C10	3.77	1.55	1.43
35	d	409	LHG	O7-C5	-3.77	1.37	1.46
41	20	201	A86	C21-C20	3.77	1.57	1.51
41	34	312	A86	C21-C20	3.77	1.57	1.51
30	33	309	CLA	C4D-ND	-3.77	1.32	1.37
30	31	307	CLA	C4D-ND	-3.77	1.32	1.37
30	15	307	CLA	C4D-ND	-3.77	1.32	1.37
41	39	311	A86	C21-C20	3.77	1.57	1.51
41	21	314	A86	C10-C11	3.76	1.45	1.34
30	B	603	CLA	C4D-ND	-3.76	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	17	305	CLA	C4D-ND	-3.76	1.32	1.37
41	11	312	A86	C10-C11	3.76	1.45	1.34
41	40	213	A86	C10-C11	3.76	1.45	1.34
30	Z	102	CLA	C1D-ND	3.76	1.42	1.37
41	38	302	A86	C9-C10	3.76	1.55	1.43
41	31	312	A86	C10-C11	3.76	1.45	1.34
32	h	101	BCR	C1-C6	-3.76	1.48	1.53
30	35	307	CLA	C4D-ND	-3.75	1.32	1.37
41	12	319	A86	C9-C10	3.75	1.55	1.43
41	13	315	A86	C9-C10	3.75	1.55	1.43
41	37	311	A86	C10-C11	3.75	1.45	1.34
30	17	308	CLA	C4D-ND	-3.75	1.32	1.37
41	33	314	A86	C10-C11	3.75	1.45	1.34
41	40	211	A86	C9-C10	3.75	1.55	1.43
41	17	315	A86	C21-C20	3.75	1.57	1.51
41	18	314	A86	C9-C10	3.75	1.55	1.43
41	14	312	A86	C21-C20	3.75	1.57	1.51
41	14	312	A86	C9-C10	3.75	1.55	1.43
41	16	310	A86	C9-C10	3.75	1.55	1.43
41	18	302	A86	C9-C10	3.75	1.55	1.43
41	32	318	A86	C9-C10	3.75	1.55	1.43
41	13	313	A86	C10-C11	3.74	1.45	1.34
41	16	313	A86	C9-C10	3.74	1.55	1.43
41	37	316	A86	C9-C10	3.74	1.55	1.43
41	12	317	A86	C5-C6	3.74	1.40	1.35
41	41	310	A86	C21-C20	3.74	1.57	1.51
30	31	303	CLA	C4D-ND	-3.74	1.32	1.37
30	37	305	CLA	C4D-ND	-3.74	1.32	1.37
41	13	317	A86	C9-C10	3.74	1.55	1.43
41	17	314	A86	C9-C10	3.74	1.55	1.43
41	36	310	A86	C9-C10	3.74	1.55	1.43
41	18	314	A86	C21-C20	3.74	1.57	1.51
30	c	504	CLA	C4D-ND	-3.74	1.32	1.37
41	20	211	A86	C9-C10	3.73	1.55	1.43
41	34	313	A86	C5-C6	3.73	1.40	1.35
41	34	312	A86	C9-C10	3.73	1.55	1.43
41	13	312	A86	C21-C20	3.73	1.57	1.51
30	C	519	CLA	C4D-ND	-3.73	1.32	1.37
41	35	311	A86	C21-C20	3.73	1.57	1.51
41	32	319	A86	C9-C10	3.73	1.55	1.43
30	19	302	CLA	C4D-ND	-3.73	1.32	1.37
41	37	315	A86	C21-C20	3.73	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	31	314	A86	C9-C10	3.73	1.55	1.43
30	38	303	CLA	C4D-ND	-3.72	1.32	1.37
41	33	315	A86	C9-C10	3.72	1.55	1.43
30	15	306	CLA	C1D-ND	3.72	1.42	1.37
41	33	317	A86	C9-C10	3.72	1.55	1.43
30	18	303	CLA	C4D-ND	-3.72	1.32	1.37
41	37	312	A86	C9-C10	3.72	1.55	1.43
41	38	314	A86	C9-C10	3.72	1.55	1.43
41	41	314	A86	C5-C6	3.72	1.40	1.35
41	17	312	A86	C9-C10	3.72	1.55	1.43
41	17	316	A86	C9-C10	3.72	1.55	1.43
41	13	314	A86	C9-C10	3.71	1.55	1.43
30	B	601	CLA	C4D-ND	-3.71	1.32	1.37
32	C	518	BCR	C30-C25	-3.71	1.48	1.53
32	H	101	BCR	C1-C6	-3.71	1.48	1.53
41	37	314	A86	C9-C10	3.71	1.54	1.43
41	17	302	A86	C9-C10	3.71	1.54	1.43
41	14	313	A86	C5-C6	3.71	1.40	1.35
41	15	311	A86	C21-C20	3.71	1.57	1.51
32	m	103	BCR	C30-C25	-3.71	1.48	1.53
41	11	311	A86	C9-C10	3.71	1.54	1.43
41	37	302	A86	C9-C10	3.71	1.54	1.43
41	14	314	A86	C9-C10	3.71	1.54	1.43
41	13	312	A86	C9-C10	3.71	1.54	1.43
41	33	313	A86	C10-C11	3.71	1.45	1.34
41	31	311	A86	C21-C20	3.71	1.57	1.51
30	b	602	CLA	C4D-ND	-3.71	1.32	1.37
41	15	312	A86	C5-C6	3.71	1.40	1.35
41	12	316	A86	C9-C10	3.71	1.54	1.43
41	15	314	A86	C9-C10	3.71	1.54	1.43
41	31	311	A86	C9-C10	3.71	1.54	1.43
30	14	308	CLA	C4D-ND	-3.70	1.32	1.37
41	15	313	A86	C9-C10	3.70	1.54	1.43
30	21	305	CLA	C1D-ND	3.70	1.42	1.37
41	21	310	A86	C21-C20	3.70	1.57	1.51
30	B	602	CLA	C4D-ND	-3.70	1.32	1.37
41	31	313	A86	C9-C10	3.70	1.54	1.43
41	38	314	A86	C21-C20	3.70	1.57	1.51
41	37	302	A86	C10-C11	3.70	1.45	1.34
41	34	314	A86	C9-C10	3.70	1.54	1.43
41	13	313	A86	C5-C6	3.70	1.40	1.35
41	13	312	A86	C10-C11	3.70	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	35	306	CLA	C1D-ND	3.70	1.42	1.37
41	35	314	A86	C9-C10	3.70	1.54	1.43
41	11	314	A86	C9-C10	3.70	1.54	1.43
41	21	313	A86	C9-C10	3.70	1.54	1.43
30	16	309	CLA	C4D-ND	-3.69	1.32	1.37
41	11	312	A86	C21-C20	3.69	1.57	1.51
41	21	312	A86	C9-C10	3.69	1.54	1.43
41	33	313	A86	C9-C10	3.69	1.54	1.43
41	11	313	A86	C9-C10	3.69	1.54	1.43
41	41	311	A86	C9-C10	3.69	1.54	1.43
30	41	301	CLA	C1D-ND	3.69	1.42	1.37
41	32	315	A86	C9-C10	3.69	1.54	1.43
41	35	311	A86	C9-C10	3.69	1.54	1.43
41	21	311	A86	C9-C10	3.69	1.54	1.43
30	21	306	CLA	C1D-ND	3.69	1.42	1.37
41	21	313	A86	C21-C20	3.69	1.57	1.51
41	35	312	A86	C5-C6	3.69	1.40	1.35
41	17	302	A86	C10-C11	3.69	1.45	1.34
41	36	311	A86	C9-C10	3.69	1.54	1.43
41	32	317	A86	C9-C10	3.68	1.54	1.43
30	c	524	CLA	C1D-ND	3.68	1.42	1.37
41	16	312	A86	C5-C6	3.68	1.40	1.35
41	35	311	A86	C10-C11	3.68	1.45	1.34
41	35	313	A86	C9-C10	3.68	1.54	1.43
41	36	312	A86	C5-C6	3.68	1.40	1.35
41	14	313	A86	C21-C20	3.68	1.57	1.51
41	15	311	A86	C9-C10	3.68	1.54	1.43
41	33	314	A86	C5-C6	3.68	1.40	1.35
41	15	311	A86	C10-C11	3.68	1.45	1.34
41	16	311	A86	C9-C10	3.68	1.54	1.43
41	16	312	A86	C21-C20	3.68	1.57	1.51
30	32	307	CLA	C4D-ND	-3.68	1.32	1.37
41	17	313	A86	C5-C6	3.67	1.40	1.35
30	18	306	CLA	C1D-ND	3.67	1.42	1.37
30	38	306	CLA	C1D-ND	3.67	1.42	1.37
41	41	312	A86	C9-C10	3.67	1.54	1.43
41	15	314	A86	C10-C11	3.67	1.45	1.34
41	13	313	A86	C21-C20	3.67	1.57	1.51
41	41	313	A86	C9-C10	3.67	1.54	1.43
30	M	101	CLA	C4D-ND	-3.67	1.32	1.37
30	12	307	CLA	C4D-ND	-3.67	1.32	1.37
30	16	304	CLA	C4D-ND	-3.67	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	601	CLA	C4D-ND	-3.67	1.32	1.37
30	40	204	CLA	C4D-ND	-3.67	1.32	1.37
41	33	314	A86	C21-C20	3.67	1.57	1.51
41	21	314	A86	C21-C20	3.67	1.57	1.51
41	12	318	A86	C9-C10	3.67	1.54	1.43
41	39	310	A86	C5-C6	3.67	1.40	1.35
41	31	312	A86	C21-C20	3.66	1.57	1.51
41	39	311	A86	C10-C11	3.66	1.45	1.34
30	12	311	CLA	C4D-ND	-3.66	1.32	1.37
30	32	311	CLA	C4D-ND	-3.66	1.32	1.37
41	40	213	A86	C5-C6	3.66	1.40	1.35
30	B	615	CLA	C4D-ND	-3.66	1.32	1.37
30	34	301	CLA	C4D-ND	-3.66	1.32	1.37
41	19	309	A86	C9-C10	3.66	1.54	1.43
30	m	101	CLA	C4D-ND	-3.66	1.32	1.37
41	12	316	A86	C10-C11	3.66	1.45	1.34
41	39	309	A86	C9-C10	3.66	1.54	1.43
41	37	312	A86	C10-C11	3.66	1.45	1.34
30	18	305	CLA	C4D-ND	-3.66	1.32	1.37
41	35	314	A86	C10-C11	3.66	1.45	1.34
30	20	208	CLA	C1D-ND	3.65	1.42	1.37
41	11	312	A86	C5-C6	3.65	1.40	1.35
41	17	312	A86	C10-C11	3.65	1.45	1.34
41	18	314	A86	C10-C11	3.65	1.45	1.34
30	37	308	CLA	C4D-ND	-3.65	1.32	1.37
41	31	312	A86	C5-C6	3.65	1.40	1.35
41	34	311	A86	C9-C10	3.65	1.54	1.43
41	13	317	A86	C10-C11	3.65	1.45	1.34
41	14	311	A86	C9-C10	3.65	1.54	1.43
30	b	615	CLA	C4D-ND	-3.65	1.32	1.37
41	14	312	A86	C10-C11	3.65	1.45	1.34
41	32	315	A86	C10-C11	3.65	1.45	1.34
30	20	204	CLA	C4D-ND	-3.65	1.32	1.37
41	19	311	A86	C10-C11	3.65	1.45	1.34
41	37	313	A86	C5-C6	3.65	1.40	1.35
41	31	311	A86	C10-C11	3.65	1.45	1.34
30	36	309	CLA	C4D-ND	-3.65	1.32	1.37
41	14	314	A86	C19-C18	3.65	1.57	1.52
41	21	310	A86	C9-C10	3.65	1.54	1.43
41	11	314	A86	C10-C11	3.65	1.45	1.34
41	12	315	A86	C10-C11	3.65	1.45	1.34
41	41	310	A86	C9-C10	3.65	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	16	310	A86	C21-C20	3.65	1.57	1.51
41	32	314	A86	C9-C10	3.64	1.54	1.43
41	20	213	A86	C5-C6	3.64	1.40	1.35
41	17	313	A86	C21-C20	3.64	1.57	1.51
30	W	102	CLA	C4D-ND	-3.64	1.32	1.37
30	39	308	CLA	C4D-ND	-3.64	1.32	1.37
41	33	317	A86	C10-C11	3.64	1.45	1.34
41	35	312	A86	C21-C20	3.64	1.57	1.51
41	41	313	A86	C21-C20	3.64	1.57	1.51
41	38	314	A86	C10-C11	3.64	1.45	1.34
41	20	213	A86	C21-C20	3.64	1.57	1.51
41	40	213	A86	C21-C20	3.64	1.57	1.51
30	21	301	CLA	C1D-ND	3.64	1.42	1.37
30	b	615	CLA	C3B-C2B	-3.64	1.35	1.40
41	34	312	A86	C10-C11	3.64	1.45	1.34
41	31	316	A86	C10-C11	3.64	1.45	1.34
41	13	316	A86	C10-C11	3.63	1.45	1.34
41	36	311	A86	C10-C11	3.63	1.45	1.34
41	34	314	A86	C19-C18	3.63	1.57	1.52
30	B	608	CLA	C4D-ND	-3.63	1.32	1.37
41	15	316	A86	C10-C11	3.63	1.45	1.34
41	35	316	A86	C10-C11	3.63	1.45	1.34
41	32	319	A86	C10-C11	3.63	1.45	1.34
41	18	315	A86	C9-C10	3.63	1.54	1.43
41	16	313	A86	C10-C11	3.63	1.45	1.34
41	35	315	A86	C5-C6	3.63	1.40	1.35
41	33	312	A86	C9-C10	3.63	1.54	1.43
41	32	318	A86	C10-C11	3.63	1.45	1.34
41	11	310	A86	C9-C10	3.63	1.54	1.43
41	33	315	A86	C19-C18	3.63	1.57	1.52
41	11	311	A86	C10-C11	3.63	1.45	1.34
41	17	315	A86	C19-C18	3.63	1.57	1.52
41	36	313	A86	C10-C11	3.63	1.45	1.34
41	32	316	A86	C21-C20	3.63	1.57	1.51
41	36	312	A86	C21-C20	3.63	1.57	1.51
41	15	310	A86	C9-C10	3.63	1.54	1.43
41	33	312	A86	C10-C11	3.63	1.45	1.34
41	13	311	A86	C9-C10	3.63	1.54	1.43
41	19	309	A86	C10-C11	3.63	1.45	1.34
32	c	515	BCR	C30-C25	-3.63	1.48	1.53
41	11	316	A86	C10-C11	3.63	1.45	1.34
41	37	313	A86	C21-C20	3.63	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	11	310	A86	C10-C11	3.63	1.45	1.34
41	16	311	A86	C10-C11	3.62	1.45	1.34
41	18	315	A86	C10-C11	3.62	1.45	1.34
41	12	318	A86	C19-C18	3.62	1.57	1.52
30	b	608	CLA	C4D-ND	-3.62	1.32	1.37
30	35	301	CLA	C4D-ND	-3.62	1.32	1.37
30	13	308	CLA	C4D-ND	-3.62	1.32	1.37
41	12	304	A86	C5-C6	3.62	1.40	1.35
41	32	317	A86	C19-C18	3.62	1.57	1.52
41	34	313	A86	C21-C20	3.62	1.57	1.51
41	12	304	A86	C10-C11	3.62	1.45	1.34
41	18	313	A86	C9-C10	3.62	1.54	1.43
41	19	310	A86	C5-C6	3.62	1.40	1.35
41	35	315	A86	C10-C11	3.62	1.45	1.34
41	13	301	A86	C10-C11	3.62	1.45	1.34
41	38	302	A86	C10-C11	3.62	1.45	1.34
32	c	521	BCR	C30-C25	-3.62	1.48	1.53
30	40	205	CLA	C1D-ND	3.62	1.42	1.37
30	15	301	CLA	C4D-ND	-3.62	1.32	1.37
41	18	302	A86	C10-C11	3.62	1.45	1.34
41	13	315	A86	C10-C11	3.62	1.45	1.34
41	38	315	A86	C10-C11	3.62	1.45	1.34
30	13	304	CLA	C4D-ND	-3.62	1.32	1.37
41	38	315	A86	C9-C10	3.62	1.54	1.43
41	38	302	A86	C5-C6	3.62	1.40	1.35
41	40	201	A86	C5-C6	3.62	1.40	1.35
41	12	315	A86	C9-C10	3.62	1.54	1.43
41	31	313	A86	C19-C18	3.62	1.57	1.52
41	37	316	A86	C10-C11	3.61	1.45	1.34
41	13	314	A86	C19-C18	3.61	1.57	1.52
41	15	312	A86	C21-C20	3.61	1.57	1.51
30	31	315	CLA	C4D-ND	-3.61	1.32	1.37
41	15	315	A86	C10-C11	3.61	1.45	1.34
41	35	310	A86	C9-C10	3.61	1.54	1.43
41	17	316	A86	C10-C11	3.61	1.45	1.34
30	18	308	CLA	C1D-ND	3.61	1.42	1.37
41	18	302	A86	C5-C6	3.61	1.40	1.35
41	13	311	A86	C10-C11	3.61	1.45	1.34
30	32	312	CLA	C4D-ND	-3.61	1.32	1.37
41	37	302	A86	C21-C20	3.61	1.57	1.51
41	38	315	A86	C19-C18	3.61	1.57	1.52
41	31	314	A86	C10-C11	3.61	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	31	310	A86	C9-C10	3.61	1.54	1.43
41	32	314	A86	C10-C11	3.61	1.45	1.34
41	15	310	A86	C10-C11	3.61	1.45	1.34
41	39	309	A86	C10-C11	3.61	1.45	1.34
41	21	314	A86	C5-C6	3.61	1.40	1.35
41	33	302	A86	C10-C11	3.61	1.45	1.34
41	33	302	A86	C5-C6	3.61	1.40	1.35
30	41	306	CLA	C1D-ND	3.60	1.42	1.37
41	33	316	A86	C10-C11	3.60	1.45	1.34
41	12	319	A86	C10-C11	3.60	1.45	1.34
41	31	310	A86	C10-C11	3.60	1.45	1.34
41	36	310	A86	C21-C20	3.60	1.57	1.51
30	b	614	CLA	C4D-ND	-3.60	1.32	1.37
30	38	305	CLA	C4D-ND	-3.60	1.32	1.37
41	14	311	A86	C10-C11	3.60	1.45	1.34
30	w	102	CLA	C4D-ND	-3.60	1.32	1.37
41	38	313	A86	C9-C10	3.60	1.54	1.43
30	C	506	CLA	C4D-ND	-3.60	1.32	1.37
41	33	316	A86	C5-C6	3.60	1.40	1.35
41	16	310	A86	C19-C18	3.60	1.57	1.52
32	c	520	BCR	C1-C6	-3.60	1.48	1.53
42	32	302	LMU	O5B-C1B	3.60	1.51	1.41
30	41	308	CLA	C1D-ND	3.60	1.42	1.37
41	37	314	A86	C19-C18	3.60	1.57	1.52
41	41	314	A86	C21-C20	3.60	1.57	1.51
41	12	317	A86	C21-C20	3.60	1.57	1.51
30	B	605	CLA	C4D-ND	-3.60	1.32	1.37
41	38	313	A86	C10-C11	3.60	1.45	1.34
30	11	307	CLA	C4D-ND	-3.59	1.32	1.37
30	33	310	CLA	C4D-ND	-3.59	1.32	1.37
41	19	309	A86	C21-C20	3.59	1.57	1.51
30	20	205	CLA	C1D-ND	3.59	1.42	1.37
41	18	313	A86	C10-C11	3.59	1.45	1.34
41	17	314	A86	C19-C18	3.59	1.57	1.52
41	13	301	A86	C5-C6	3.59	1.40	1.35
41	35	313	A86	C19-C18	3.59	1.57	1.52
41	41	310	A86	C10-C11	3.59	1.45	1.34
41	11	313	A86	C10-C11	3.59	1.45	1.34
30	40	208	CLA	C1D-ND	3.59	1.42	1.37
42	12	302	LMU	O5B-C1B	3.59	1.51	1.41
41	21	311	A86	C10-C11	3.59	1.45	1.34
41	18	315	A86	C19-C18	3.58	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	35	310	A86	C10-C11	3.58	1.45	1.34
30	19	306	CLA	C4D-ND	-3.58	1.32	1.37
30	C	520	CLA	C4D-ND	-3.58	1.32	1.37
41	32	304	A86	C10-C11	3.58	1.45	1.34
32	B	616	BCR	C1-C6	-3.58	1.48	1.53
41	36	310	A86	C19-C18	3.58	1.57	1.52
30	c	506	CLA	C4D-ND	-3.58	1.32	1.37
41	37	314	A86	C10-C11	3.58	1.45	1.34
41	37	315	A86	C19-C18	3.58	1.57	1.52
41	34	311	A86	C10-C11	3.58	1.45	1.34
41	20	201	A86	C5-C6	3.57	1.40	1.35
41	32	317	A86	C10-C11	3.57	1.44	1.34
41	35	313	A86	C10-C11	3.57	1.44	1.34
41	34	314	A86	C10-C11	3.57	1.44	1.34
41	15	316	A86	C5-C6	3.57	1.40	1.35
41	15	313	A86	C19-C18	3.57	1.57	1.52
41	31	316	A86	C5-C6	3.57	1.40	1.35
30	40	202	CLA	C1D-ND	3.57	1.42	1.37
30	B	614	CLA	C4D-ND	-3.57	1.32	1.37
41	21	310	A86	C10-C11	3.57	1.44	1.34
41	41	311	A86	C21-C20	3.57	1.57	1.51
30	20	206	CLA	C1D-ND	3.57	1.42	1.37
41	39	309	A86	C21-C20	3.57	1.57	1.51
30	12	312	CLA	C4D-ND	-3.57	1.32	1.37
30	14	304	CLA	C4D-ND	-3.57	1.32	1.37
41	41	311	A86	C10-C11	3.57	1.44	1.34
30	19	308	CLA	C4D-ND	-3.57	1.32	1.37
30	21	308	CLA	C1D-ND	3.57	1.42	1.37
30	32	303	CLA	C4D-ND	-3.57	1.32	1.37
30	15	305	CLA	C1D-ND	3.57	1.42	1.37
30	38	307	CLA	C1D-ND	3.57	1.42	1.37
41	11	313	A86	C19-C18	3.56	1.57	1.52
30	14	306	CLA	C1D-ND	3.56	1.42	1.37
41	15	315	A86	C5-C6	3.56	1.40	1.35
30	11	303	CLA	C4D-ND	-3.56	1.32	1.37
41	31	313	A86	C10-C11	3.56	1.44	1.34
30	35	305	CLA	C1D-ND	3.56	1.42	1.37
30	38	308	CLA	C1D-ND	3.56	1.42	1.37
41	13	316	A86	C5-C6	3.55	1.40	1.35
41	12	318	A86	C10-C11	3.55	1.44	1.34
41	17	315	A86	C5-C6	3.55	1.40	1.35
41	21	312	A86	C10-C11	3.55	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	11	316	A86	C5-C6	3.55	1.40	1.35
30	b	612	CLA	CMD-C2D	-3.55	1.43	1.50
41	41	312	A86	C10-C11	3.55	1.44	1.34
32	Y	101	BCR	C1-C6	-3.55	1.48	1.53
41	40	211	A86	C10-C11	3.55	1.44	1.34
32	Z	101	BCR	C30-C25	-3.55	1.48	1.53
41	14	314	A86	C10-C11	3.55	1.44	1.34
41	32	304	A86	C5-C6	3.55	1.40	1.35
41	17	302	A86	C21-C20	3.54	1.57	1.51
41	35	314	A86	C5-C6	3.54	1.40	1.35
30	31	308	CLA	C4D-ND	-3.54	1.32	1.37
41	17	314	A86	C10-C11	3.54	1.44	1.34
30	c	522	CLA	C4D-ND	-3.54	1.32	1.37
41	20	211	A86	C10-C11	3.54	1.44	1.34
41	13	314	A86	C10-C11	3.54	1.44	1.34
41	40	211	A86	C21-C20	3.54	1.57	1.51
32	m	103	BCR	C1-C6	-3.54	1.48	1.53
41	21	311	A86	C21-C20	3.54	1.57	1.51
30	34	309	CLA	C4D-ND	-3.54	1.32	1.37
30	39	306	CLA	C4D-ND	-3.54	1.32	1.37
41	15	313	A86	C10-C11	3.54	1.44	1.34
41	33	315	A86	C10-C11	3.54	1.44	1.34
41	16	310	A86	C5-C6	3.53	1.40	1.35
30	c	523	CLA	C4D-ND	-3.53	1.32	1.37
30	20	202	CLA	C1D-ND	3.53	1.42	1.37
39	d	405	PL9	C3-C4	-3.53	1.43	1.49
41	16	310	A86	C10-C11	3.53	1.44	1.34
30	32	309	CLA	C4D-ND	-3.52	1.32	1.37
30	11	305	CLA	C1D-ND	3.52	1.42	1.37
41	36	310	A86	C10-C11	3.51	1.44	1.34
41	21	313	A86	C10-C11	3.51	1.44	1.34
30	31	305	CLA	C4D-ND	-3.51	1.32	1.37
41	37	315	A86	C5-C6	3.51	1.40	1.35
30	C	521	CLA	C4D-ND	-3.51	1.32	1.37
41	35	316	A86	C5-C6	3.50	1.40	1.35
41	37	311	A86	C5-C6	3.50	1.40	1.35
30	18	310	CLA	C1D-ND	3.50	1.42	1.37
30	b	605	CLA	C4D-ND	-3.50	1.32	1.37
30	11	315	CLA	C4D-ND	-3.50	1.32	1.37
41	20	211	A86	C21-C20	3.50	1.57	1.51
41	36	310	A86	C5-C6	3.50	1.40	1.35
30	18	307	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	41	302	CLA	C1D-ND	3.50	1.42	1.37
30	38	310	CLA	C1D-ND	3.49	1.42	1.37
30	32	306	CLA	C4D-ND	-3.49	1.32	1.37
32	c	515	BCR	C1-C6	-3.49	1.49	1.53
30	19	305	CLA	C4D-ND	-3.49	1.32	1.37
39	D	404	PL9	C3-C4	-3.49	1.43	1.49
30	33	301	CLA	C4D-ND	-3.48	1.32	1.37
41	14	314	A86	C5-C6	3.48	1.40	1.35
30	16	305	CLA	C1D-ND	3.48	1.42	1.37
41	38	314	A86	C5-C6	3.48	1.40	1.35
41	41	313	A86	C10-C11	3.48	1.44	1.34
30	37	307	CLA	C4D-ND	-3.48	1.32	1.37
41	32	318	A86	C5-C6	3.48	1.40	1.35
30	c	503	CLA	C3B-C2B	-3.48	1.35	1.40
41	17	311	A86	C5-C6	3.47	1.40	1.35
30	B	608	CLA	C3B-C2B	-3.46	1.35	1.40
41	13	317	A86	C5-C6	3.46	1.40	1.35
31	d	403	PHO	CAC-C3C	-3.46	1.46	1.52
30	33	307	CLA	C4D-ND	-3.46	1.32	1.37
41	33	317	A86	C5-C6	3.46	1.40	1.35
41	40	213	A86	C19-C18	3.46	1.57	1.52
30	40	206	CLA	C1D-ND	3.46	1.42	1.37
41	15	314	A86	C5-C6	3.46	1.40	1.35
31	A	403	PHO	CAC-C3C	-3.45	1.46	1.52
30	b	602	CLA	C1D-ND	3.45	1.42	1.37
40	E	101	HEM	C3C-CAC	3.45	1.54	1.47
30	38	312	CLA	C1D-ND	3.45	1.42	1.37
30	39	305	CLA	C4D-ND	-3.45	1.32	1.37
30	41	304	CLA	C1D-ND	3.45	1.42	1.37
30	21	302	CLA	C1D-ND	3.45	1.42	1.37
41	37	316	A86	C5-C6	3.45	1.40	1.35
30	21	304	CLA	C1D-ND	3.45	1.42	1.37
41	34	314	A86	C5-C6	3.44	1.40	1.35
30	B	612	CLA	CMD-C2D	-3.44	1.43	1.50
41	11	313	A86	C5-C6	3.44	1.40	1.35
41	20	201	A86	C17-C18	-3.44	1.47	1.52
30	C	503	CLA	C3B-C2B	-3.44	1.35	1.40
30	20	207	CLA	C4D-ND	-3.44	1.33	1.37
30	B	609	CLA	C4D-ND	-3.44	1.33	1.37
30	12	303	CLA	C4D-ND	-3.44	1.33	1.37
41	32	314	A86	C19-C18	3.44	1.57	1.52
30	b	609	CLA	C4D-ND	-3.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	602	CLA	C1D-ND	3.43	1.42	1.37
41	31	314	A86	C5-C6	3.43	1.40	1.35
30	33	308	CLA	C4D-ND	-3.43	1.33	1.37
41	18	314	A86	C5-C6	3.43	1.40	1.35
41	20	211	A86	C5-C6	3.43	1.40	1.35
30	11	308	CLA	C4D-ND	-3.42	1.33	1.37
30	34	308	CLA	C1D-ND	3.42	1.42	1.37
30	20	209	CLA	C4D-ND	-3.42	1.33	1.37
32	a	404	BCR	C1-C6	-3.42	1.49	1.53
30	37	306	CLA	C1D-ND	3.42	1.42	1.37
30	17	310	CLA	C4D-ND	-3.42	1.33	1.37
30	31	302	CLA	C4D-ND	-3.42	1.33	1.37
30	11	309	CLA	C1D-ND	3.42	1.42	1.37
30	17	310	CLA	C1D-ND	3.41	1.42	1.37
32	C	515	BCR	C1-C6	-3.41	1.49	1.53
30	40	207	CLA	C4D-ND	-3.41	1.33	1.37
41	20	213	A86	C19-C18	3.41	1.57	1.52
30	z	101	CLA	C1D-ND	3.41	1.42	1.37
30	17	306	CLA	C1D-ND	3.41	1.42	1.37
30	33	306	CLA	C4D-ND	-3.41	1.33	1.37
30	36	305	CLA	C1D-ND	3.41	1.42	1.37
30	34	306	CLA	C4D-ND	-3.41	1.33	1.37
30	a	403	CLA	C3B-C2B	-3.41	1.35	1.40
41	18	315	A86	C5-C6	3.41	1.40	1.35
30	A	404	CLA	C3B-C2B	-3.41	1.35	1.40
30	c	510	CLA	CMB-C2B	-3.41	1.44	1.51
30	12	313	CLA	C4D-ND	-3.41	1.33	1.37
30	21	302	CLA	C4D-ND	-3.41	1.33	1.37
30	15	302	CLA	C1D-ND	3.40	1.42	1.37
41	21	314	A86	C19-C18	3.40	1.57	1.52
30	34	310	CLA	C4D-ND	-3.40	1.33	1.37
41	17	316	A86	C5-C6	3.40	1.40	1.35
30	12	306	CLA	C4D-ND	-3.40	1.33	1.37
41	33	315	A86	C5-C6	3.40	1.40	1.35
30	40	209	CLA	C4D-ND	-3.40	1.33	1.37
41	12	315	A86	C19-C18	3.40	1.57	1.52
30	36	301	CLA	C1D-ND	3.40	1.42	1.37
30	15	309	CLA	C1D-ND	3.40	1.42	1.37
30	35	309	CLA	C1D-ND	3.40	1.42	1.37
41	38	315	A86	C5-C6	3.40	1.40	1.35
30	C	510	CLA	CMB-C2B	-3.40	1.44	1.51
41	41	314	A86	C19-C18	3.39	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	35	302	CLA	C1D-ND	3.39	1.42	1.37
30	16	301	CLA	C1D-ND	3.39	1.42	1.37
41	11	314	A86	C5-C6	3.39	1.40	1.35
30	18	312	CLA	C1D-ND	3.39	1.42	1.37
41	31	313	A86	C5-C6	3.39	1.40	1.35
41	33	312	A86	C19-C18	3.39	1.57	1.52
41	18	313	A86	C19-C18	3.39	1.57	1.52
30	17	304	CLA	C1D-ND	3.39	1.41	1.37
30	21	303	CLA	C1D-ND	3.39	1.41	1.37
30	41	307	CLA	C1D-ND	3.39	1.41	1.37
30	14	309	CLA	C4D-ND	-3.38	1.33	1.37
30	20	209	CLA	C1D-ND	3.38	1.41	1.37
41	40	201	A86	C17-C18	-3.38	1.47	1.52
30	40	208	CLA	C4D-ND	-3.38	1.33	1.37
41	12	319	A86	C5-C6	3.38	1.40	1.35
41	41	312	A86	C21-C20	3.38	1.57	1.51
41	21	312	A86	C21-C20	3.38	1.57	1.51
41	13	314	A86	C5-C6	3.38	1.40	1.35
30	11	302	CLA	C4D-ND	-3.38	1.33	1.37
32	c	516	BCR	C1-C6	-3.38	1.49	1.53
30	c	523	CLA	C1D-ND	3.38	1.41	1.37
41	15	313	A86	C5-C6	3.38	1.40	1.35
30	b	608	CLA	C3B-C2B	-3.37	1.35	1.40
40	e	101	HEM	C3C-CAC	3.37	1.54	1.47
30	37	304	CLA	C1D-ND	3.37	1.41	1.37
30	32	310	CLA	C4D-ND	-3.37	1.33	1.37
30	40	203	CLA	C1D-ND	3.37	1.41	1.37
30	31	309	CLA	C4D-ND	-3.37	1.33	1.37
30	41	303	CLA	C1D-ND	3.37	1.41	1.37
30	37	310	CLA	C4D-ND	-3.37	1.33	1.37
41	35	313	A86	C5-C6	3.37	1.40	1.35
41	14	311	A86	C19-C18	3.37	1.57	1.52
30	38	301	CLA	C4D-ND	-3.36	1.33	1.37
30	13	306	CLA	C1D-ND	3.36	1.41	1.37
30	14	308	CLA	C1D-ND	3.36	1.41	1.37
30	41	302	CLA	C4D-ND	-3.36	1.33	1.37
30	B	612	CLA	MG-ND	-3.36	1.99	2.05
30	13	303	CLA	C4D-ND	-3.36	1.33	1.37
30	20	208	CLA	C4D-ND	-3.36	1.33	1.37
41	34	311	A86	C19-C18	3.36	1.57	1.52
41	38	313	A86	C19-C18	3.36	1.57	1.52
30	19	304	CLA	C1D-ND	3.36	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	21	311	A86	C5-C6	3.36	1.40	1.35
30	20	206	CLA	C4D-ND	-3.35	1.33	1.37
30	36	308	CLA	C4D-ND	-3.35	1.33	1.37
30	c	503	CLA	C1D-ND	3.35	1.41	1.37
30	37	309	CLA	C1D-ND	3.35	1.41	1.37
30	32	313	CLA	C4D-ND	-3.35	1.33	1.37
30	21	307	CLA	C1D-ND	3.35	1.41	1.37
39	D	407	PL9	C53-C6	-3.35	1.43	1.50
30	15	303	CLA	C4D-ND	-3.35	1.33	1.37
30	39	304	CLA	C1D-ND	3.35	1.41	1.37
30	17	307	CLA	C4D-ND	-3.35	1.33	1.37
30	17	309	CLA	C1D-ND	3.35	1.41	1.37
41	41	311	A86	C5-C6	3.35	1.40	1.35
30	33	307	CLA	C1D-ND	3.35	1.41	1.37
30	34	305	CLA	C4D-ND	-3.35	1.33	1.37
30	36	303	CLA	C4D-ND	-3.35	1.33	1.37
30	34	303	CLA	C4D-ND	-3.35	1.33	1.37
30	11	305	CLA	C4D-ND	-3.35	1.33	1.37
30	20	203	CLA	C1D-ND	3.35	1.41	1.37
41	37	302	A86	C5-C6	3.35	1.40	1.35
30	37	310	CLA	C1D-ND	3.34	1.41	1.37
41	41	313	A86	C5-C6	3.34	1.40	1.35
30	33	309	CLA	C1D-ND	3.34	1.41	1.37
30	38	307	CLA	C4D-ND	-3.34	1.33	1.37
30	11	307	CLA	C1D-ND	3.34	1.41	1.37
30	35	303	CLA	C4D-ND	-3.34	1.33	1.37
30	12	312	CLA	C1D-ND	3.34	1.41	1.37
30	38	304	CLA	C1D-ND	3.34	1.41	1.37
41	21	310	A86	C5-C6	3.34	1.40	1.35
41	32	319	A86	C5-C6	3.34	1.40	1.35
30	14	301	CLA	C4D-ND	-3.34	1.33	1.37
30	19	303	CLA	C4D-ND	-3.34	1.33	1.37
32	A	405	BCR	C1-C6	-3.34	1.49	1.53
30	18	307	CLA	C4D-ND	-3.34	1.33	1.37
30	13	310	CLA	C1D-ND	3.34	1.41	1.37
30	11	309	CLA	C4D-ND	-3.34	1.33	1.37
32	Z	101	BCR	C1-C6	-3.33	1.49	1.53
30	11	304	CLA	C1D-ND	3.33	1.41	1.37
30	16	308	CLA	C4D-ND	-3.33	1.33	1.37
30	33	304	CLA	C4D-ND	-3.33	1.33	1.37
32	b	623	BCR	C1-C6	-3.33	1.49	1.53
41	34	312	A86	C5-C6	3.33	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	18	301	CLA	C4D-ND	-3.33	1.33	1.37
41	13	315	A86	C5-C6	3.33	1.40	1.35
41	16	313	A86	C5-C6	3.33	1.40	1.35
41	17	314	A86	C5-C6	3.33	1.40	1.35
41	40	211	A86	C5-C6	3.33	1.40	1.35
30	b	615	CLA	C1D-ND	3.33	1.41	1.37
30	18	309	CLA	C1D-ND	3.32	1.41	1.37
30	c	524	CLA	C4D-ND	-3.32	1.33	1.37
30	40	209	CLA	C1D-ND	3.32	1.41	1.37
30	13	306	CLA	C4D-ND	-3.32	1.33	1.37
30	C	521	CLA	C1D-ND	3.32	1.41	1.37
41	21	313	A86	C5-C6	3.32	1.40	1.35
30	16	303	CLA	C4D-ND	-3.32	1.33	1.37
30	32	308	CLA	C4D-ND	-3.32	1.33	1.37
41	13	311	A86	C19-C18	3.31	1.57	1.52
41	12	318	A86	C5-C6	3.31	1.40	1.35
30	40	203	CLA	C4D-ND	-3.31	1.33	1.37
30	40	206	CLA	C4D-ND	-3.31	1.33	1.37
30	b	612	CLA	MG-ND	-3.31	1.99	2.05
30	34	306	CLA	C1D-ND	3.31	1.41	1.37
41	15	310	A86	C19-C18	3.31	1.57	1.52
30	14	310	CLA	C1D-ND	3.31	1.41	1.37
41	11	310	A86	C19-C18	3.31	1.57	1.52
41	32	317	A86	C5-C6	3.31	1.40	1.35
30	12	314	CLA	C1D-ND	3.31	1.41	1.37
30	11	301	CLA	C1D-ND	3.31	1.41	1.37
30	13	305	CLA	C1D-ND	3.31	1.41	1.37
30	38	309	CLA	C1D-ND	3.31	1.41	1.37
40	v	201	HEM	C3C-CAC	3.31	1.54	1.47
40	V	201	HEM	C3C-CAC	3.30	1.54	1.47
30	41	303	CLA	C4D-ND	-3.30	1.33	1.37
30	C	512	CLA	C1D-ND	3.30	1.41	1.37
41	21	312	A86	C5-C6	3.30	1.40	1.35
30	40	202	CLA	C4D-ND	-3.30	1.33	1.37
41	35	310	A86	C19-C18	3.30	1.57	1.52
30	14	306	CLA	C4D-ND	-3.30	1.33	1.37
30	12	308	CLA	C4D-ND	-3.30	1.33	1.37
30	14	310	CLA	C4D-ND	-3.30	1.33	1.37
41	37	314	A86	C5-C6	3.30	1.40	1.35
30	b	610	CLA	C3B-C2B	-3.30	1.35	1.40
30	20	203	CLA	C4D-ND	-3.30	1.33	1.37
30	39	303	CLA	C1D-ND	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	19	311	A86	C5-C6	3.29	1.40	1.35
30	32	311	CLA	C1D-ND	3.29	1.41	1.37
41	36	313	A86	C5-C6	3.29	1.40	1.35
30	16	302	CLA	C1D-ND	3.29	1.41	1.37
30	20	207	CLA	C1D-ND	3.29	1.41	1.37
30	18	308	CLA	C4D-ND	-3.29	1.33	1.37
41	14	312	A86	C19-C18	3.29	1.57	1.52
41	17	302	A86	C5-C6	3.29	1.40	1.35
30	B	615	CLA	C1D-ND	3.29	1.41	1.37
30	c	511	CLA	CMD-C2D	-3.29	1.43	1.50
30	36	302	CLA	C1D-ND	3.29	1.41	1.37
30	Z	102	CLA	C4D-ND	-3.29	1.33	1.37
30	16	303	CLA	C1D-ND	3.29	1.41	1.37
30	35	303	CLA	C1D-ND	3.29	1.41	1.37
30	13	309	CLA	C4D-ND	-3.29	1.33	1.37
41	41	310	A86	C5-C6	3.29	1.40	1.35
41	38	314	A86	C19-C18	3.29	1.57	1.52
30	20	202	CLA	C4D-ND	-3.28	1.33	1.37
30	35	307	CLA	C1D-ND	3.28	1.41	1.37
30	C	519	CLA	C1D-ND	3.28	1.41	1.37
41	41	312	A86	C5-C6	3.28	1.40	1.35
30	D	401	CLA	CMB-C2B	-3.28	1.44	1.51
30	31	304	CLA	C4D-ND	-3.28	1.33	1.37
30	13	309	CLA	C1D-ND	3.28	1.41	1.37
41	39	311	A86	C19-C18	3.28	1.57	1.52
30	12	311	CLA	C1D-ND	3.28	1.41	1.37
41	31	310	A86	C19-C18	3.28	1.57	1.52
30	16	306	CLA	C4D-ND	-3.28	1.33	1.37
30	38	311	CLA	C1D-ND	3.27	1.41	1.37
41	37	312	A86	C5-C6	3.27	1.40	1.35
30	36	301	CLA	C4D-ND	-3.27	1.33	1.37
30	39	303	CLA	C4D-ND	-3.27	1.33	1.37
30	b	604	CLA	C1D-ND	3.27	1.41	1.37
30	16	301	CLA	C4D-ND	-3.27	1.33	1.37
30	32	308	CLA	C1D-ND	3.27	1.41	1.37
30	C	511	CLA	CMD-C2D	-3.27	1.43	1.50
30	35	309	CLA	C4D-ND	-3.27	1.33	1.37
30	12	309	CLA	C1D-ND	3.27	1.41	1.37
30	d	401	CLA	CMB-C2B	-3.27	1.44	1.51
30	34	307	CLA	C4D-ND	-3.27	1.33	1.37
30	C	503	CLA	C1D-ND	3.27	1.41	1.37
30	19	308	CLA	C1D-ND	3.27	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	308	CLA	C1D-ND	3.27	1.41	1.37
30	17	308	CLA	C1D-ND	3.27	1.41	1.37
30	36	303	CLA	C1D-ND	3.27	1.41	1.37
30	12	309	CLA	C4D-ND	-3.27	1.33	1.37
41	37	302	A86	C19-C18	3.27	1.57	1.52
30	14	302	CLA	C1D-ND	3.26	1.41	1.37
30	39	302	CLA	C1D-ND	3.26	1.41	1.37
30	18	304	CLA	C1D-ND	3.26	1.41	1.37
30	21	303	CLA	C4D-ND	-3.26	1.33	1.37
30	33	311	CLA	C4D-ND	-3.26	1.33	1.37
30	32	309	CLA	C1D-ND	3.26	1.41	1.37
41	17	302	A86	C19-C18	3.26	1.57	1.52
30	19	303	CLA	C1D-ND	3.26	1.41	1.37
39	d	408	PL9	C53-C6	-3.26	1.43	1.50
30	15	306	CLA	C4D-ND	-3.26	1.33	1.37
30	37	307	CLA	C1D-ND	3.26	1.41	1.37
30	17	304	CLA	C4D-ND	-3.26	1.33	1.37
30	33	311	CLA	C1D-ND	3.26	1.41	1.37
30	39	308	CLA	C1D-ND	3.26	1.41	1.37
41	31	311	A86	C19-C18	3.26	1.57	1.52
41	19	309	A86	C5-C6	3.26	1.40	1.35
30	40	207	CLA	C1D-ND	3.25	1.41	1.37
41	13	312	A86	C5-C6	3.25	1.40	1.35
30	17	307	CLA	C1D-ND	3.25	1.41	1.37
41	17	312	A86	C5-C6	3.25	1.40	1.35
30	35	306	CLA	C4D-ND	-3.25	1.33	1.37
41	11	311	A86	C19-C18	3.25	1.57	1.52
41	14	312	A86	C5-C6	3.25	1.40	1.35
30	19	301	CLA	C1D-ND	3.25	1.41	1.37
30	W	103	CLA	C4D-ND	-3.25	1.33	1.37
30	31	309	CLA	C1D-ND	3.25	1.41	1.37
30	39	301	CLA	C1D-ND	3.25	1.41	1.37
30	15	307	CLA	C1D-ND	3.25	1.41	1.37
30	13	302	CLA	C1D-ND	3.25	1.41	1.37
30	31	307	CLA	C1D-ND	3.25	1.41	1.37
32	F	101	BCR	C1-C6	-3.24	1.49	1.53
41	18	314	A86	C19-C18	3.24	1.57	1.52
41	34	312	A86	C19-C18	3.24	1.57	1.52
30	19	302	CLA	C1D-ND	3.24	1.41	1.37
30	17	306	CLA	C4D-ND	-3.24	1.33	1.37
30	14	309	CLA	C1D-ND	3.24	1.41	1.37
30	36	306	CLA	C4D-ND	-3.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	37	306	CLA	C4D-ND	-3.24	1.33	1.37
41	39	311	A86	C5-C6	3.24	1.40	1.35
41	12	316	A86	C5-C6	3.23	1.40	1.35
30	c	512	CLA	C1D-ND	3.23	1.41	1.37
30	18	311	CLA	C4D-ND	-3.23	1.33	1.37
30	B	604	CLA	C1D-ND	3.23	1.41	1.37
41	39	309	A86	C5-C6	3.23	1.40	1.35
30	38	308	CLA	C4D-ND	-3.23	1.33	1.37
32	f	101	BCR	C1-C6	-3.23	1.49	1.53
30	21	304	CLA	C4D-ND	-3.23	1.33	1.37
41	35	311	A86	C19-C18	3.23	1.57	1.52
30	B	611	CLA	C3B-C2B	-3.23	1.35	1.40
30	15	308	CLA	C4D-ND	-3.23	1.33	1.37
30	38	312	CLA	C4D-ND	-3.23	1.33	1.37
30	31	305	CLA	C1D-ND	3.22	1.41	1.37
30	40	205	CLA	C4D-ND	-3.22	1.33	1.37
30	11	308	CLA	C1D-ND	3.22	1.41	1.37
30	41	304	CLA	C4D-ND	-3.22	1.33	1.37
30	12	305	CLA	C1D-ND	3.22	1.41	1.37
41	39	309	A86	C19-C18	3.22	1.57	1.52
30	14	305	CLA	C4D-ND	-3.22	1.33	1.37
30	a	403	CLA	C3B-CAB	-3.22	1.41	1.47
30	38	311	CLA	C4D-ND	-3.21	1.33	1.37
41	11	311	A86	C5-C6	3.21	1.40	1.35
30	36	308	CLA	C1D-ND	3.21	1.41	1.37
30	13	310	CLA	C4D-ND	-3.21	1.33	1.37
30	37	304	CLA	C4D-ND	-3.21	1.33	1.37
30	16	308	CLA	C1D-ND	3.21	1.41	1.37
30	40	204	CLA	C1D-ND	3.21	1.41	1.37
30	15	309	CLA	C4D-ND	-3.21	1.33	1.37
30	18	311	CLA	C1D-ND	3.21	1.41	1.37
30	B	605	CLA	C3B-C2B	-3.21	1.35	1.40
30	14	303	CLA	C4D-ND	-3.21	1.33	1.37
41	19	311	A86	C19-C18	3.21	1.56	1.52
30	12	308	CLA	C1D-ND	3.20	1.41	1.37
30	15	303	CLA	C1D-ND	3.20	1.41	1.37
41	33	313	A86	C19-C18	3.20	1.56	1.52
30	B	610	CLA	C3B-C2B	-3.20	1.35	1.40
30	14	301	CLA	C1D-ND	3.20	1.41	1.37
41	39	310	A86	C25-C24	3.20	1.42	1.34
30	32	313	CLA	C1D-ND	3.20	1.41	1.37
41	13	311	A86	C5-C6	3.20	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	314	CLA	C4D-ND	-3.20	1.33	1.37
30	13	305	CLA	C4D-ND	-3.20	1.33	1.37
30	17	308	CLA	CMB-C2B	-3.20	1.45	1.51
30	41	308	CLA	C4D-ND	-3.20	1.33	1.37
41	32	315	A86	C19-C18	3.20	1.56	1.52
30	41	305	CLA	C4D-ND	-3.20	1.33	1.37
32	B	624	BCR	C1-C6	-3.20	1.49	1.53
30	C	503	CLA	CMB-C2B	-3.20	1.45	1.51
41	19	309	A86	C19-C18	3.20	1.56	1.52
30	33	306	CLA	C1D-ND	3.20	1.41	1.37
30	21	305	CLA	C4D-ND	-3.20	1.33	1.37
30	38	304	CLA	C4D-ND	-3.19	1.33	1.37
30	37	308	CLA	CMB-C2B	-3.19	1.45	1.51
41	13	312	A86	C19-C18	3.19	1.56	1.52
30	b	605	CLA	C3B-C2B	-3.19	1.35	1.40
41	15	311	A86	C19-C18	3.19	1.56	1.52
41	35	311	A86	C25-C24	3.19	1.42	1.34
41	17	312	A86	C25-C24	3.19	1.42	1.34
30	14	305	CLA	C1D-ND	3.19	1.41	1.37
41	33	313	A86	C5-C6	3.19	1.40	1.35
41	41	313	A86	C19-C18	3.19	1.56	1.52
30	20	205	CLA	C4D-ND	-3.19	1.33	1.37
41	35	311	A86	C5-C6	3.19	1.40	1.35
41	19	310	A86	C25-C24	3.19	1.42	1.34
30	13	303	CLA	C1D-ND	3.19	1.41	1.37
41	36	311	A86	C25-C24	3.19	1.42	1.34
41	21	313	A86	C19-C18	3.19	1.56	1.52
30	12	303	CLA	C1D-ND	3.19	1.41	1.37
41	15	311	A86	C5-C6	3.18	1.40	1.35
41	15	311	A86	C25-C24	3.18	1.42	1.34
30	12	310	CLA	C1D-ND	3.18	1.41	1.37
41	11	311	A86	C25-C24	3.18	1.42	1.34
41	16	311	A86	C25-C24	3.18	1.42	1.34
41	37	312	A86	C25-C24	3.18	1.42	1.34
30	A	404	CLA	C3B-CAB	-3.18	1.41	1.47
32	c	521	BCR	C1-C6	-3.18	1.49	1.53
30	w	103	CLA	C4D-ND	-3.18	1.33	1.37
30	11	304	CLA	C4D-ND	-3.18	1.33	1.37
30	18	312	CLA	C4D-ND	-3.18	1.33	1.37
30	35	308	CLA	C4D-ND	-3.18	1.33	1.37
41	31	311	A86	C25-C24	3.18	1.42	1.34
30	20	204	CLA	C1D-ND	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	41	309	CLA	C4D-ND	-3.18	1.33	1.37
30	b	608	CLA	CMB-C2B	-3.17	1.45	1.51
30	34	305	CLA	C1D-ND	3.17	1.41	1.37
30	18	303	CLA	C1D-ND	3.17	1.41	1.37
41	16	311	A86	C5-C6	3.17	1.40	1.35
30	37	308	CLA	C1D-ND	3.17	1.41	1.37
30	38	303	CLA	C1D-ND	3.17	1.41	1.37
41	32	315	A86	C25-C24	3.17	1.42	1.34
41	12	316	A86	C25-C24	3.17	1.42	1.34
30	11	315	CLA	C1D-ND	3.17	1.41	1.37
30	37	301	CLA	C1D-ND	3.17	1.41	1.37
30	21	308	CLA	C4D-ND	-3.17	1.33	1.37
30	C	505	CLA	CMB-C2B	-3.16	1.45	1.51
30	c	506	CLA	C3B-C2B	-3.16	1.36	1.40
30	36	307	CLA	CHC-C1C	3.16	1.43	1.35
30	17	308	CLA	C3B-C2B	-3.16	1.36	1.40
30	b	611	CLA	C3B-C2B	-3.16	1.36	1.40
30	17	301	CLA	C1D-ND	3.16	1.41	1.37
41	34	312	A86	C25-C24	3.15	1.42	1.34
41	32	315	A86	C5-C6	3.15	1.40	1.35
41	13	312	A86	C25-C24	3.15	1.42	1.34
41	33	313	A86	C25-C24	3.15	1.42	1.34
41	33	312	A86	C5-C6	3.15	1.40	1.35
41	36	311	A86	C5-C6	3.15	1.40	1.35
41	12	316	A86	C19-C18	3.15	1.56	1.52
41	21	311	A86	C19-C18	3.15	1.56	1.52
38	C	517	DGD	O2G-C2G	-3.15	1.38	1.46
30	31	306	CLA	C4D-ND	-3.15	1.33	1.37
41	31	311	A86	C5-C6	3.15	1.40	1.35
30	31	304	CLA	C1D-ND	3.15	1.41	1.37
30	34	301	CLA	C1D-ND	3.15	1.41	1.37
41	17	312	A86	C19-C18	3.14	1.56	1.52
41	37	312	A86	C19-C18	3.14	1.56	1.52
41	20	201	A86	C25-C24	3.14	1.42	1.34
30	14	307	CLA	C4D-ND	-3.14	1.33	1.37
41	34	311	A86	C5-C6	3.14	1.39	1.35
30	35	301	CLA	C1D-ND	3.14	1.41	1.37
30	C	507	CLA	C3B-C2B	-3.14	1.36	1.40
30	15	305	CLA	CHC-C1C	3.14	1.43	1.35
30	16	307	CLA	CHC-C1C	3.14	1.43	1.35
30	41	301	CLA	C4D-ND	-3.14	1.33	1.37
41	20	212	A86	C25-C24	3.14	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	603	CLA	CMB-C2B	-3.14	1.45	1.51
41	40	212	A86	C25-C24	3.14	1.42	1.34
30	35	308	CLA	C1D-ND	3.14	1.41	1.37
30	21	301	CLA	C4D-ND	-3.13	1.33	1.37
30	B	604	CLA	CMB-C2B	-3.13	1.45	1.51
30	12	307	CLA	C1D-ND	3.13	1.41	1.37
30	14	307	CLA	C1D-ND	3.13	1.41	1.37
32	B	618	BCR	C1-C6	-3.13	1.49	1.53
30	b	604	CLA	CMB-C2B	-3.13	1.45	1.51
30	c	503	CLA	CMB-C2B	-3.13	1.45	1.51
30	38	301	CLA	C1D-ND	3.13	1.41	1.37
41	16	311	A86	C19-C18	3.13	1.56	1.52
41	36	311	A86	C19-C18	3.13	1.56	1.52
38	c	518	DGD	O2G-C2G	-3.13	1.38	1.46
32	b	616	BCR	C1-C6	-3.13	1.49	1.53
30	c	507	CLA	C3B-C2B	-3.13	1.36	1.40
41	40	201	A86	C25-C24	3.13	1.42	1.34
30	21	307	CLA	C4D-ND	-3.12	1.33	1.37
30	21	309	CLA	C4D-ND	-3.12	1.33	1.37
30	13	307	CLA	C4D-ND	-3.12	1.33	1.37
30	31	315	CLA	C1D-ND	3.12	1.41	1.37
30	35	305	CLA	CHC-C1C	3.12	1.43	1.35
41	20	211	A86	C19-C18	3.12	1.56	1.52
30	12	313	CLA	C1D-ND	3.12	1.41	1.37
41	38	313	A86	C5-C6	3.12	1.39	1.35
30	11	302	CLA	C1D-ND	3.12	1.41	1.37
41	20	210	A86	C25-C24	3.12	1.42	1.34
30	35	305	CLA	C4D-ND	-3.12	1.33	1.37
41	11	312	A86	C25-C24	3.12	1.42	1.34
30	32	305	CLA	C1D-ND	3.12	1.41	1.37
41	31	312	A86	C25-C24	3.12	1.42	1.34
41	41	311	A86	C19-C18	3.11	1.56	1.52
30	15	301	CLA	C1D-ND	3.11	1.41	1.37
30	18	304	CLA	C4D-ND	-3.11	1.33	1.37
35	L	102	LHG	O7-C5	-3.11	1.38	1.46
41	39	311	A86	C25-C24	3.11	1.42	1.34
32	B	617	BCR	C1-C6	-3.11	1.49	1.53
30	b	605	CLA	C1D-ND	3.11	1.41	1.37
30	18	301	CLA	C1D-ND	3.11	1.41	1.37
30	B	605	CLA	C1D-ND	3.11	1.41	1.37
41	14	312	A86	C25-C24	3.11	1.42	1.34
41	19	311	A86	C25-C24	3.11	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	40	210	A86	C25-C24	3.11	1.42	1.34
42	32	302	LMU	O5'-C1'	3.11	1.49	1.41
41	40	211	A86	C19-C18	3.10	1.56	1.52
30	d	401	CLA	C3B-C2B	-3.10	1.36	1.40
42	12	302	LMU	O5'-C1'	3.10	1.49	1.41
41	37	313	A86	C25-C24	3.10	1.42	1.34
36	b	619	LMG	O8-C9	-3.10	1.38	1.45
30	B	608	CLA	CMB-C2B	-3.10	1.45	1.51
30	12	306	CLA	C1D-ND	3.10	1.41	1.37
39	d	408	PL9	C36-C34	-3.10	1.44	1.51
41	14	311	A86	C5-C6	3.10	1.39	1.35
41	15	312	A86	C25-C24	3.10	1.42	1.34
30	37	308	CLA	C3B-C2B	-3.10	1.36	1.40
30	C	505	CLA	C3B-C2B	-3.10	1.36	1.40
30	15	308	CLA	C1D-ND	3.09	1.41	1.37
30	12	310	CLA	C4D-ND	-3.09	1.33	1.37
30	35	301	CLA	CHC-C1C	3.09	1.42	1.35
32	b	617	BCR	C1-C6	-3.09	1.49	1.53
30	41	307	CLA	C4D-ND	-3.09	1.33	1.37
41	35	312	A86	C25-C24	3.09	1.42	1.34
30	17	309	CLA	C4D-ND	-3.09	1.33	1.37
30	32	303	CLA	C1D-ND	3.09	1.41	1.37
30	c	505	CLA	C3B-C2B	-3.08	1.36	1.40
32	B	618	BCR	C30-C25	-3.08	1.49	1.53
41	12	315	A86	C5-C6	3.08	1.39	1.35
30	18	305	CLA	C1D-ND	3.08	1.41	1.37
30	34	302	CLA	C1D-ND	3.08	1.41	1.37
41	33	314	A86	C25-C24	3.08	1.42	1.34
39	D	407	PL9	C36-C34	-3.08	1.44	1.51
41	18	313	A86	C5-C6	3.08	1.39	1.35
30	38	305	CLA	C1D-ND	3.08	1.41	1.37
30	c	505	CLA	CMB-C2B	-3.08	1.45	1.51
30	36	305	CLA	C4D-ND	-3.08	1.33	1.37
41	41	311	A86	C25-C24	3.08	1.42	1.34
41	14	313	A86	C25-C24	3.08	1.42	1.34
41	37	311	A86	C25-C24	3.08	1.42	1.34
41	34	313	A86	C25-C24	3.07	1.42	1.34
30	b	603	CLA	CMB-C2B	-3.07	1.45	1.51
41	18	314	A86	C25-C24	3.07	1.42	1.34
41	16	312	A86	C25-C24	3.07	1.42	1.34
30	15	301	CLA	CHC-C1C	3.07	1.42	1.35
41	17	313	A86	C25-C24	3.07	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	620	LMG	O8-C9	-3.07	1.38	1.45
30	33	303	CLA	C1D-ND	3.07	1.41	1.37
30	34	307	CLA	C1D-ND	3.07	1.41	1.37
41	38	314	A86	C25-C24	3.07	1.42	1.34
30	15	304	CLA	C4D-ND	-3.07	1.33	1.37
32	C	518	BCR	C1-C6	-3.07	1.49	1.53
41	21	313	A86	C25-C24	3.06	1.42	1.34
41	32	314	A86	C5-C6	3.06	1.39	1.35
41	17	311	A86	C25-C24	3.06	1.42	1.34
30	16	305	CLA	C4D-ND	-3.06	1.33	1.37
30	15	305	CLA	C4D-ND	-3.06	1.33	1.37
30	37	309	CLA	C4D-ND	-3.06	1.33	1.37
30	31	301	CLA	C1D-ND	3.06	1.41	1.37
30	C	511	CLA	CHC-C1C	3.06	1.42	1.35
31	D	403	PHO	CAC-C3C	-3.06	1.46	1.52
41	41	313	A86	C25-C24	3.06	1.42	1.34
33	L	103	SQD	O47-C7	3.06	1.42	1.34
41	21	311	A86	C25-C24	3.06	1.42	1.34
36	c	519	LMG	O7-C8	-3.06	1.38	1.46
30	38	310	CLA	C4D-ND	-3.06	1.33	1.37
30	21	306	CLA	C4D-ND	-3.05	1.33	1.37
41	13	313	A86	C25-C24	3.05	1.42	1.34
30	W	102	CLA	C1D-ND	3.05	1.41	1.37
30	34	304	CLA	C1D-ND	3.05	1.41	1.37
30	33	310	CLA	C1D-ND	3.05	1.41	1.37
41	11	312	A86	C19-C18	3.05	1.56	1.52
35	l	102	LHG	O7-C5	-3.05	1.39	1.46
30	11	306	CLA	C4D-ND	-3.05	1.33	1.37
30	33	304	CLA	C1D-ND	3.05	1.41	1.37
41	36	312	A86	C25-C24	3.04	1.42	1.34
30	36	306	CLA	CMB-C2B	-3.04	1.45	1.51
36	Q	301	LMG	O7-C8	-3.04	1.39	1.46
30	b	601	CLA	C1D-ND	3.04	1.41	1.37
41	35	312	A86	C19-C18	3.04	1.56	1.52
30	b	615	CLA	CMB-C2B	-3.04	1.45	1.51
30	37	303	CLA	C1D-ND	3.04	1.41	1.37
30	b	606	CLA	CMB-C2B	-3.04	1.45	1.51
30	38	307	CLA	CHC-C1C	3.04	1.42	1.35
32	a	404	BCR	C30-C25	-3.04	1.49	1.53
30	13	307	CLA	C1D-ND	3.04	1.41	1.37
30	C	520	CLA	C1D-ND	3.04	1.41	1.37
30	41	306	CLA	C4D-ND	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	35	304	CLA	C4D-ND	-3.04	1.33	1.37
41	20	211	A86	C25-C24	3.04	1.42	1.34
41	39	310	A86	C21-C20	3.03	1.56	1.51
30	33	308	CLA	C1D-ND	3.03	1.41	1.37
41	40	211	A86	C25-C24	3.03	1.42	1.34
30	34	310	CLA	C1D-ND	3.03	1.41	1.37
41	32	304	A86	C19-C18	3.03	1.56	1.52
32	A	405	BCR	C30-C25	-3.03	1.49	1.53
41	12	317	A86	C25-C24	3.03	1.42	1.34
30	19	306	CLA	C1D-ND	3.03	1.41	1.37
41	32	316	A86	C25-C24	3.03	1.42	1.34
41	31	312	A86	C19-C18	3.03	1.56	1.52
41	17	302	A86	C25-C24	3.03	1.42	1.34
38	J	101	DGD	O2G-C2G	-3.02	1.39	1.46
38	j	101	DGD	O2G-C2G	-3.02	1.39	1.46
30	18	310	CLA	C4D-ND	-3.02	1.33	1.37
36	c	519	LMG	O1-C7	-3.02	1.38	1.43
30	32	310	CLA	C1D-ND	3.02	1.41	1.37
41	12	304	A86	C19-C18	3.02	1.56	1.52
30	19	304	CLA	C4D-ND	-3.02	1.33	1.37
30	c	512	CLA	CHC-C1C	3.02	1.42	1.35
30	39	304	CLA	C4D-ND	-3.02	1.33	1.37
33	l	101	SQD	O47-C7	3.01	1.42	1.34
41	19	310	A86	C17-C18	-3.01	1.48	1.52
30	b	606	CLA	C1D-ND	3.01	1.41	1.37
38	c	517	DGD	O1G-C1G	-3.01	1.38	1.45
30	17	303	CLA	C1D-ND	3.01	1.41	1.37
30	c	522	CLA	C1D-ND	3.01	1.41	1.37
30	20	202	CLA	CHC-C1C	3.01	1.42	1.35
30	40	202	CLA	CHC-C1C	3.01	1.42	1.35
30	C	506	CLA	C3B-C2B	-3.01	1.36	1.40
30	c	511	CLA	CHC-C1C	3.01	1.42	1.35
41	41	312	A86	C25-C24	3.01	1.42	1.34
41	31	310	A86	C5-C6	3.01	1.39	1.35
30	13	304	CLA	C1D-ND	3.01	1.41	1.37
30	b	609	CLA	CMB-C2B	-3.01	1.45	1.51
30	18	307	CLA	CHC-C1C	3.01	1.42	1.35
41	16	310	A86	C25-C24	3.00	1.42	1.34
30	16	306	CLA	CMB-C2B	-3.00	1.45	1.51
30	39	306	CLA	C1D-ND	3.00	1.41	1.37
31	d	404	PHO	CAC-C3C	-3.00	1.46	1.52
30	C	506	CLA	C1D-ND	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	38	315	A86	C25-C24	3.00	1.42	1.34
30	D	401	CLA	C3B-C2B	-3.00	1.36	1.40
41	13	314	A86	C25-C24	3.00	1.42	1.34
41	39	310	A86	C17-C18	-3.00	1.48	1.52
30	32	306	CLA	C1D-ND	3.00	1.41	1.37
41	12	317	A86	C19-C18	3.00	1.56	1.52
30	B	623	CLA	CMD-C2D	-3.00	1.44	1.50
30	W	103	CLA	CHC-C1C	3.00	1.42	1.35
30	B	615	CLA	CMB-C2B	-3.00	1.45	1.51
41	33	315	A86	C25-C24	2.99	1.42	1.34
30	B	610	CLA	CMB-C2B	-2.99	1.45	1.51
30	35	307	CLA	CHC-C1C	2.99	1.42	1.35
30	14	304	CLA	C1D-ND	2.99	1.41	1.37
30	41	301	CLA	CHC-C1C	2.99	1.42	1.35
30	d	402	CLA	C1D-ND	2.99	1.41	1.37
41	32	316	A86	C19-C18	2.99	1.56	1.52
41	11	313	A86	C25-C24	2.99	1.42	1.34
30	21	301	CLA	CHC-C1C	2.99	1.42	1.35
41	14	313	A86	C19-C18	2.99	1.56	1.52
41	35	310	A86	C5-C6	2.99	1.39	1.35
41	36	310	A86	C25-C24	2.99	1.42	1.34
30	21	309	CLA	CHC-C1C	2.99	1.42	1.35
41	15	312	A86	C19-C18	2.99	1.56	1.52
41	34	313	A86	C19-C18	2.99	1.56	1.52
30	18	305	CLA	CHC-C1C	2.99	1.42	1.35
30	31	301	CLA	CHC-C1C	2.99	1.42	1.35
30	14	303	CLA	C1D-ND	2.99	1.41	1.37
41	13	313	A86	C19-C18	2.99	1.56	1.52
41	19	310	A86	C21-C20	2.99	1.56	1.51
41	13	316	A86	C25-C24	2.99	1.42	1.34
41	34	314	A86	C25-C24	2.99	1.42	1.34
36	Q	301	LMG	O1-C7	-2.99	1.38	1.43
41	21	314	A86	C25-C24	2.99	1.42	1.34
30	33	303	CLA	CHC-C1C	2.99	1.42	1.35
30	B	605	CLA	CMB-C2B	-2.98	1.45	1.51
41	20	213	A86	C25-C24	2.98	1.42	1.34
30	B	606	CLA	CMB-C2B	-2.98	1.45	1.51
41	15	313	A86	C25-C24	2.98	1.42	1.34
41	15	310	A86	C5-C6	2.98	1.39	1.35
41	40	213	A86	C25-C24	2.98	1.42	1.34
30	14	302	CLA	CHC-C1C	2.98	1.42	1.35
30	41	309	CLA	CHC-C1C	2.98	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	31	313	A86	C25-C24	2.98	1.42	1.34
30	33	301	CLA	C1D-ND	2.98	1.41	1.37
41	17	314	A86	C25-C24	2.98	1.42	1.34
41	37	315	A86	C25-C24	2.98	1.42	1.34
30	13	302	CLA	CHC-C1C	2.97	1.42	1.35
30	31	306	CLA	C1D-ND	2.97	1.41	1.37
30	C	512	CLA	CHC-C1C	2.97	1.42	1.35
41	41	314	A86	C25-C24	2.97	1.42	1.34
30	35	302	CLA	C4D-ND	-2.97	1.33	1.37
30	34	309	CLA	C1D-ND	2.97	1.41	1.37
41	37	313	A86	C19-C18	2.97	1.56	1.52
30	12	305	CLA	CHC-C1C	2.97	1.42	1.35
41	21	312	A86	C25-C24	2.97	1.42	1.34
36	D	408	LMG	O7-C8	-2.97	1.39	1.46
41	21	312	A86	C19-C18	2.97	1.56	1.52
41	37	302	A86	C25-C24	2.97	1.42	1.34
41	14	314	A86	C25-C24	2.97	1.42	1.34
30	11	306	CLA	C1D-ND	2.97	1.41	1.37
30	40	209	CLA	CMB-C2B	-2.97	1.45	1.51
41	33	316	A86	C25-C24	2.97	1.42	1.34
41	35	315	A86	C19-C18	2.97	1.56	1.52
41	37	314	A86	C25-C24	2.97	1.42	1.34
41	41	312	A86	C19-C18	2.97	1.56	1.52
41	11	310	A86	C5-C6	2.97	1.39	1.35
30	11	301	CLA	CHC-C1C	2.97	1.42	1.35
41	13	301	A86	C19-C18	2.97	1.56	1.52
30	15	302	CLA	C4D-ND	-2.97	1.33	1.37
30	A	404	CLA	CMB-C2B	-2.97	1.45	1.51
32	c	520	BCR	C30-C25	-2.96	1.49	1.53
30	b	622	CLA	CMD-C2D	-2.96	1.44	1.50
30	15	307	CLA	CHC-C1C	2.96	1.42	1.35
30	35	304	CLA	CHC-C1C	2.96	1.42	1.35
30	38	305	CLA	CHC-C1C	2.96	1.42	1.35
38	C	516	DGD	O1G-C1G	-2.96	1.38	1.45
41	12	304	A86	C25-C24	2.96	1.42	1.34
41	32	317	A86	C25-C24	2.96	1.42	1.34
30	31	302	CLA	C1D-ND	2.96	1.41	1.37
30	15	303	CLA	CHC-C1C	2.96	1.42	1.35
30	35	303	CLA	CHC-C1C	2.96	1.42	1.35
41	17	315	A86	C25-C24	2.96	1.42	1.34
41	12	318	A86	C25-C24	2.96	1.42	1.34
41	15	315	A86	C19-C18	2.96	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	15	316	A86	C19-C18	2.96	1.56	1.52
30	38	303	CLA	CHC-C1C	2.96	1.42	1.35
30	b	610	CLA	CMB-C2B	-2.96	1.45	1.51
30	21	308	CLA	CHC-C1C	2.96	1.42	1.35
30	b	605	CLA	CMB-C2B	-2.96	1.45	1.51
41	18	315	A86	C25-C24	2.96	1.42	1.34
41	36	312	A86	C19-C18	2.95	1.56	1.52
30	B	607	CLA	CMB-C2B	-2.95	1.45	1.51
41	35	313	A86	C25-C24	2.95	1.42	1.34
32	b	616	BCR	C30-C25	-2.95	1.49	1.53
41	16	312	A86	C19-C18	2.95	1.56	1.52
30	d	407	CLA	CMB-C2B	-2.95	1.45	1.51
30	38	306	CLA	C4D-ND	-2.95	1.33	1.37
30	18	303	CLA	CHC-C1C	2.95	1.42	1.35
30	16	304	CLA	CMB-C2B	-2.95	1.45	1.51
30	17	301	CLA	CMB-C2B	-2.95	1.45	1.51
33	B	621	SQD	O48-C23	2.95	1.41	1.33
30	37	301	CLA	CMB-C2B	-2.95	1.45	1.51
30	15	304	CLA	CHC-C1C	2.95	1.42	1.35
32	b	617	BCR	C30-C25	-2.95	1.49	1.53
41	13	301	A86	C25-C24	2.94	1.42	1.34
30	c	508	CLA	CMB-C2B	-2.94	1.45	1.51
36	d	410	LMG	O7-C8	-2.94	1.39	1.46
30	B	601	CLA	C1D-ND	2.94	1.41	1.37
30	20	209	CLA	CHC-C1C	2.94	1.42	1.35
41	17	313	A86	C19-C18	2.94	1.56	1.52
41	32	304	A86	C25-C24	2.94	1.42	1.34
30	C	504	CLA	C1D-ND	2.94	1.41	1.37
30	19	307	CLA	C1D-ND	2.94	1.41	1.37
32	a	408	BCR	C1-C6	-2.94	1.49	1.53
30	w	103	CLA	CHC-C1C	2.94	1.42	1.35
30	a	403	CLA	CMB-C2B	-2.94	1.45	1.51
30	c	506	CLA	C1D-ND	2.93	1.41	1.37
30	31	308	CLA	C1D-ND	2.93	1.41	1.37
30	C	508	CLA	CMB-C2B	-2.93	1.45	1.51
41	39	309	A86	C25-C24	2.93	1.42	1.34
30	18	306	CLA	C4D-ND	-2.93	1.33	1.37
41	21	310	A86	O-C13	-2.93	1.17	1.23
41	41	310	A86	O-C13	-2.93	1.17	1.23
30	B	606	CLA	C1D-ND	2.93	1.41	1.37
30	41	308	CLA	CHC-C1C	2.93	1.42	1.35
30	b	601	CLA	CMB-C2B	-2.93	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	308	CLA	CHC-C1C	2.93	1.42	1.35
33	b	620	SQD	O48-C23	2.93	1.41	1.33
30	40	209	CLA	CHC-C1C	2.93	1.42	1.35
30	31	303	CLA	C1D-ND	2.93	1.41	1.37
30	C	503	CLA	MG-ND	-2.93	2.00	2.05
30	C	511	CLA	MG-ND	-2.93	2.00	2.05
30	B	609	CLA	C3B-C2B	-2.93	1.36	1.40
30	c	504	CLA	C1D-ND	2.93	1.41	1.37
30	11	303	CLA	C1D-ND	2.93	1.41	1.37
41	31	316	A86	C25-C24	2.93	1.42	1.34
41	35	316	A86	C19-C18	2.93	1.56	1.52
41	33	302	A86	C25-C24	2.93	1.42	1.34
30	M	101	CLA	CHC-C1C	2.93	1.42	1.35
41	35	315	A86	C25-C24	2.93	1.42	1.34
30	B	601	CLA	CMB-C2B	-2.92	1.45	1.51
41	15	315	A86	C25-C24	2.92	1.42	1.34
41	19	309	A86	C25-C24	2.92	1.42	1.34
30	11	307	CLA	CHC-C1C	2.92	1.42	1.35
41	18	302	A86	C19-C18	2.92	1.56	1.52
30	32	312	CLA	C1D-ND	2.92	1.41	1.37
30	34	310	CLA	CHC-C1C	2.92	1.42	1.35
30	20	209	CLA	CMB-C2B	-2.92	1.45	1.51
41	38	302	A86	C25-C24	2.92	1.42	1.34
30	c	509	CLA	C3B-C2B	-2.92	1.36	1.40
41	33	302	A86	C19-C18	2.92	1.56	1.52
30	21	307	CLA	CHC-C1C	2.92	1.42	1.35
41	11	316	A86	C25-C24	2.92	1.42	1.34
41	18	302	A86	C25-C24	2.92	1.42	1.34
30	36	302	CLA	CMB-C2B	-2.92	1.45	1.51
30	36	304	CLA	CMB-C2B	-2.92	1.45	1.51
30	32	305	CLA	CHC-C1C	2.92	1.42	1.35
41	33	314	A86	C19-C18	2.92	1.56	1.52
41	38	302	A86	C19-C18	2.92	1.56	1.52
30	b	622	CLA	CHC-C1C	2.92	1.42	1.35
30	36	309	CLA	CHC-C1C	2.92	1.42	1.35
30	14	310	CLA	CHC-C1C	2.91	1.42	1.35
30	12	314	CLA	CHC-C1C	2.91	1.42	1.35
30	21	306	CLA	CHC-C1C	2.91	1.42	1.35
30	41	307	CLA	CHC-C1C	2.91	1.42	1.35
30	41	306	CLA	CHC-C1C	2.91	1.42	1.35
30	12	309	CLA	CHC-C1C	2.91	1.42	1.35
30	b	608	CLA	CHC-C1C	2.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	311	CLA	CHC-C1C	2.91	1.42	1.35
30	34	302	CLA	CHC-C1C	2.91	1.42	1.35
30	b	609	CLA	C1D-ND	2.90	1.41	1.37
30	36	304	CLA	C1D-ND	2.90	1.41	1.37
30	38	312	CLA	CHC-C1C	2.90	1.42	1.35
39	d	408	PL9	C26-C24	-2.90	1.45	1.51
30	w	102	CLA	C1D-ND	2.90	1.41	1.37
41	31	316	A86	C19-C18	2.90	1.56	1.52
30	35	309	CLA	CHC-C1C	2.90	1.42	1.35
32	Y	101	BCR	C30-C25	-2.90	1.49	1.53
30	C	514	CLA	C1D-ND	2.90	1.41	1.37
35	B	622	LHG	O7-C5	-2.90	1.39	1.46
30	16	302	CLA	CMB-C2B	-2.90	1.45	1.51
30	B	623	CLA	CHC-C1C	2.90	1.42	1.35
30	39	305	CLA	C1D-ND	2.90	1.41	1.37
41	11	316	A86	C19-C18	2.90	1.56	1.52
30	31	309	CLA	CHC-C1C	2.90	1.42	1.35
30	41	303	CLA	CHC-C1C	2.90	1.42	1.35
30	m	101	CLA	CHC-C1C	2.90	1.42	1.35
30	18	309	CLA	CHC-C1C	2.90	1.42	1.35
30	c	503	CLA	CMC-C2C	-2.89	1.44	1.50
30	D	402	CLA	C1D-ND	2.89	1.41	1.37
30	16	309	CLA	CHC-C1C	2.89	1.42	1.35
41	17	316	A86	C19-C18	2.89	1.56	1.52
30	38	309	CLA	CHC-C1C	2.89	1.42	1.35
30	39	305	CLA	CMB-C2B	-2.89	1.45	1.51
30	18	308	CLA	CHC-C1C	2.89	1.42	1.35
30	C	508	CLA	MG-ND	-2.89	2.00	2.05
30	14	308	CLA	CHC-C1C	2.89	1.42	1.35
30	15	309	CLA	CHC-C1C	2.89	1.42	1.35
30	c	503	CLA	MG-ND	-2.89	2.00	2.05
30	38	308	CLA	CHC-C1C	2.89	1.42	1.35
30	B	602	CLA	CHC-C1C	2.89	1.42	1.35
35	b	621	LHG	O7-C5	-2.88	1.39	1.46
30	b	601	CLA	C3B-C2B	-2.88	1.36	1.40
30	a	402	CLA	C1D-ND	2.88	1.41	1.37
30	D	406	CLA	CMB-C2B	-2.88	1.45	1.51
30	14	306	CLA	CHC-C1C	2.88	1.42	1.35
30	C	509	CLA	C3B-C2B	-2.88	1.36	1.40
30	13	306	CLA	CHC-C1C	2.88	1.42	1.35
30	D	401	CLA	C3B-CAB	-2.88	1.42	1.47
41	13	316	A86	C19-C18	2.88	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	32	307	CLA	C1D-ND	2.88	1.41	1.37
30	35	306	CLA	CHC-C1C	2.88	1.42	1.35
30	c	514	CLA	CHC-C1C	2.88	1.42	1.35
30	b	622	CLA	CMB-C2B	-2.88	1.45	1.51
30	18	312	CLA	CHC-C1C	2.88	1.42	1.35
30	M	101	CLA	CMB-C2B	-2.88	1.45	1.51
30	19	305	CLA	C1D-ND	2.88	1.41	1.37
30	15	306	CLA	CHC-C1C	2.87	1.42	1.35
41	15	316	A86	C25-C24	2.87	1.42	1.34
30	40	208	CLA	CHC-C1C	2.87	1.42	1.35
30	21	303	CLA	CHC-C1C	2.87	1.42	1.35
30	32	313	CLA	CHC-C1C	2.87	1.42	1.35
30	12	310	CLA	CMB-C2B	-2.87	1.45	1.51
30	16	308	CLA	CMB-C2B	-2.87	1.45	1.51
41	33	312	A86	C25-C24	2.87	1.42	1.34
30	c	523	CLA	CHC-C1C	2.87	1.42	1.35
30	18	306	CLA	CHC-C1C	2.87	1.42	1.35
30	20	208	CLA	CHC-C1C	2.87	1.42	1.35
30	B	609	CLA	CMB-C2B	-2.87	1.45	1.51
30	B	623	CLA	CMB-C2B	-2.87	1.45	1.51
30	D	402	CLA	CMB-C2B	-2.87	1.45	1.51
30	B	609	CLA	C1D-ND	2.87	1.41	1.37
30	39	307	CLA	C1D-ND	2.87	1.41	1.37
30	C	508	CLA	C1D-ND	2.87	1.41	1.37
30	34	303	CLA	C1D-ND	2.87	1.41	1.37
30	34	306	CLA	CHC-C1C	2.87	1.42	1.35
41	35	316	A86	C25-C24	2.87	1.42	1.34
30	D	405	CLA	CMD-C2D	-2.86	1.44	1.50
30	35	308	CLA	CHC-C1C	2.86	1.42	1.35
30	38	309	CLA	CMB-C2B	-2.86	1.45	1.51
41	40	201	A86	C24-C1	2.86	1.52	1.45
30	19	306	CLA	C3B-C2B	-2.86	1.36	1.40
30	13	307	CLA	CMB-C2B	-2.86	1.45	1.51
30	c	511	CLA	MG-ND	-2.86	2.00	2.05
30	m	101	CLA	CMB-C2B	-2.86	1.45	1.51
41	33	316	A86	C19-C18	2.86	1.56	1.52
30	36	304	CLA	CHC-C1C	2.86	1.42	1.35
30	w	102	CLA	CMB-C2B	-2.86	1.45	1.51
30	19	305	CLA	CMB-C2B	-2.86	1.45	1.51
30	C	514	CLA	CHC-C1C	2.86	1.42	1.35
30	32	309	CLA	CHC-C1C	2.86	1.42	1.35
30	17	305	CLA	C1D-ND	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	608	CLA	CHC-C1C	2.86	1.42	1.35
30	21	304	CLA	CHC-C1C	2.86	1.42	1.35
32	B	617	BCR	C30-C25	-2.86	1.49	1.53
32	H	101	BCR	C30-C25	-2.86	1.49	1.53
30	W	102	CLA	CMB-C2B	-2.86	1.45	1.51
30	36	307	CLA	C1D-ND	2.86	1.41	1.37
30	13	310	CLA	CHC-C1C	2.86	1.42	1.35
30	31	306	CLA	CMB-C2B	-2.86	1.45	1.51
30	b	606	CLA	CMD-C2D	-2.86	1.44	1.50
30	d	406	CLA	CMD-C2D	-2.85	1.44	1.50
30	B	614	CLA	C1D-ND	2.85	1.41	1.37
33	A	406	SQD	O48-C23	2.85	1.41	1.33
30	39	303	CLA	CHC-C1C	2.85	1.42	1.35
41	38	313	A86	C25-C24	2.85	1.41	1.34
30	16	304	CLA	CHC-C1C	2.85	1.42	1.35
30	C	513	CLA	C1D-ND	2.85	1.41	1.37
30	16	309	CLA	C1D-ND	2.85	1.41	1.37
30	16	307	CLA	C1D-ND	2.85	1.41	1.37
39	d	408	PL9	C11-C9	-2.85	1.45	1.51
41	18	313	A86	C25-C24	2.85	1.41	1.34
30	33	309	CLA	CHC-C1C	2.85	1.42	1.35
41	33	317	A86	C25-C24	2.85	1.41	1.34
30	c	513	CLA	C1D-ND	2.85	1.41	1.37
41	13	311	A86	C25-C24	2.85	1.41	1.34
30	b	609	CLA	C3B-C2B	-2.85	1.36	1.40
30	33	305	CLA	C1D-ND	2.85	1.41	1.37
30	B	611	CLA	CMC-C2C	-2.84	1.44	1.50
30	19	303	CLA	CHC-C1C	2.84	1.42	1.35
30	37	303	CLA	CHC-C1C	2.84	1.42	1.35
30	15	308	CLA	CHC-C1C	2.84	1.42	1.35
30	18	309	CLA	CMB-C2B	-2.84	1.45	1.51
41	41	310	A86	C25-C24	2.84	1.41	1.34
30	34	308	CLA	CHC-C1C	2.84	1.42	1.35
30	19	301	CLA	CHC-C1C	2.84	1.42	1.35
30	c	508	CLA	MG-ND	-2.84	2.00	2.05
30	36	308	CLA	CMB-C2B	-2.84	1.45	1.51
30	33	307	CLA	CHC-C1C	2.84	1.42	1.35
30	40	207	CLA	CHC-C1C	2.84	1.42	1.35
30	31	305	CLA	CHC-C1C	2.84	1.42	1.35
39	D	407	PL9	C11-C9	-2.84	1.45	1.51
30	d	402	CLA	CMB-C2B	-2.84	1.45	1.51
30	17	303	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	33	308	CLA	CMB-C2B	-2.84	1.45	1.51
30	11	306	CLA	CHC-C1C	2.84	1.42	1.35
41	20	201	A86	C24-C1	2.84	1.52	1.45
32	A	409	BCR	C1-C6	-2.83	1.49	1.53
30	B	605	CLA	CHC-C1C	2.83	1.42	1.35
30	c	506	CLA	CMD-C2D	-2.83	1.44	1.50
30	c	508	CLA	C1D-ND	2.83	1.41	1.37
30	C	503	CLA	CMC-C2C	-2.83	1.44	1.50
30	20	207	CLA	CHC-C1C	2.83	1.42	1.35
41	13	317	A86	C19-C18	2.83	1.56	1.52
30	C	512	CLA	CMB-C2B	-2.83	1.45	1.51
30	37	308	CLA	C3B-CAB	-2.83	1.42	1.47
41	16	313	A86	C25-C24	2.83	1.41	1.34
30	17	306	CLA	CHC-C1C	2.83	1.42	1.35
30	21	302	CLA	CHC-C1C	2.83	1.42	1.35
30	C	521	CLA	CHC-C1C	2.83	1.42	1.35
41	15	314	A86	C25-C24	2.83	1.41	1.34
30	b	614	CLA	C1D-ND	2.83	1.41	1.37
32	A	409	BCR	C30-C25	-2.83	1.49	1.53
30	b	611	CLA	CMC-C2C	-2.83	1.44	1.50
30	34	307	CLA	CMB-C2B	-2.83	1.45	1.51
30	11	309	CLA	CHC-C1C	2.83	1.42	1.35
30	31	301	CLA	CMB-C2B	-2.82	1.45	1.51
41	11	314	A86	C25-C24	2.82	1.41	1.34
30	31	307	CLA	CHC-C1C	2.82	1.42	1.35
30	41	305	CLA	CHC-C1C	2.82	1.42	1.35
30	b	604	CLA	MG-ND	-2.82	2.00	2.05
30	c	514	CLA	C1D-ND	2.82	1.41	1.37
30	16	304	CLA	C1D-ND	2.82	1.41	1.37
41	21	310	A86	C25-C24	2.82	1.41	1.34
30	11	305	CLA	CHC-C1C	2.82	1.42	1.35
30	36	309	CLA	C1D-ND	2.82	1.41	1.37
31	A	403	PHO	CBD-CGD	-2.82	1.48	1.52
30	B	612	CLA	CMB-C2B	-2.82	1.45	1.51
30	19	306	CLA	CMB-C2B	-2.82	1.45	1.51
30	32	311	CLA	CHC-C1C	2.82	1.42	1.35
41	37	316	A86	C19-C18	2.82	1.56	1.52
30	19	305	CLA	CHC-C1C	2.82	1.42	1.35
30	37	306	CLA	CHC-C1C	2.82	1.42	1.35
30	21	305	CLA	CHC-C1C	2.82	1.42	1.35
30	17	308	CLA	C3B-CAB	-2.82	1.42	1.47
41	35	314	A86	C25-C24	2.82	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	612	CLA	CMB-C2B	-2.82	1.45	1.51
41	31	314	A86	C25-C24	2.82	1.41	1.34
30	32	310	CLA	CMB-C2B	-2.82	1.45	1.51
41	19	309	A86	O-C13	-2.82	1.17	1.23
30	39	306	CLA	CMB-C2B	-2.82	1.45	1.51
30	38	306	CLA	CHC-C1C	2.82	1.42	1.35
30	39	301	CLA	CHC-C1C	2.82	1.42	1.35
41	13	317	A86	C25-C24	2.81	1.41	1.34
30	B	607	CLA	C1D-ND	2.81	1.41	1.37
30	c	506	CLA	CMB-C2B	-2.81	1.45	1.51
30	39	305	CLA	CHC-C1C	2.81	1.42	1.35
30	d	401	CLA	C3B-CAB	-2.81	1.42	1.47
41	37	316	A86	C25-C24	2.81	1.41	1.34
30	c	524	CLA	CHC-C1C	2.81	1.42	1.35
30	32	311	CLA	CMB-C2B	-2.81	1.45	1.51
41	17	316	A86	C25-C24	2.81	1.41	1.34
30	12	313	CLA	CHC-C1C	2.81	1.42	1.35
30	33	311	CLA	CHC-C1C	2.81	1.42	1.35
30	39	306	CLA	C3B-C2B	-2.81	1.36	1.40
41	37	315	A86	C14-C15	2.81	1.58	1.52
41	32	318	A86	C19-C18	2.81	1.56	1.52
30	D	401	CLA	CMD-C2D	-2.81	1.44	1.50
30	41	304	CLA	CHC-C1C	2.81	1.42	1.35
30	B	601	CLA	C3B-C2B	-2.81	1.36	1.40
30	11	306	CLA	CMB-C2B	-2.81	1.45	1.51
33	a	405	SQD	O48-C23	2.81	1.41	1.33
32	a	408	BCR	C30-C25	-2.80	1.49	1.53
30	b	607	CLA	CMB-C2B	-2.80	1.45	1.51
41	12	319	A86	C25-C24	2.80	1.41	1.34
39	d	405	PL9	C53-C6	-2.80	1.44	1.50
41	36	313	A86	C25-C24	2.80	1.41	1.34
41	13	315	A86	C25-C24	2.80	1.41	1.34
30	31	307	CLA	CMB-C2B	-2.80	1.45	1.51
41	20	213	A86	O-C13	-2.80	1.17	1.23
31	d	403	PHO	CBD-CGD	-2.80	1.48	1.52
41	32	319	A86	C19-C18	2.80	1.56	1.52
30	40	204	CLA	CHC-C1C	2.80	1.42	1.35
41	17	302	A86	O-C13	-2.80	1.17	1.23
41	39	309	A86	O-C13	-2.80	1.17	1.23
30	35	302	CLA	CHC-C1C	2.80	1.42	1.35
41	15	310	A86	C25-C24	2.80	1.41	1.34
30	c	512	CLA	CMB-C2B	-2.79	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	17	315	A86	C14-C15	2.79	1.58	1.52
30	C	506	CLA	CMD-C2D	-2.79	1.44	1.50
30	34	308	CLA	CMB-C2B	-2.79	1.45	1.51
30	b	602	CLA	CHC-C1C	2.79	1.42	1.35
41	21	314	A86	O-C13	-2.79	1.17	1.23
30	13	309	CLA	CHC-C1C	2.79	1.42	1.35
30	19	302	CLA	CHC-C1C	2.79	1.42	1.35
41	34	311	A86	C25-C24	2.79	1.41	1.34
32	c	516	BCR	C30-C25	-2.79	1.49	1.53
32	h	101	BCR	C30-C25	-2.79	1.49	1.53
30	C	504	CLA	CMD-C2D	-2.79	1.44	1.50
30	12	306	CLA	CHC-C1C	2.79	1.42	1.35
30	32	308	CLA	CMD-C2D	-2.79	1.44	1.50
30	Z	102	CLA	CHC-C1C	2.79	1.42	1.35
41	32	318	A86	C25-C24	2.78	1.41	1.34
30	B	603	CLA	C3B-C2B	-2.78	1.36	1.40
30	A	402	CLA	C1D-ND	2.78	1.41	1.37
30	18	311	CLA	CHC-C1C	2.78	1.42	1.35
30	41	302	CLA	CHC-C1C	2.78	1.42	1.35
30	c	513	CLA	CMB-C2B	-2.78	1.45	1.51
30	b	605	CLA	CHC-C1C	2.78	1.42	1.35
30	39	302	CLA	CHC-C1C	2.78	1.42	1.35
30	d	402	CLA	CHC-C1C	2.78	1.42	1.35
39	D	404	PL9	C6-C1	-2.78	1.43	1.48
30	B	606	CLA	CMD-C2D	-2.78	1.44	1.50
41	35	310	A86	C25-C24	2.78	1.41	1.34
30	20	204	CLA	CHC-C1C	2.78	1.42	1.35
41	31	310	A86	C25-C24	2.78	1.41	1.34
30	b	612	CLA	CMC-C2C	-2.78	1.44	1.50
30	B	604	CLA	MG-ND	-2.78	2.00	2.05
39	D	407	PL9	C26-C24	-2.78	1.45	1.51
30	36	301	CLA	CHC-C1C	2.78	1.42	1.35
30	B	612	CLA	CMC-C2C	-2.78	1.44	1.50
30	b	603	CLA	C3B-C2B	-2.78	1.36	1.40
41	11	312	A86	C-C1	2.78	1.56	1.50
38	J	101	DGD	O5D-C6D	-2.77	1.38	1.43
30	C	506	CLA	CMB-C2B	-2.77	1.45	1.51
30	13	304	CLA	CHC-C1C	2.77	1.42	1.35
30	37	305	CLA	C1D-ND	2.77	1.41	1.37
30	37	307	CLA	CHC-C1C	2.77	1.42	1.35
41	21	310	A86	C19-C18	2.77	1.56	1.52
41	32	319	A86	C25-C24	2.77	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	38	315	A86	O-C13	-2.77	1.17	1.23
40	v	201	HEM	CAB-C3B	2.77	1.55	1.47
30	C	520	CLA	CHC-C1C	2.77	1.42	1.35
41	11	310	A86	C25-C24	2.77	1.41	1.34
40	E	101	HEM	CAB-C3B	2.77	1.55	1.47
30	16	301	CLA	CHC-C1C	2.77	1.42	1.35
39	D	407	PL9	C41-C39	-2.77	1.45	1.51
41	33	317	A86	C19-C18	2.77	1.56	1.52
41	14	311	A86	C25-C24	2.77	1.41	1.34
40	e	101	HEM	CAB-C3B	2.77	1.55	1.47
30	13	307	CLA	CHC-C1C	2.77	1.42	1.35
30	14	309	CLA	CHC-C1C	2.77	1.42	1.35
38	c	518	DGD	O6D-C5D	-2.77	1.37	1.44
30	C	513	CLA	CHC-C1C	2.77	1.42	1.35
30	11	304	CLA	CHC-C1C	2.77	1.42	1.35
41	16	310	A86	O-C13	-2.77	1.17	1.23
30	12	307	CLA	CHC-C1C	2.77	1.42	1.35
30	18	310	CLA	CHC-C1C	2.77	1.42	1.35
30	38	311	CLA	CHC-C1C	2.77	1.42	1.35
30	17	303	CLA	CMB-C2B	-2.77	1.45	1.51
30	c	509	CLA	CMC-C2C	-2.76	1.44	1.50
30	d	402	CLA	C3B-C2B	-2.76	1.36	1.40
30	a	403	CLA	CMD-C2D	-2.76	1.44	1.50
30	33	309	CLA	CMB-C2B	-2.76	1.45	1.51
30	34	305	CLA	CHC-C1C	2.76	1.42	1.35
41	32	314	A86	C25-C24	2.76	1.41	1.34
30	c	522	CLA	CHC-C1C	2.76	1.42	1.35
41	40	213	A86	O-C13	-2.76	1.17	1.23
30	11	303	CLA	CHC-C1C	2.76	1.42	1.35
30	13	303	CLA	CHC-C1C	2.76	1.42	1.35
30	37	303	CLA	CMB-C2B	-2.76	1.45	1.51
30	c	504	CLA	CMD-C2D	-2.76	1.44	1.50
41	36	310	A86	O-C13	-2.76	1.17	1.23
30	31	308	CLA	C3B-C2B	-2.76	1.36	1.40
30	17	304	CLA	CMB-C2B	-2.76	1.45	1.51
30	B	613	CLA	CHC-C1C	2.76	1.42	1.35
30	15	302	CLA	CHC-C1C	2.76	1.42	1.35
30	14	305	CLA	CHC-C1C	2.75	1.42	1.35
41	31	312	A86	C-C1	2.75	1.56	1.50
30	34	309	CLA	C3B-C2B	-2.75	1.36	1.40
30	33	310	CLA	CMB-C2B	-2.75	1.45	1.51
30	34	301	CLA	CMB-C2B	-2.75	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	615	CLA	CHC-C1C	2.75	1.42	1.35
41	37	302	A86	O-C13	-2.75	1.17	1.23
30	A	402	CLA	CMB-C2B	-2.75	1.45	1.51
30	32	312	CLA	CMB-C2B	-2.75	1.45	1.51
41	33	315	A86	O-C13	-2.75	1.17	1.23
41	41	310	A86	C19-C18	2.75	1.56	1.52
30	D	402	CLA	CHC-C1C	2.75	1.42	1.35
30	14	307	CLA	CMB-C2B	-2.75	1.45	1.51
30	38	310	CLA	CHC-C1C	2.75	1.42	1.35
30	b	611	CLA	C1D-ND	2.75	1.41	1.37
39	d	408	PL9	C41-C39	-2.75	1.45	1.51
30	37	304	CLA	CMB-C2B	-2.75	1.45	1.51
30	c	512	CLA	C3B-C2B	-2.75	1.36	1.40
30	11	302	CLA	CHC-C1C	2.75	1.42	1.35
30	38	301	CLA	CHC-C1C	2.75	1.42	1.35
30	36	309	CLA	CMB-C2B	-2.75	1.45	1.51
39	d	405	PL9	C6-C1	-2.75	1.43	1.48
30	37	305	CLA	CHC-C1C	2.75	1.42	1.35
30	c	507	CLA	MG-ND	-2.75	2.00	2.05
40	V	201	HEM	CAB-C3B	2.75	1.54	1.47
30	37	310	CLA	CHC-C1C	2.75	1.42	1.35
30	C	504	CLA	CMB-C2B	-2.74	1.45	1.51
30	b	603	CLA	C1D-ND	2.74	1.41	1.37
30	19	301	CLA	CMB-C2B	-2.74	1.45	1.51
41	17	314	A86	O-C13	-2.74	1.17	1.23
38	c	518	DGD	O5D-C6D	-2.74	1.38	1.43
30	14	308	CLA	CMB-C2B	-2.74	1.45	1.51
30	A	404	CLA	CMD-C2D	-2.74	1.45	1.50
30	17	307	CLA	CHC-C1C	2.74	1.42	1.35
30	14	304	CLA	CHC-C1C	2.74	1.42	1.35
30	C	505	CLA	C1D-ND	2.74	1.41	1.37
41	18	313	A86	O-C13	-2.74	1.17	1.23
30	B	602	CLA	CMB-C2B	-2.74	1.45	1.51
41	12	319	A86	C19-C18	2.74	1.56	1.52
30	39	301	CLA	CMB-C2B	-2.74	1.45	1.51
41	12	318	A86	O-C13	-2.74	1.17	1.23
30	17	310	CLA	CHC-C1C	2.74	1.42	1.35
41	21	311	A86	O-C13	-2.74	1.17	1.23
30	16	309	CLA	CMB-C2B	-2.74	1.45	1.51
30	18	301	CLA	CHC-C1C	2.74	1.42	1.35
41	13	315	A86	C19-C18	2.74	1.56	1.52
41	41	314	A86	O-C13	-2.74	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	32	303	CLA	CMB-C2B	-2.74	1.45	1.51
30	b	613	CLA	CHC-C1C	2.74	1.42	1.35
30	38	310	CLA	CMB-C2B	-2.74	1.46	1.51
41	11	313	A86	O-C13	-2.73	1.17	1.23
30	b	614	CLA	CMB-C2B	-2.73	1.46	1.51
30	c	522	CLA	CMB-C2B	-2.73	1.46	1.51
41	12	315	A86	C25-C24	2.73	1.41	1.34
30	b	615	CLA	CMD-C2D	-2.73	1.45	1.50
30	33	310	CLA	C3B-C2B	-2.73	1.36	1.40
39	d	408	PL9	C46-C44	-2.73	1.45	1.51
30	C	507	CLA	MG-ND	-2.73	2.00	2.05
30	32	308	CLA	CHC-C1C	2.73	1.42	1.35
30	d	401	CLA	CMD-C2D	-2.73	1.45	1.50
30	a	402	CLA	CMB-C2B	-2.73	1.46	1.51
30	c	513	CLA	CHC-C1C	2.73	1.42	1.35
30	16	302	CLA	C3B-C2B	-2.73	1.36	1.40
30	C	509	CLA	MG-ND	-2.73	2.00	2.05
30	39	307	CLA	CHC-C1C	2.73	1.42	1.35
41	18	315	A86	O-C13	-2.73	1.17	1.23
33	L	103	SQD	O48-C23	2.73	1.41	1.33
30	C	503	CLA	C3B-CAB	-2.73	1.42	1.47
30	14	309	CLA	CMB-C2B	-2.73	1.46	1.51
30	17	309	CLA	CHC-C1C	2.73	1.42	1.35
30	34	307	CLA	CHC-C1C	2.73	1.42	1.35
30	40	203	CLA	CMB-C2B	-2.73	1.46	1.51
41	13	314	A86	O-C13	-2.73	1.17	1.23
30	B	604	CLA	CMD-C2D	-2.73	1.45	1.50
30	31	304	CLA	CMD-C2D	-2.72	1.45	1.50
41	20	211	A86	O-C13	-2.72	1.17	1.23
41	40	212	A86	C24-C1	2.72	1.51	1.45
30	18	301	CLA	CMB-C2B	-2.72	1.46	1.51
30	17	305	CLA	CHC-C1C	2.72	1.41	1.35
30	W	103	CLA	CMD-C2D	-2.72	1.45	1.50
32	C	515	BCR	C30-C25	-2.72	1.50	1.53
30	36	302	CLA	C3B-C2B	-2.72	1.36	1.40
30	17	308	CLA	CHC-C1C	2.72	1.41	1.35
30	b	613	CLA	MG-ND	-2.72	2.00	2.05
30	34	303	CLA	CMB-C2B	-2.72	1.46	1.51
30	11	307	CLA	CMB-C2B	-2.72	1.46	1.51
41	11	310	A86	O-C13	-2.72	1.17	1.23
41	35	313	A86	O-C13	-2.72	1.17	1.23
41	40	211	A86	O-C13	-2.72	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	504	CLA	CMB-C2B	-2.72	1.46	1.51
30	b	602	CLA	CMB-C2B	-2.72	1.46	1.51
41	20	212	A86	C-C1	2.72	1.56	1.50
30	38	304	CLA	CMB-C2B	-2.72	1.46	1.51
30	34	304	CLA	CHC-C1C	2.72	1.41	1.35
41	12	315	A86	O-C13	-2.72	1.17	1.23
41	32	314	A86	O-C13	-2.72	1.17	1.23
30	39	304	CLA	CMB-C2B	-2.72	1.46	1.51
30	b	602	CLA	CMC-C2C	-2.72	1.45	1.50
30	b	604	CLA	CMD-C2D	-2.72	1.45	1.50
30	14	301	CLA	CMB-C2B	-2.72	1.46	1.51
30	16	307	CLA	CMB-C2B	-2.72	1.46	1.51
30	34	309	CLA	CMB-C2B	-2.72	1.46	1.51
30	34	305	CLA	CMD-C2D	-2.72	1.45	1.50
41	31	313	A86	O-C13	-2.71	1.17	1.23
30	C	509	CLA	CMC-C2C	-2.71	1.45	1.50
30	12	310	CLA	CHC-C1C	2.71	1.41	1.35
30	20	203	CLA	CHC-C1C	2.71	1.41	1.35
30	34	305	CLA	MG-ND	-2.71	2.00	2.05
30	B	613	CLA	MG-ND	-2.71	2.00	2.05
30	13	305	CLA	CHC-C1C	2.71	1.41	1.35
30	36	302	CLA	CHC-C1C	2.71	1.41	1.35
30	19	303	CLA	CMB-C2B	-2.71	1.46	1.51
30	B	615	CLA	CMC-C2C	-2.71	1.45	1.50
30	33	306	CLA	CMD-C2D	-2.71	1.45	1.50
30	a	402	CLA	CHC-C1C	2.71	1.41	1.35
41	41	311	A86	O-C13	-2.71	1.17	1.23
30	31	303	CLA	CMB-C2B	-2.71	1.46	1.51
30	17	306	CLA	CMD-C2D	-2.71	1.45	1.50
41	14	311	A86	O-C13	-2.71	1.17	1.23
30	39	303	CLA	CMB-C2B	-2.71	1.46	1.51
41	11	313	A86	C-C1	2.71	1.56	1.50
38	C	517	DGD	O4D-C4D	-2.71	1.36	1.43
30	20	203	CLA	CMB-C2B	-2.71	1.46	1.51
33	l	101	SQD	O48-C23	2.71	1.41	1.33
30	37	309	CLA	CHC-C1C	2.71	1.41	1.35
30	c	509	CLA	MG-ND	-2.71	2.00	2.05
30	16	307	CLA	CMC-C2C	-2.71	1.45	1.50
30	18	304	CLA	CMB-C2B	-2.71	1.46	1.51
30	19	307	CLA	CHC-C1C	2.71	1.41	1.35
41	14	314	A86	O-C13	-2.71	1.17	1.23
30	11	308	CLA	CHC-C1C	2.71	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	520	CLA	CMB-C2B	-2.70	1.46	1.51
30	31	304	CLA	MG-ND	-2.70	2.00	2.05
30	A	402	CLA	CHC-C1C	2.70	1.41	1.35
41	35	313	A86	C-C1	2.70	1.56	1.50
41	31	310	A86	O-C13	-2.70	1.17	1.23
41	13	315	A86	C-C1	2.70	1.56	1.50
41	16	312	A86	C-C1	2.70	1.56	1.50
41	37	314	A86	O-C13	-2.70	1.17	1.23
36	12	301	LMG	O1-C1	2.70	1.44	1.40
30	M	101	CLA	CMD-C2D	-2.70	1.45	1.50
30	34	309	CLA	CHC-C1C	2.70	1.41	1.35
30	40	203	CLA	CHC-C1C	2.70	1.41	1.35
30	18	310	CLA	CMB-C2B	-2.70	1.46	1.51
30	37	308	CLA	CHC-C1C	2.70	1.41	1.35
30	36	307	CLA	CMB-C2B	-2.70	1.46	1.51
30	12	303	CLA	CHC-C1C	2.70	1.41	1.35
30	31	304	CLA	CHC-C1C	2.70	1.41	1.35
30	B	614	CLA	CMB-C2B	-2.70	1.46	1.51
30	38	301	CLA	CMB-C2B	-2.70	1.46	1.51
30	14	303	CLA	CHC-C1C	2.70	1.41	1.35
30	21	302	CLA	CMB-C2B	-2.70	1.46	1.51
30	m	101	CLA	C1D-ND	2.70	1.41	1.37
41	33	314	A86	C14-C15	2.70	1.58	1.52
30	33	308	CLA	CHC-C1C	2.70	1.41	1.35
30	36	307	CLA	CMC-C2C	-2.70	1.45	1.50
31	D	403	PHO	CBD-CGD	-2.70	1.48	1.52
41	15	313	A86	C-C1	2.70	1.56	1.50
41	13	313	A86	C14-C15	2.69	1.58	1.52
30	D	405	CLA	CMB-C2B	-2.69	1.46	1.51
30	32	312	CLA	C3B-C2B	-2.69	1.36	1.40
30	c	507	CLA	CHC-C1C	2.69	1.41	1.35
41	14	313	A86	C14-C15	2.69	1.58	1.52
41	38	313	A86	O-C13	-2.69	1.17	1.23
41	17	313	A86	C14-C15	2.69	1.58	1.52
30	16	302	CLA	CHC-C1C	2.69	1.41	1.35
30	33	306	CLA	CHC-C1C	2.69	1.41	1.35
30	12	311	CLA	CMB-C2B	-2.69	1.46	1.51
30	32	305	CLA	CMB-C2B	-2.69	1.46	1.51
30	31	308	CLA	CMB-C2B	-2.69	1.46	1.51
30	12	308	CLA	CHC-C1C	2.69	1.41	1.35
41	40	212	A86	C-C1	2.69	1.56	1.50
30	33	303	CLA	CMB-C2B	-2.69	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	31	303	CLA	CHC-C1C	2.69	1.41	1.35
41	35	310	A86	O-C13	-2.69	1.17	1.23
30	C	513	CLA	CMB-C2B	-2.69	1.46	1.51
30	19	304	CLA	CMB-C2B	-2.69	1.46	1.51
30	14	307	CLA	CHC-C1C	2.69	1.41	1.35
30	19	302	CLA	CMB-C2B	-2.69	1.46	1.51
30	37	306	CLA	CMD-C2D	-2.69	1.45	1.50
30	C	502	CLA	C1D-ND	2.69	1.41	1.37
30	c	502	CLA	CMD-C2D	-2.69	1.45	1.50
39	D	404	PL9	C53-C6	-2.69	1.45	1.50
30	37	305	CLA	CMB-C2B	-2.69	1.46	1.51
30	B	615	CLA	CMD-C2D	-2.69	1.45	1.50
30	13	308	CLA	CMB-C2B	-2.69	1.46	1.51
39	D	407	PL9	C46-C44	-2.69	1.45	1.51
41	37	313	A86	C14-C15	2.69	1.58	1.52
30	17	305	CLA	CMB-C2B	-2.69	1.46	1.51
30	B	602	CLA	CMC-C2C	-2.69	1.45	1.50
41	35	314	A86	C19-C18	2.69	1.56	1.52
30	b	615	CLA	CMC-C2C	-2.69	1.45	1.50
33	A	406	SQD	O47-C7	2.69	1.41	1.34
41	20	212	A86	C24-C1	2.69	1.51	1.45
30	33	307	CLA	CMB-C2B	-2.69	1.46	1.51
30	11	315	CLA	CHC-C1C	2.69	1.41	1.35
41	13	311	A86	O-C13	-2.68	1.17	1.23
30	c	502	CLA	C1D-ND	2.68	1.41	1.37
30	c	505	CLA	C1D-ND	2.68	1.41	1.37
30	35	306	CLA	CMB-C2B	-2.68	1.46	1.51
39	D	407	PL9	C5-C4	-2.68	1.37	1.47
30	39	302	CLA	CMB-C2B	-2.68	1.46	1.51
38	C	517	DGD	O5D-C6D	-2.68	1.38	1.43
41	32	319	A86	C-C1	2.68	1.56	1.50
41	33	312	A86	O-C13	-2.68	1.17	1.23
30	c	511	CLA	C3B-CAB	-2.68	1.42	1.47
30	b	607	CLA	C1D-ND	2.68	1.41	1.37
41	12	318	A86	C-C1	2.68	1.56	1.50
41	40	210	A86	C-C1	2.68	1.56	1.50
30	C	502	CLA	CMD-C2D	-2.68	1.45	1.50
30	c	502	CLA	CMB-C2B	-2.68	1.46	1.51
41	14	313	A86	C-C1	2.68	1.56	1.50
41	34	313	A86	C14-C15	2.68	1.58	1.52
30	31	306	CLA	CHC-C1C	2.68	1.41	1.35
30	31	308	CLA	CHC-C1C	2.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	40	210	A86	C24-C1	2.68	1.51	1.45
30	B	613	CLA	C1D-ND	2.68	1.41	1.37
30	31	315	CLA	CMD-C2D	-2.68	1.45	1.50
30	B	606	CLA	C3B-C2B	-2.68	1.36	1.40
41	15	312	A86	C-C1	2.68	1.56	1.50
30	34	302	CLA	CMB-C2B	-2.68	1.46	1.51
41	20	210	A86	C24-C1	2.68	1.51	1.45
41	34	311	A86	O-C13	-2.67	1.17	1.23
30	41	302	CLA	CMB-C2B	-2.67	1.46	1.51
41	31	314	A86	C-C1	2.67	1.56	1.50
30	16	305	CLA	CHC-C1C	2.67	1.41	1.35
41	17	314	A86	C14-C15	2.67	1.57	1.52
41	14	314	A86	C-C1	2.67	1.56	1.50
41	17	316	A86	C-C1	2.67	1.56	1.50
30	32	307	CLA	CHC-C1C	2.67	1.41	1.35
30	M	101	CLA	C1D-ND	2.67	1.41	1.37
30	d	406	CLA	CMB-C2B	-2.67	1.46	1.51
30	12	312	CLA	CHC-C1C	2.67	1.41	1.35
41	33	314	A86	C-C1	2.67	1.56	1.50
41	37	316	A86	C-C1	2.67	1.56	1.50
30	b	601	CLA	C3B-CAB	-2.67	1.42	1.47
30	B	611	CLA	C1D-ND	2.67	1.41	1.37
30	13	309	CLA	C3B-C2B	-2.67	1.36	1.40
30	16	306	CLA	CHC-C1C	2.67	1.41	1.35
41	31	313	A86	C-C1	2.67	1.56	1.50
30	B	603	CLA	CMD-C2D	-2.67	1.45	1.50
41	13	313	A86	O-C13	-2.67	1.17	1.23
30	33	305	CLA	CHC-C1C	2.67	1.41	1.35
41	32	317	A86	O-C13	-2.67	1.17	1.23
30	b	615	CLA	CHC-C1C	2.67	1.41	1.35
41	36	313	A86	C19-C18	2.67	1.56	1.52
30	w	103	CLA	CMD-C2D	-2.67	1.45	1.50
31	d	404	PHO	CBD-CGD	-2.67	1.48	1.52
30	B	604	CLA	C3B-C2B	-2.66	1.36	1.40
30	D	401	CLA	CHC-C1C	2.66	1.41	1.35
41	12	317	A86	C-C1	2.66	1.56	1.50
41	36	312	A86	C-C1	2.66	1.56	1.50
30	14	301	CLA	CHC-C1C	2.66	1.41	1.35
30	C	502	CLA	CMB-C2B	-2.66	1.46	1.51
30	15	301	CLA	CMB-C2B	-2.66	1.46	1.51
30	15	306	CLA	CMB-C2B	-2.66	1.46	1.51
30	38	303	CLA	CMB-C2B	-2.66	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	33	314	A86	O-C13	-2.66	1.17	1.23
41	37	314	A86	C14-C15	2.66	1.57	1.52
41	12	317	A86	C14-C15	2.66	1.57	1.52
41	15	314	A86	C19-C18	2.66	1.56	1.52
30	m	101	CLA	CMD-C2D	-2.66	1.45	1.50
41	41	313	A86	C-C1	2.66	1.56	1.50
30	32	310	CLA	CHC-C1C	2.66	1.41	1.35
41	34	314	A86	O-C13	-2.66	1.17	1.23
38	j	101	DGD	O5D-C6D	-2.66	1.38	1.43
30	13	309	CLA	CMB-C2B	-2.66	1.46	1.51
41	39	310	A86	O-C13	-2.66	1.17	1.23
41	13	317	A86	C-C1	2.66	1.56	1.50
41	38	315	A86	C-C1	2.66	1.56	1.50
30	33	301	CLA	CMB-C2B	-2.66	1.46	1.51
30	b	622	CLA	C3B-C2B	-2.66	1.36	1.40
30	11	304	CLA	CMD-C2D	-2.66	1.45	1.50
30	c	503	CLA	C3B-CAB	-2.66	1.42	1.47
41	39	310	A86	C24-C1	2.66	1.51	1.45
30	18	303	CLA	CMB-C2B	-2.66	1.46	1.51
30	40	206	CLA	CMB-C2B	-2.66	1.46	1.51
41	33	317	A86	C-C1	2.66	1.56	1.50
30	C	507	CLA	CHC-C1C	2.66	1.41	1.35
30	17	304	CLA	CHC-C1C	2.66	1.41	1.35
30	34	301	CLA	CHC-C1C	2.66	1.41	1.35
30	31	315	CLA	CHC-C1C	2.66	1.41	1.35
41	13	313	A86	C-C1	2.66	1.56	1.50
30	M	101	CLA	C3B-C2B	-2.66	1.36	1.40
30	m	101	CLA	C3B-C2B	-2.66	1.36	1.40
41	35	312	A86	C-C1	2.66	1.56	1.50
30	36	306	CLA	CHC-C1C	2.66	1.41	1.35
30	16	305	CLA	CMD-C2D	-2.66	1.45	1.50
41	41	312	A86	O-C13	-2.65	1.17	1.23
38	C	517	DGD	O4E-C4E	-2.65	1.36	1.43
30	35	301	CLA	CMB-C2B	-2.65	1.46	1.51
41	11	316	A86	C24-C1	2.65	1.51	1.45
41	32	317	A86	C-C1	2.65	1.56	1.50
38	C	517	DGD	O6D-C5D	-2.65	1.37	1.44
41	16	312	A86	C14-C15	2.65	1.57	1.52
41	31	312	A86	C14-C15	2.65	1.57	1.52
30	d	401	CLA	C1D-ND	2.65	1.41	1.37
41	20	210	A86	C-C1	2.65	1.56	1.50
41	19	310	A86	O-C13	-2.65	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	34	314	A86	C14-C15	2.65	1.57	1.52
30	34	305	CLA	CMB-C2B	-2.65	1.46	1.51
39	d	408	PL9	C5-C4	-2.65	1.37	1.47
30	39	308	CLA	CHC-C1C	2.65	1.41	1.35
30	b	603	CLA	CMD-C2D	-2.65	1.45	1.50
30	b	604	CLA	C3B-C2B	-2.65	1.36	1.40
41	32	317	A86	C14-C15	2.65	1.57	1.52
30	C	511	CLA	C3B-CAB	-2.65	1.42	1.47
30	b	602	CLA	C3B-C2B	-2.65	1.36	1.40
30	18	308	CLA	CMB-C2B	-2.65	1.46	1.51
36	b	619	LMG	O4-C4	-2.65	1.36	1.43
38	c	518	DGD	O4E-C4E	-2.65	1.36	1.43
30	39	301	CLA	C3B-C2B	-2.65	1.36	1.40
30	C	510	CLA	MG-ND	-2.65	2.00	2.05
41	16	313	A86	C19-C18	2.65	1.56	1.52
41	20	213	A86	C-C1	2.65	1.56	1.50
36	w	101	LMG	O7-C8	-2.65	1.40	1.46
41	21	314	A86	C-C1	2.65	1.56	1.50
30	36	305	CLA	CHC-C1C	2.65	1.41	1.35
30	31	315	CLA	CMB-C2B	-2.65	1.46	1.51
41	17	311	A86	C-C1	2.65	1.56	1.50
30	34	304	CLA	CMB-C2B	-2.65	1.46	1.51
30	36	308	CLA	CHC-C1C	2.65	1.41	1.35
41	11	314	A86	C-C1	2.64	1.56	1.50
30	33	310	CLA	CHC-C1C	2.64	1.41	1.35
41	12	318	A86	C14-C15	2.64	1.57	1.52
30	33	304	CLA	CHC-C1C	2.64	1.41	1.35
41	16	313	A86	C-C1	2.64	1.56	1.50
30	33	306	CLA	MG-ND	-2.64	2.00	2.05
41	15	313	A86	O-C13	-2.64	1.17	1.23
30	12	313	CLA	CMB-C2B	-2.64	1.46	1.51
30	B	601	CLA	C3B-CAB	-2.64	1.42	1.47
30	B	623	CLA	MG-ND	-2.64	2.00	2.05
30	32	308	CLA	MG-ND	-2.64	2.00	2.05
30	32	306	CLA	CHC-C1C	2.64	1.41	1.35
41	11	314	A86	C19-C18	2.64	1.56	1.52
30	32	312	CLA	CHC-C1C	2.64	1.41	1.35
41	21	312	A86	O-C13	-2.64	1.17	1.23
41	36	310	A86	C-C1	2.64	1.56	1.50
41	40	213	A86	C-C1	2.64	1.56	1.50
30	16	308	CLA	CHC-C1C	2.64	1.41	1.35
41	34	314	A86	C-C1	2.64	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	41	314	A86	C-C1	2.64	1.56	1.50
30	12	303	CLA	CMB-C2B	-2.64	1.46	1.51
30	16	301	CLA	CMB-C2B	-2.64	1.46	1.51
41	15	313	A86	C14-C15	2.64	1.57	1.52
41	32	316	A86	O-C13	-2.64	1.17	1.23
41	37	313	A86	C-C1	2.64	1.56	1.50
30	z	101	CLA	CMB-C2B	-2.64	1.46	1.51
30	37	304	CLA	CHC-C1C	2.64	1.41	1.35
36	W	101	LMG	O7-C8	-2.64	1.40	1.46
41	32	316	A86	C-C1	2.64	1.56	1.50
41	32	318	A86	C-C1	2.64	1.56	1.50
30	D	401	CLA	MG-ND	-2.64	2.00	2.05
30	B	610	CLA	CMC-C2C	-2.64	1.45	1.50
30	12	308	CLA	CMD-C2D	-2.64	1.45	1.50
41	15	314	A86	C-C1	2.64	1.56	1.50
41	21	313	A86	C-C1	2.64	1.56	1.50
41	38	314	A86	O-C13	-2.64	1.17	1.23
30	b	622	CLA	MG-ND	-2.64	2.00	2.05
30	12	305	CLA	CMB-C2B	-2.64	1.46	1.51
30	33	305	CLA	CMB-C2B	-2.64	1.46	1.51
41	21	313	A86	O-C13	-2.64	1.17	1.23
30	11	315	CLA	CMB-C2B	-2.64	1.46	1.51
30	39	306	CLA	CHC-C1C	2.63	1.41	1.35
38	c	518	DGD	O4D-C4D	-2.63	1.36	1.43
41	31	314	A86	C19-C18	2.63	1.56	1.52
41	19	311	A86	C24-C1	2.63	1.51	1.45
30	36	301	CLA	CMB-C2B	-2.63	1.46	1.51
41	32	316	A86	C14-C15	2.63	1.57	1.52
30	17	301	CLA	CHC-C1C	2.63	1.41	1.35
41	34	313	A86	C-C1	2.63	1.56	1.50
30	b	603	CLA	MG-ND	-2.63	2.00	2.05
41	18	315	A86	C-C1	2.63	1.56	1.50
41	35	314	A86	C-C1	2.63	1.56	1.50
30	20	206	CLA	CMB-C2B	-2.63	1.46	1.51
41	17	302	A86	C-C1	2.63	1.56	1.50
30	C	521	CLA	CMB-C2B	-2.63	1.46	1.51
41	36	311	A86	O-C13	-2.63	1.17	1.23
30	c	504	CLA	CHC-C1C	2.63	1.41	1.35
41	41	313	A86	O-C13	-2.63	1.17	1.23
30	19	308	CLA	CHC-C1C	2.63	1.41	1.35
41	13	312	A86	O-C13	-2.63	1.17	1.23
41	15	310	A86	O-C13	-2.63	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	36	312	A86	C14-C15	2.63	1.57	1.52
30	B	602	CLA	C3B-C2B	-2.63	1.36	1.40
30	d	401	CLA	MG-ND	-2.63	2.00	2.05
41	33	302	A86	C24-C1	2.63	1.51	1.45
30	15	309	CLA	CMB-C2B	-2.63	1.46	1.51
30	d	401	CLA	CHC-C1C	2.63	1.41	1.35
41	17	315	A86	O-C13	-2.63	1.17	1.23
30	C	519	CLA	CMB-C2B	-2.63	1.46	1.51
30	37	301	CLA	CHC-C1C	2.63	1.41	1.35
30	32	308	CLA	CMB-C2B	-2.63	1.46	1.51
30	15	307	CLA	CMB-C2B	-2.63	1.46	1.51
41	31	311	A86	O-C13	-2.63	1.17	1.23
41	13	314	A86	C-C1	2.63	1.56	1.50
41	19	310	A86	C24-C1	2.63	1.51	1.45
31	d	403	PHO	C3B-C2B	-2.63	1.36	1.40
41	36	313	A86	C-C1	2.62	1.56	1.50
30	35	309	CLA	CMB-C2B	-2.62	1.46	1.51
30	32	305	CLA	CMC-C2C	-2.62	1.45	1.50
31	A	403	PHO	C3B-C2B	-2.62	1.36	1.40
30	C	503	CLA	CMD-C2D	-2.62	1.45	1.50
30	b	610	CLA	CMC-C2C	-2.62	1.45	1.50
30	11	308	CLA	CMB-C2B	-2.62	1.46	1.51
30	c	510	CLA	MG-ND	-2.62	2.00	2.05
30	c	523	CLA	CMB-C2B	-2.62	1.46	1.51
31	A	403	PHO	CMD-C2D	-2.62	1.45	1.51
30	14	302	CLA	CMB-C2B	-2.62	1.46	1.51
30	13	305	CLA	CMD-C2D	-2.62	1.45	1.50
30	34	303	CLA	CHC-C1C	2.62	1.41	1.35
41	17	315	A86	C24-C1	2.62	1.51	1.45
30	12	307	CLA	CMB-C2B	-2.62	1.46	1.51
30	d	407	CLA	CHC-C1C	2.62	1.41	1.35
30	11	301	CLA	CMB-C2B	-2.62	1.46	1.51
30	14	305	CLA	CMB-C2B	-2.62	1.46	1.51
30	18	312	CLA	CMB-C2B	-2.62	1.46	1.51
41	14	312	A86	O-C13	-2.62	1.17	1.23
30	d	406	CLA	CHC-C1C	2.62	1.41	1.35
30	B	612	CLA	CMA-C3A	-2.62	1.47	1.53
30	b	613	CLA	C1D-ND	2.62	1.41	1.37
30	31	304	CLA	CMB-C2B	-2.62	1.46	1.51
30	b	612	CLA	CHC-C1C	2.62	1.41	1.35
30	38	308	CLA	CMB-C2B	-2.62	1.46	1.51
30	C	511	CLA	CMB-C2B	-2.62	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	17	313	A86	C-C1	2.62	1.56	1.50
30	17	307	CLA	CMD-C2D	-2.62	1.45	1.50
30	B	612	CLA	CHC-C1C	2.62	1.41	1.35
30	B	610	CLA	C1D-ND	2.62	1.41	1.37
30	12	312	CLA	CMB-C2B	-2.61	1.46	1.51
41	18	302	A86	C24-C1	2.61	1.51	1.45
36	B	620	LMG	O4-C4	-2.61	1.36	1.43
41	37	311	A86	C24-C1	2.61	1.51	1.45
30	20	204	CLA	CMB-C2B	-2.61	1.46	1.51
30	17	309	CLA	CMB-C2B	-2.61	1.46	1.51
30	B	613	CLA	CMB-C2B	-2.61	1.46	1.51
30	13	304	CLA	CMB-C2B	-2.61	1.46	1.51
30	c	510	CLA	CMC-C2C	-2.61	1.45	1.50
30	D	402	CLA	C3B-C2B	-2.61	1.36	1.40
30	18	304	CLA	CHC-C1C	2.61	1.41	1.35
30	19	304	CLA	CHC-C1C	2.61	1.41	1.35
41	16	310	A86	C-C1	2.61	1.56	1.50
41	37	311	A86	C-C1	2.61	1.56	1.50
30	11	304	CLA	CMB-C2B	-2.61	1.46	1.51
30	34	302	CLA	CMC-C2C	-2.61	1.45	1.50
30	37	307	CLA	CMD-C2D	-2.61	1.45	1.50
41	17	311	A86	C24-C1	2.61	1.51	1.45
41	38	302	A86	C24-C1	2.61	1.51	1.45
41	11	313	A86	C14-C15	2.61	1.57	1.52
41	38	315	A86	C14-C15	2.61	1.57	1.52
41	35	316	A86	C-C1	2.61	1.56	1.50
41	13	301	A86	C24-C1	2.61	1.51	1.45
30	b	613	CLA	CMB-C2B	-2.61	1.46	1.51
30	33	310	CLA	MG-ND	-2.61	2.00	2.05
30	37	309	CLA	CMB-C2B	-2.61	1.46	1.51
30	36	305	CLA	CMD-C2D	-2.61	1.45	1.50
30	C	504	CLA	CHC-C1C	2.61	1.41	1.35
30	C	510	CLA	CMC-C2C	-2.61	1.45	1.50
30	38	312	CLA	CMB-C2B	-2.61	1.46	1.51
30	c	506	CLA	CHC-C1C	2.61	1.41	1.35
30	C	503	CLA	C4B-CHC	-2.61	1.33	1.41
30	20	205	CLA	CHC-C1C	2.61	1.41	1.35
30	31	302	CLA	CMB-C2B	-2.61	1.46	1.51
41	14	314	A86	C14-C15	2.61	1.57	1.52
30	b	611	CLA	CHC-C1C	2.61	1.41	1.35
41	15	312	A86	C14-C15	2.61	1.57	1.52
30	c	503	CLA	CMD-C2D	-2.61	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	34	313	A86	O-C13	-2.61	1.17	1.23
30	19	306	CLA	CHC-C1C	2.60	1.41	1.35
30	D	405	CLA	MG-ND	-2.60	2.00	2.05
41	37	302	A86	C-C1	2.60	1.56	1.50
30	11	305	CLA	CMB-C2B	-2.60	1.46	1.51
41	12	317	A86	O-C13	-2.60	1.17	1.23
41	37	313	A86	O-C13	-2.60	1.17	1.23
41	11	312	A86	C14-C15	2.60	1.57	1.52
30	34	309	CLA	MG-ND	-2.60	2.00	2.05
30	a	403	CLA	CHC-C1C	2.60	1.41	1.35
41	31	316	A86	C24-C1	2.60	1.51	1.45
41	37	315	A86	C24-C1	2.60	1.51	1.45
36	B	619	LMG	O7-C8	-2.60	1.40	1.46
41	31	313	A86	C14-C15	2.60	1.57	1.52
36	Q	301	LMG	O8-C9	-2.60	1.39	1.45
30	31	308	CLA	CMD-C2D	-2.60	1.45	1.50
30	C	519	CLA	CHC-C1C	2.60	1.41	1.35
30	D	405	CLA	CHC-C1C	2.60	1.41	1.35
30	35	308	CLA	CMB-C2B	-2.60	1.46	1.51
30	40	207	CLA	CMB-C2B	-2.60	1.46	1.51
30	11	303	CLA	CMB-C2B	-2.60	1.46	1.51
30	B	608	CLA	C1D-ND	2.60	1.41	1.37
41	11	311	A86	O-C13	-2.60	1.17	1.23
41	16	311	A86	O-C13	-2.60	1.17	1.23
41	16	312	A86	O-C13	-2.60	1.17	1.23
38	c	518	DGD	O3G-C1D	-2.60	1.35	1.40
41	16	312	A86	C24-C1	2.60	1.51	1.45
41	17	312	A86	O-C13	-2.60	1.17	1.23
41	36	312	A86	C24-C1	2.60	1.51	1.45
30	z	101	CLA	CHC-C1C	2.60	1.41	1.35
41	21	310	A86	C-C1	2.60	1.56	1.50
36	c	519	LMG	O8-C9	-2.60	1.39	1.45
36	b	618	LMG	O7-C8	-2.60	1.40	1.46
30	35	307	CLA	CMB-C2B	-2.60	1.46	1.51
41	35	313	A86	C14-C15	2.60	1.57	1.52
41	39	311	A86	C24-C1	2.60	1.51	1.45
30	b	608	CLA	C1D-ND	2.60	1.41	1.37
30	34	310	CLA	CMB-C2B	-2.60	1.46	1.51
41	41	310	A86	C-C1	2.60	1.56	1.50
41	33	313	A86	O-C13	-2.60	1.17	1.23
30	D	406	CLA	CHC-C1C	2.60	1.41	1.35
30	32	313	CLA	CMB-C2B	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	404	CLA	CHC-C1C	2.59	1.41	1.35
33	a	405	SQD	O47-C7	2.59	1.41	1.34
41	15	311	A86	O-C13	-2.59	1.17	1.23
30	33	301	CLA	CMD-C2D	-2.59	1.45	1.50
30	B	603	CLA	MG-ND	-2.59	2.00	2.05
41	34	312	A86	O-C13	-2.59	1.17	1.23
30	20	207	CLA	CMB-C2B	-2.59	1.46	1.51
41	12	319	A86	C-C1	2.59	1.56	1.50
31	d	403	PHO	CMD-C2D	-2.59	1.45	1.51
41	17	313	A86	O-C13	-2.59	1.17	1.23
41	13	314	A86	C14-C15	2.59	1.57	1.52
30	39	304	CLA	CHC-C1C	2.59	1.41	1.35
30	14	309	CLA	CMD-C2D	-2.59	1.45	1.50
30	14	304	CLA	CMB-C2B	-2.59	1.46	1.51
30	32	312	CLA	MG-ND	-2.59	2.00	2.05
41	33	315	A86	C-C1	2.59	1.56	1.50
38	C	517	DGD	O3G-C1D	-2.59	1.35	1.40
41	20	213	A86	C24-C1	2.59	1.51	1.45
30	40	206	CLA	CHC-C1C	2.59	1.41	1.35
41	13	316	A86	C-C1	2.59	1.56	1.50
30	36	308	CLA	C3B-C2B	-2.59	1.36	1.40
30	c	512	CLA	MG-ND	-2.59	2.00	2.05
30	38	304	CLA	CHC-C1C	2.59	1.41	1.35
30	40	204	CLA	CMB-C2B	-2.59	1.46	1.51
41	39	311	A86	C-C1	2.59	1.56	1.50
41	17	314	A86	C-C1	2.59	1.56	1.50
30	c	513	CLA	CMD-C2D	-2.59	1.45	1.50
41	18	315	A86	C14-C15	2.59	1.57	1.52
30	B	604	CLA	CAC-C3C	-2.59	1.44	1.51
30	34	306	CLA	CMB-C2B	-2.59	1.46	1.51
41	15	316	A86	C-C1	2.59	1.56	1.50
41	34	313	A86	C24-C1	2.59	1.51	1.45
30	D	401	CLA	CMC-C2C	-2.58	1.45	1.50
30	12	312	CLA	CMD-C2D	-2.58	1.45	1.50
30	31	302	CLA	CHC-C1C	2.58	1.41	1.35
30	14	310	CLA	CMB-C2B	-2.58	1.46	1.51
41	31	316	A86	C-C1	2.58	1.56	1.50
41	14	313	A86	C24-C1	2.58	1.51	1.45
41	40	213	A86	C24-C1	2.58	1.51	1.45
30	b	609	CLA	CHC-C1C	2.58	1.41	1.35
30	33	301	CLA	CHC-C1C	2.58	1.41	1.35
41	35	316	A86	C24-C1	2.58	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	35	311	A86	O-C13	-2.58	1.17	1.23
41	15	312	A86	O-C13	-2.58	1.17	1.23
41	37	312	A86	O-C13	-2.58	1.17	1.23
30	34	301	CLA	CMD-C2D	-2.58	1.45	1.50
30	w	102	CLA	CHC-C1C	2.58	1.41	1.35
30	c	503	CLA	C4B-CHC	-2.58	1.33	1.41
30	b	606	CLA	C3B-C2B	-2.58	1.36	1.40
30	B	613	CLA	CAA-C2A	-2.58	1.49	1.54
30	31	305	CLA	CMB-C2B	-2.58	1.46	1.51
30	W	102	CLA	CHC-C1C	2.58	1.41	1.35
30	13	310	CLA	CMB-C2B	-2.58	1.46	1.51
30	b	609	CLA	CMD-C2D	-2.58	1.45	1.50
41	15	316	A86	C24-C1	2.58	1.51	1.45
30	C	512	CLA	MG-ND	-2.58	2.00	2.05
30	b	610	CLA	C1D-ND	2.58	1.41	1.37
30	11	309	CLA	CMB-C2B	-2.58	1.46	1.51
30	B	605	CLA	CMD-C2D	-2.58	1.45	1.50
30	C	508	CLA	CMD-C2D	-2.58	1.45	1.50
41	36	312	A86	O-C13	-2.58	1.17	1.23
30	b	610	CLA	MG-ND	-2.58	2.00	2.05
41	12	317	A86	C24-C1	2.58	1.51	1.45
30	B	610	CLA	CHC-C1C	2.58	1.41	1.35
30	19	301	CLA	C3B-C2B	-2.58	1.36	1.40
30	c	510	CLA	CHC-C1C	2.58	1.41	1.35
41	18	314	A86	O-C13	-2.58	1.17	1.23
30	12	303	CLA	CMD-C2D	-2.58	1.45	1.50
41	37	315	A86	O-C13	-2.58	1.17	1.23
30	c	505	CLA	CAC-C3C	-2.58	1.44	1.51
30	13	302	CLA	CMB-C2B	-2.58	1.46	1.51
30	B	603	CLA	C1D-ND	2.58	1.41	1.37
30	11	304	CLA	MG-ND	-2.58	2.00	2.05
41	21	314	A86	C24-C1	2.58	1.51	1.45
41	33	316	A86	C-C1	2.57	1.56	1.50
41	14	313	A86	O-C13	-2.57	1.17	1.23
41	32	315	A86	O-C13	-2.57	1.17	1.23
30	C	512	CLA	C3B-C2B	-2.57	1.36	1.40
30	14	306	CLA	CMB-C2B	-2.57	1.46	1.51
30	18	305	CLA	CMB-C2B	-2.57	1.46	1.51
36	32	301	LMG	O1-C1	2.57	1.44	1.40
41	37	314	A86	C-C1	2.57	1.56	1.50
30	B	611	CLA	CHC-C1C	2.57	1.41	1.35
41	33	314	A86	C24-C1	2.57	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	316	A86	C24-C1	2.57	1.51	1.45
30	D	405	CLA	CMC-C2C	-2.57	1.45	1.50
30	B	623	CLA	C3B-C2B	-2.57	1.36	1.40
30	b	606	CLA	CHC-C1C	2.57	1.41	1.35
41	15	315	A86	C24-C1	2.57	1.51	1.45
41	11	312	A86	O-C13	-2.57	1.17	1.23
30	32	303	CLA	CMD-C2D	-2.57	1.45	1.50
41	15	315	A86	C-C1	2.57	1.56	1.50
30	12	305	CLA	CMC-C2C	-2.57	1.45	1.50
30	13	305	CLA	CMB-C2B	-2.57	1.46	1.51
30	c	504	CLA	C3B-C2B	-2.57	1.36	1.40
30	B	609	CLA	CMD-C2D	-2.57	1.45	1.50
30	c	514	CLA	CMB-C2B	-2.57	1.46	1.51
30	32	307	CLA	CMB-C2B	-2.57	1.46	1.51
30	40	205	CLA	CHC-C1C	2.57	1.41	1.35
30	B	610	CLA	MG-ND	-2.57	2.00	2.05
41	17	311	A86	O-C13	-2.57	1.17	1.23
38	c	518	DGD	O3G-C3G	-2.57	1.39	1.43
30	12	308	CLA	CMB-C2B	-2.57	1.46	1.51
30	d	401	CLA	CMC-C2C	-2.57	1.45	1.50
30	32	312	CLA	CMD-C2D	-2.57	1.45	1.50
41	37	311	A86	O-C13	-2.57	1.17	1.23
30	33	311	CLA	CMB-C2B	-2.57	1.46	1.51
30	36	309	CLA	CMD-C2D	-2.57	1.45	1.50
30	20	206	CLA	CHC-C1C	2.57	1.41	1.35
30	16	308	CLA	C3B-C2B	-2.56	1.36	1.40
41	32	314	A86	C-C1	2.56	1.56	1.50
30	C	505	CLA	CAC-C3C	-2.56	1.44	1.51
30	B	606	CLA	CMC-C2C	-2.56	1.45	1.50
41	33	315	A86	C14-C15	2.56	1.57	1.52
41	11	312	A86	C24-C1	2.56	1.51	1.45
30	B	610	CLA	CMD-C2D	-2.56	1.45	1.50
30	33	303	CLA	CMC-C2C	-2.56	1.45	1.50
41	19	311	A86	O-C13	-2.56	1.17	1.23
30	31	308	CLA	C3B-CAB	-2.56	1.42	1.47
41	33	302	A86	C-C1	2.56	1.56	1.50
41	17	313	A86	C24-C1	2.56	1.51	1.45
41	31	312	A86	O-C13	-2.56	1.17	1.23
30	12	314	CLA	CMB-C2B	-2.56	1.46	1.51
30	31	309	CLA	CMB-C2B	-2.56	1.46	1.51
30	C	504	CLA	C3B-C2B	-2.56	1.36	1.40
41	12	316	A86	O-C13	-2.56	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	31	301	CLA	CMC-C2C	-2.56	1.45	1.50
30	36	303	CLA	CMB-C2B	-2.56	1.46	1.51
30	37	307	CLA	CMB-C2B	-2.56	1.46	1.51
41	39	311	A86	O-C13	-2.56	1.17	1.23
30	32	309	CLA	CMB-C2B	-2.56	1.46	1.51
30	B	606	CLA	CHC-C1C	2.56	1.41	1.35
41	35	315	A86	C24-C1	2.56	1.51	1.45
30	15	308	CLA	C3B-C2B	-2.56	1.36	1.40
30	36	309	CLA	C3B-C2B	-2.56	1.36	1.40
30	31	307	CLA	C3B-C2B	-2.56	1.36	1.40
30	B	609	CLA	CHC-C1C	2.56	1.41	1.35
41	35	312	A86	O-C13	-2.56	1.17	1.23
30	34	308	CLA	MG-ND	-2.56	2.00	2.05
30	C	512	CLA	C3B-CAB	-2.56	1.42	1.47
41	35	314	A86	O-C13	-2.56	1.17	1.23
30	21	309	CLA	CMB-C2B	-2.56	1.46	1.51
30	b	610	CLA	CHC-C1C	2.55	1.41	1.35
30	15	308	CLA	CMB-C2B	-2.55	1.46	1.51
30	b	608	CLA	CMD-C2D	-2.55	1.45	1.50
30	14	302	CLA	CMC-C2C	-2.55	1.45	1.50
41	35	312	A86	C14-C15	2.55	1.57	1.52
41	19	311	A86	C-C1	2.55	1.56	1.50
30	B	605	CLA	C3B-CAB	-2.55	1.42	1.47
30	18	301	CLA	C3B-C2B	-2.55	1.36	1.40
30	B	608	CLA	CMD-C2D	-2.55	1.45	1.50
30	38	305	CLA	CMB-C2B	-2.55	1.46	1.51
30	33	306	CLA	CMB-C2B	-2.55	1.46	1.51
30	B	601	CLA	CHC-C1C	2.55	1.41	1.35
41	38	313	A86	C-C1	2.55	1.56	1.50
36	W	101	LMG	O8-C9	-2.55	1.39	1.45
30	11	308	CLA	C3B-C2B	-2.55	1.36	1.40
30	16	303	CLA	CHC-C1C	2.55	1.41	1.35
30	C	510	CLA	CHC-C1C	2.55	1.41	1.35
30	12	309	CLA	CMB-C2B	-2.55	1.46	1.51
30	b	610	CLA	CMD-C2D	-2.55	1.45	1.50
41	17	316	A86	O-C13	-2.55	1.17	1.23
30	b	612	CLA	CMA-C3A	-2.55	1.47	1.53
41	33	316	A86	C24-C1	2.55	1.51	1.45
41	37	313	A86	C24-C1	2.54	1.51	1.45
36	w	101	LMG	O8-C9	-2.54	1.39	1.45
30	32	306	CLA	CMB-C2B	-2.54	1.46	1.51
30	39	308	CLA	CMB-C2B	-2.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	33	309	CLA	C3B-C2B	-2.54	1.36	1.40
41	12	304	A86	C-C1	2.54	1.56	1.50
41	13	316	A86	C24-C1	2.54	1.51	1.45
30	C	510	CLA	C1D-ND	2.54	1.40	1.37
41	20	212	A86	C35-C34	2.54	1.56	1.51
41	13	313	A86	C24-C1	2.54	1.51	1.45
30	c	511	CLA	CMB-C2B	-2.54	1.46	1.51
41	15	314	A86	O-C13	-2.54	1.17	1.23
30	C	506	CLA	CHC-C1C	2.54	1.41	1.35
30	b	613	CLA	CAA-C2A	-2.54	1.49	1.54
30	b	601	CLA	CHC-C1C	2.54	1.41	1.35
41	40	201	A86	O-C13	-2.54	1.17	1.23
41	13	301	A86	C-C1	2.54	1.56	1.50
30	w	102	CLA	C3B-C2B	-2.54	1.36	1.40
30	36	302	CLA	CMC-C2C	-2.54	1.45	1.50
41	32	304	A86	C-C1	2.54	1.56	1.50
30	36	305	CLA	CMB-C2B	-2.54	1.46	1.51
30	16	309	CLA	C3B-C2B	-2.54	1.36	1.40
30	14	309	CLA	C3B-C2B	-2.54	1.36	1.40
30	16	303	CLA	CMB-C2B	-2.54	1.46	1.51
30	19	308	CLA	CMB-C2B	-2.54	1.46	1.51
30	12	308	CLA	MG-ND	-2.54	2.00	2.05
30	13	305	CLA	MG-ND	-2.54	2.00	2.05
41	32	304	A86	C24-C1	2.54	1.51	1.45
30	15	303	CLA	CMB-C2B	-2.54	1.46	1.51
41	41	314	A86	C24-C1	2.54	1.51	1.45
30	b	603	CLA	CHC-C1C	2.53	1.41	1.35
30	39	307	CLA	CMB-C2B	-2.53	1.46	1.51
30	a	403	CLA	CMC-C2C	-2.53	1.45	1.50
30	z	101	CLA	MG-ND	-2.53	2.00	2.05
30	17	307	CLA	CMB-C2B	-2.53	1.46	1.51
30	13	303	CLA	CMB-C2B	-2.53	1.46	1.51
41	35	315	A86	O-C13	-2.53	1.18	1.23
30	41	306	CLA	CMB-C2B	-2.53	1.46	1.51
30	d	406	CLA	MG-ND	-2.53	2.00	2.05
30	12	306	CLA	CMB-C2B	-2.53	1.46	1.51
30	b	607	CLA	CHC-C1C	2.53	1.41	1.35
41	37	316	A86	O-C13	-2.53	1.18	1.23
30	b	607	CLA	CMD-C2D	-2.53	1.45	1.50
41	18	313	A86	C-C1	2.53	1.56	1.50
30	b	604	CLA	C4B-CHC	-2.53	1.34	1.41
30	14	301	CLA	CMD-C2D	-2.53	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	38	301	CLA	C3B-C2B	-2.53	1.36	1.40
42	12	302	LMU	O3'-C3'	2.53	1.48	1.43
30	41	309	CLA	CMB-C2B	-2.53	1.46	1.51
41	15	310	A86	C-C1	2.53	1.56	1.50
30	13	306	CLA	CMB-C2B	-2.53	1.46	1.51
30	35	303	CLA	CMB-C2B	-2.53	1.46	1.51
41	20	201	A86	O-C13	-2.53	1.18	1.23
41	12	315	A86	C-C1	2.53	1.56	1.50
30	B	607	CLA	CHC-C1C	2.53	1.41	1.35
38	C	517	DGD	O3G-C3G	-2.53	1.39	1.43
38	J	101	DGD	O1G-C1G	-2.53	1.39	1.45
41	20	201	A86	C-C1	2.53	1.56	1.50
30	B	604	CLA	C4B-CHC	-2.53	1.34	1.41
41	40	212	A86	C35-C34	2.53	1.56	1.51
30	32	303	CLA	CHC-C1C	2.53	1.41	1.35
36	12	301	LMG	O4-C4	-2.53	1.37	1.43
30	37	306	CLA	CMB-C2B	-2.53	1.46	1.51
30	C	509	CLA	CMD-C2D	-2.53	1.45	1.50
41	31	312	A86	C24-C1	2.52	1.51	1.45
30	36	303	CLA	CHC-C1C	2.52	1.41	1.35
41	13	317	A86	O-C13	-2.52	1.18	1.23
41	11	316	A86	C-C1	2.52	1.56	1.50
41	35	312	A86	C24-C1	2.52	1.51	1.45
30	d	402	CLA	C3B-CAB	-2.52	1.42	1.47
30	16	302	CLA	CMC-C2C	-2.52	1.45	1.50
36	D	408	LMG	O1-C7	-2.52	1.39	1.43
35	a	407	LHG	O7-C5	-2.52	1.40	1.46
30	34	309	CLA	CMD-C2D	-2.52	1.45	1.50
30	16	305	CLA	CMB-C2B	-2.52	1.46	1.51
41	18	302	A86	C-C1	2.52	1.56	1.50
30	36	307	CLA	CMD-C2D	-2.52	1.45	1.50
41	12	304	A86	C24-C1	2.52	1.51	1.45
30	18	307	CLA	CMB-C2B	-2.52	1.46	1.51
41	40	201	A86	C-C1	2.52	1.56	1.50
30	21	308	CLA	CMB-C2B	-2.52	1.46	1.51
30	b	604	CLA	CAC-C3C	-2.52	1.44	1.51
30	19	307	CLA	CMB-C2B	-2.52	1.46	1.51
41	35	315	A86	C-C1	2.52	1.56	1.50
36	32	301	LMG	O7-C8	-2.52	1.40	1.46
30	D	401	CLA	C1D-ND	2.52	1.40	1.37
33	B	621	SQD	O47-C7	2.52	1.41	1.34
30	32	311	CLA	C3B-C2B	-2.52	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	614	CLA	CMD-C2D	-2.51	1.45	1.50
30	13	309	CLA	CMD-C2D	-2.51	1.45	1.50
30	17	309	CLA	C3B-C2B	-2.51	1.36	1.40
30	d	407	CLA	CMD-C2D	-2.51	1.45	1.50
30	c	508	CLA	CMD-C2D	-2.51	1.45	1.50
30	B	603	CLA	CHC-C1C	2.51	1.41	1.35
35	A	408	LHG	O7-C5	-2.51	1.40	1.46
30	w	102	CLA	CMC-C2C	-2.51	1.45	1.50
30	D	406	CLA	C1D-ND	2.51	1.40	1.37
30	C	513	CLA	C3B-C2B	-2.51	1.36	1.40
30	38	307	CLA	CMB-C2B	-2.51	1.46	1.51
30	13	309	CLA	MG-ND	-2.51	2.00	2.05
30	14	305	CLA	CMD-C2D	-2.51	1.45	1.50
30	14	309	CLA	MG-ND	-2.51	2.00	2.05
41	31	310	A86	C-C1	2.51	1.56	1.50
30	21	306	CLA	CMB-C2B	-2.51	1.46	1.51
33	a	405	SQD	O2-C2	-2.51	1.37	1.43
30	11	301	CLA	CMC-C2C	-2.51	1.45	1.50
30	c	508	CLA	CMC-C2C	-2.51	1.45	1.50
30	b	605	CLA	C3B-CAB	-2.51	1.42	1.47
30	b	605	CLA	CMD-C2D	-2.51	1.45	1.50
30	c	509	CLA	CMD-C2D	-2.51	1.45	1.50
30	b	614	CLA	CMD-C2D	-2.51	1.45	1.50
30	37	310	CLA	CMB-C2B	-2.51	1.46	1.51
30	35	308	CLA	C3B-C2B	-2.51	1.36	1.40
30	33	304	CLA	CMB-C2B	-2.51	1.46	1.51
30	14	305	CLA	MG-ND	-2.51	2.00	2.05
30	B	607	CLA	CMD-C2D	-2.51	1.45	1.50
41	32	319	A86	O-C13	-2.51	1.18	1.23
30	34	308	CLA	C3B-C2B	-2.50	1.36	1.40
41	36	310	A86	C24-C1	2.50	1.51	1.45
33	b	620	SQD	O47-C7	2.50	1.41	1.34
41	14	311	A86	C-C1	2.50	1.56	1.50
41	13	316	A86	O-C13	-2.50	1.18	1.23
30	31	308	CLA	MG-ND	-2.50	2.00	2.05
30	17	310	CLA	CMB-C2B	-2.50	1.46	1.51
41	37	315	A86	C-C1	2.50	1.56	1.50
30	C	513	CLA	CMD-C2D	-2.50	1.45	1.50
30	b	606	CLA	CMC-C2C	-2.50	1.45	1.50
30	12	313	CLA	MG-ND	-2.50	2.00	2.05
30	11	302	CLA	CMB-C2B	-2.50	1.46	1.51
30	14	303	CLA	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	41	308	CLA	CMB-C2B	-2.50	1.46	1.51
30	d	406	CLA	CMC-C2C	-2.50	1.45	1.50
41	21	312	A86	C24-C1	2.50	1.51	1.45
41	38	302	A86	C-C1	2.50	1.56	1.50
30	20	205	CLA	CMB-C2B	-2.50	1.46	1.51
30	16	307	CLA	CMD-C2D	-2.50	1.45	1.50
30	31	307	CLA	CMD-C2D	-2.50	1.45	1.50
41	15	312	A86	C24-C1	2.50	1.51	1.45
30	D	406	CLA	C3B-C2B	-2.50	1.36	1.40
41	14	314	A86	C24-C1	2.50	1.51	1.45
41	35	310	A86	C-C1	2.50	1.56	1.50
41	13	315	A86	O-C13	-2.50	1.18	1.23
41	34	314	A86	C24-C1	2.50	1.51	1.45
41	34	311	A86	C-C1	2.49	1.56	1.50
30	c	510	CLA	C1D-ND	2.49	1.40	1.37
30	17	306	CLA	CMB-C2B	-2.49	1.46	1.51
30	11	308	CLA	CMD-C2D	-2.49	1.45	1.50
30	37	301	CLA	MG-ND	-2.49	2.00	2.05
30	c	514	CLA	CMC-C2C	-2.49	1.45	1.50
30	41	303	CLA	CMB-C2B	-2.49	1.46	1.51
41	31	314	A86	O-C13	-2.49	1.18	1.23
30	19	305	CLA	C3B-C2B	-2.49	1.36	1.40
41	16	310	A86	C24-C1	2.49	1.51	1.45
41	41	312	A86	C24-C1	2.49	1.51	1.45
30	c	502	CLA	CHC-C1C	2.49	1.41	1.35
30	13	302	CLA	CMC-C2C	-2.49	1.45	1.50
31	A	403	PHO	CMC-C2C	-2.49	1.45	1.51
30	A	402	CLA	CMC-C2C	-2.49	1.45	1.50
30	17	301	CLA	MG-ND	-2.49	2.00	2.05
30	16	309	CLA	CMD-C2D	-2.49	1.45	1.50
41	11	314	A86	O-C13	-2.49	1.18	1.23
30	B	610	CLA	C3B-CAB	-2.49	1.42	1.47
30	D	402	CLA	C3B-CAB	-2.49	1.42	1.47
30	c	512	CLA	C3B-CAB	-2.49	1.42	1.47
30	12	313	CLA	C3B-C2B	-2.49	1.36	1.40
41	11	310	A86	C-C1	2.49	1.56	1.50
41	33	312	A86	C-C1	2.49	1.56	1.50
30	40	205	CLA	CMB-C2B	-2.49	1.46	1.51
30	39	305	CLA	C3B-C2B	-2.49	1.36	1.40
30	c	507	CLA	C1D-ND	2.49	1.40	1.37
30	16	308	CLA	MG-ND	-2.49	2.00	2.05
30	18	309	CLA	MG-ND	-2.49	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	32	311	CLA	CMD-C2D	-2.49	1.45	1.50
30	b	614	CLA	CHC-C1C	2.49	1.41	1.35
30	C	508	CLA	CMC-C2C	-2.49	1.45	1.50
30	32	312	CLA	C3B-CAB	-2.49	1.42	1.47
30	a	402	CLA	CMD-C2D	-2.49	1.45	1.50
41	18	315	A86	C24-C1	2.49	1.51	1.45
30	21	301	CLA	CMB-C2B	-2.49	1.46	1.51
33	A	406	SQD	O2-C2	-2.48	1.37	1.43
30	c	524	CLA	CMB-C2B	-2.48	1.46	1.51
30	11	315	CLA	CMD-C2D	-2.48	1.45	1.50
41	17	315	A86	C-C1	2.48	1.56	1.50
30	A	402	CLA	CMD-C2D	-2.48	1.45	1.50
30	C	514	CLA	CMB-C2B	-2.48	1.46	1.51
30	C	502	CLA	CHC-C1C	2.48	1.41	1.35
30	B	613	CLA	CMC-C2C	-2.48	1.45	1.50
30	14	308	CLA	C3B-C2B	-2.48	1.36	1.40
30	b	613	CLA	CMD-C2D	-2.48	1.45	1.50
30	b	610	CLA	C3B-CAB	-2.48	1.42	1.47
41	21	313	A86	C24-C1	2.48	1.51	1.45
30	a	403	CLA	MG-ND	-2.48	2.00	2.05
30	C	519	CLA	MG-ND	-2.48	2.00	2.05
30	Z	102	CLA	CMB-C2B	-2.48	1.46	1.51
30	16	307	CLA	C3B-CAB	-2.48	1.42	1.47
30	32	311	CLA	MG-ND	-2.48	2.00	2.05
30	B	614	CLA	CHC-C1C	2.47	1.41	1.35
41	33	302	A86	O-C13	-2.47	1.18	1.23
30	c	510	CLA	CMD-C2D	-2.47	1.45	1.50
30	18	311	CLA	CMB-C2B	-2.47	1.46	1.51
30	c	505	CLA	C3B-CAB	-2.47	1.42	1.47
30	36	308	CLA	MG-ND	-2.47	2.00	2.05
41	34	312	A86	C14-C15	2.47	1.57	1.52
30	41	307	CLA	CMB-C2B	-2.47	1.46	1.51
30	C	507	CLA	CMD-C2D	-2.47	1.45	1.50
41	15	315	A86	O-C13	-2.47	1.18	1.23
30	41	301	CLA	CMB-C2B	-2.47	1.46	1.51
30	B	615	CLA	MG-ND	-2.47	2.00	2.05
30	33	309	CLA	MG-ND	-2.47	2.00	2.05
30	12	313	CLA	CMD-C2D	-2.47	1.45	1.50
30	W	102	CLA	C3B-C2B	-2.47	1.36	1.40
36	m	102	LMG	O4-C4	-2.47	1.37	1.43
41	39	310	A86	C-C1	2.47	1.56	1.50
30	b	615	CLA	MG-ND	-2.47	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	21	303	CLA	CMB-C2B	-2.47	1.46	1.51
30	b	611	CLA	CMD-C2D	-2.47	1.45	1.50
41	35	313	A86	C24-C1	2.47	1.51	1.45
30	B	613	CLA	CMD-C2D	-2.47	1.45	1.50
30	d	407	CLA	C1D-ND	2.47	1.40	1.37
36	M	102	LMG	O4-C4	-2.47	1.37	1.43
30	c	504	CLA	MG-ND	-2.46	2.00	2.05
30	D	406	CLA	CMD-C2D	-2.46	1.45	1.50
41	15	311	A86	C14-C15	2.46	1.57	1.52
41	32	318	A86	O-C13	-2.46	1.18	1.23
41	14	312	A86	C14-C15	2.46	1.57	1.52
36	d	410	LMG	O1-C7	-2.46	1.39	1.43
30	38	309	CLA	MG-ND	-2.46	2.00	2.05
30	33	310	CLA	C3B-CAB	-2.46	1.42	1.47
41	15	316	A86	O-C13	-2.46	1.18	1.23
30	33	309	CLA	CMD-C2D	-2.46	1.45	1.50
41	35	316	A86	O-C13	-2.46	1.18	1.23
30	C	514	CLA	CMC-C2C	-2.46	1.45	1.50
41	33	316	A86	O-C13	-2.46	1.18	1.23
30	W	103	CLA	CMB-C2B	-2.46	1.46	1.51
30	a	402	CLA	CMC-C2C	-2.46	1.45	1.50
41	41	312	A86	C-C1	2.46	1.56	1.50
41	13	314	A86	C24-C1	2.46	1.51	1.45
30	w	103	CLA	CMB-C2B	-2.46	1.46	1.51
41	31	311	A86	C14-C15	2.46	1.57	1.52
30	35	305	CLA	CMB-C2B	-2.46	1.46	1.51
30	c	507	CLA	CMD-C2D	-2.46	1.45	1.50
41	13	311	A86	C-C1	2.46	1.56	1.50
41	33	317	A86	O-C13	-2.46	1.18	1.23
30	B	614	CLA	C3B-C2B	-2.46	1.37	1.40
41	37	302	A86	C24-C1	2.46	1.51	1.45
41	11	311	A86	C14-C15	2.45	1.57	1.52
31	d	403	PHO	CMC-C2C	-2.45	1.45	1.51
31	D	403	PHO	CMC-C2C	-2.45	1.45	1.51
30	38	311	CLA	CMB-C2B	-2.45	1.46	1.51
30	33	309	CLA	C3B-CAB	-2.45	1.42	1.47
41	12	319	A86	O-C13	-2.45	1.18	1.23
30	33	310	CLA	CMD-C2D	-2.45	1.45	1.50
30	c	506	CLA	CMC-C2C	-2.45	1.45	1.50
30	37	308	CLA	MG-ND	-2.45	2.00	2.05
30	b	613	CLA	CMC-C2C	-2.45	1.45	1.50
41	38	302	A86	O-C13	-2.45	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	D	407	PL9	C31-C29	-2.45	1.46	1.51
41	16	313	A86	O-C13	-2.45	1.18	1.23
41	32	304	A86	O-C13	-2.45	1.18	1.23
41	19	309	A86	C-C1	2.45	1.55	1.50
41	18	314	A86	C14-C15	2.45	1.57	1.52
30	21	307	CLA	CMB-C2B	-2.45	1.46	1.51
41	39	309	A86	C-C1	2.45	1.55	1.50
30	c	505	CLA	MG-ND	-2.45	2.00	2.05
30	c	509	CLA	C3B-CAB	-2.45	1.42	1.47
30	18	310	CLA	CMD-C2D	-2.45	1.45	1.50
41	33	313	A86	C14-C15	2.45	1.57	1.52
41	41	313	A86	C24-C1	2.45	1.51	1.45
30	38	311	CLA	CMD-C2D	-2.45	1.45	1.50
30	A	404	CLA	MG-ND	-2.45	2.00	2.05
30	C	503	CLA	CAC-C3C	-2.45	1.44	1.51
30	11	308	CLA	MG-ND	-2.45	2.00	2.05
41	21	312	A86	C-C1	2.45	1.55	1.50
30	c	502	CLA	MG-ND	-2.45	2.00	2.05
30	34	309	CLA	C3B-CAB	-2.44	1.43	1.47
30	A	404	CLA	CMC-C2C	-2.44	1.45	1.50
30	c	503	CLA	CAC-C3C	-2.44	1.44	1.51
30	C	504	CLA	MG-ND	-2.44	2.00	2.05
30	33	304	CLA	CMD-C2D	-2.44	1.45	1.50
38	j	101	DGD	O1G-C1G	-2.44	1.39	1.45
30	C	505	CLA	C3B-CAB	-2.44	1.43	1.47
30	36	307	CLA	C3B-CAB	-2.44	1.43	1.47
41	36	313	A86	O-C13	-2.44	1.18	1.23
30	13	308	CLA	C3B-C2B	-2.44	1.37	1.40
30	32	306	CLA	CMD-C2D	-2.44	1.45	1.50
30	B	611	CLA	CMD-C2D	-2.44	1.45	1.50
30	18	311	CLA	CMD-C2D	-2.44	1.45	1.50
30	C	505	CLA	MG-ND	-2.44	2.01	2.05
30	15	305	CLA	CMB-C2B	-2.44	1.46	1.51
41	18	302	A86	O-C13	-2.44	1.18	1.23
30	c	505	CLA	CMC-C2C	-2.43	1.45	1.50
30	C	510	CLA	C3B-C2B	-2.43	1.37	1.40
30	38	310	CLA	CMD-C2D	-2.43	1.45	1.50
41	40	210	A86	O-C13	-2.43	1.18	1.23
30	38	306	CLA	CMB-C2B	-2.43	1.46	1.51
32	b	623	BCR	C30-C25	-2.43	1.50	1.53
30	17	307	CLA	C3B-CAB	-2.43	1.43	1.47
30	41	305	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	19	310	A86	C-C1	2.43	1.55	1.50
30	31	302	CLA	CMD-C2D	-2.43	1.45	1.50
39	d	408	PL9	C31-C29	-2.43	1.46	1.51
41	31	316	A86	O-C13	-2.43	1.18	1.23
41	38	315	A86	C24-C1	2.43	1.51	1.45
41	36	311	A86	C14-C15	2.43	1.57	1.52
30	c	514	CLA	MG-ND	-2.43	2.01	2.05
30	17	308	CLA	MG-ND	-2.43	2.01	2.05
31	d	403	PHO	CMB-C2B	-2.43	1.45	1.51
31	A	403	PHO	CMB-C2B	-2.43	1.45	1.51
38	C	516	DGD	O5D-C6D	-2.43	1.39	1.43
41	20	212	A86	O-C13	-2.43	1.18	1.23
30	31	308	CLA	CMC-C2C	-2.43	1.45	1.50
30	34	309	CLA	CMC-C2C	-2.43	1.45	1.50
41	38	314	A86	C14-C15	2.43	1.57	1.52
30	D	402	CLA	MG-ND	-2.43	2.01	2.05
41	35	311	A86	C14-C15	2.43	1.57	1.52
41	20	210	A86	O-C13	-2.43	1.18	1.23
30	C	506	CLA	CMC-C2C	-2.43	1.45	1.50
41	12	318	A86	C24-C1	2.43	1.51	1.45
41	17	302	A86	C24-C1	2.43	1.51	1.45
30	12	311	CLA	C3B-C2B	-2.42	1.37	1.40
41	12	304	A86	O-C13	-2.42	1.18	1.23
30	31	315	CLA	C3B-C2B	-2.42	1.37	1.40
30	C	509	CLA	C3B-CAB	-2.42	1.43	1.47
30	40	202	CLA	CMB-C2B	-2.42	1.46	1.51
41	16	311	A86	C14-C15	2.42	1.57	1.52
41	18	314	A86	C-C1	2.42	1.55	1.50
41	15	313	A86	C24-C1	2.42	1.51	1.45
30	11	307	CLA	C3B-C2B	-2.42	1.37	1.40
41	13	301	A86	O-C13	-2.42	1.18	1.23
30	39	303	CLA	C3B-C2B	-2.42	1.37	1.40
30	15	304	CLA	CMB-C2B	-2.42	1.46	1.51
30	W	102	CLA	CMC-C2C	-2.42	1.45	1.50
30	17	301	CLA	CMD-C2D	-2.42	1.45	1.50
30	C	508	CLA	C4B-CHC	-2.42	1.34	1.41
30	18	306	CLA	CMB-C2B	-2.42	1.46	1.51
41	37	314	A86	C24-C1	2.42	1.51	1.45
41	11	316	A86	O-C13	-2.42	1.18	1.23
30	12	311	CLA	MG-ND	-2.42	2.01	2.05
30	c	522	CLA	MG-ND	-2.42	2.01	2.05
41	40	211	A86	C-C1	2.42	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	37	309	CLA	C3B-C2B	-2.42	1.37	1.40
30	20	202	CLA	CMB-C2B	-2.41	1.46	1.51
30	37	303	CLA	C3B-CAB	-2.41	1.43	1.47
41	37	312	A86	C14-C15	2.41	1.57	1.52
30	C	505	CLA	CMD-C2D	-2.41	1.45	1.50
30	17	309	CLA	CMD-C2D	-2.41	1.45	1.50
30	d	407	CLA	C3B-C2B	-2.41	1.37	1.40
30	19	303	CLA	C3B-C2B	-2.41	1.37	1.40
41	19	309	A86	C24-C1	2.41	1.51	1.45
30	c	505	CLA	CMD-C2D	-2.41	1.45	1.50
30	c	502	CLA	CMC-C2C	-2.41	1.45	1.50
30	14	308	CLA	CMD-C2D	-2.41	1.45	1.50
30	11	302	CLA	CMD-C2D	-2.41	1.45	1.50
31	d	404	PHO	CMC-C2C	-2.41	1.45	1.51
32	B	624	BCR	C30-C25	-2.41	1.50	1.53
40	v	201	HEM	C3D-C2D	-2.41	1.31	1.36
41	20	211	A86	C-C1	2.41	1.55	1.50
30	37	307	CLA	C3B-CAB	-2.41	1.43	1.47
30	18	301	CLA	CMD-C2D	-2.41	1.45	1.50
30	14	309	CLA	CMC-C2C	-2.41	1.45	1.50
30	35	302	CLA	CMB-C2B	-2.40	1.46	1.51
41	33	315	A86	C24-C1	2.40	1.51	1.45
30	C	511	CLA	CMC-C2C	-2.40	1.45	1.50
30	12	311	CLA	C3B-CAB	-2.40	1.43	1.47
30	b	614	CLA	CMC-C2C	-2.40	1.45	1.50
30	12	311	CLA	CMD-C2D	-2.40	1.45	1.50
41	12	316	A86	C14-C15	2.40	1.57	1.52
30	32	311	CLA	C3B-CAB	-2.40	1.43	1.47
30	17	303	CLA	C3B-C2B	-2.40	1.37	1.40
38	c	517	DGD	O5D-C6D	-2.40	1.39	1.43
30	21	305	CLA	CMB-C2B	-2.40	1.46	1.51
30	b	602	CLA	C3B-CAB	-2.40	1.43	1.47
30	32	307	CLA	MG-ND	-2.40	2.01	2.05
30	15	302	CLA	CMB-C2B	-2.40	1.46	1.51
30	b	603	CLA	CMC-C2C	-2.40	1.45	1.50
41	32	317	A86	C24-C1	2.40	1.51	1.45
41	31	313	A86	C24-C1	2.40	1.51	1.45
30	13	308	CLA	CMD-C2D	-2.40	1.45	1.50
30	41	304	CLA	CMB-C2B	-2.40	1.46	1.51
41	40	212	A86	O-C13	-2.40	1.18	1.23
30	36	309	CLA	CMC-C2C	-2.40	1.45	1.50
30	16	303	CLA	MG-ND	-2.40	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	32	315	A86	C14-C15	2.40	1.57	1.52
36	32	301	LMG	O4-C4	-2.40	1.37	1.43
30	c	508	CLA	C4B-CHC	-2.40	1.34	1.41
41	17	312	A86	C14-C15	2.40	1.57	1.52
30	B	607	CLA	MG-ND	-2.40	2.01	2.05
30	b	607	CLA	MG-ND	-2.39	2.01	2.05
30	c	507	CLA	CMC-C2C	-2.39	1.45	1.50
30	34	308	CLA	CMD-C2D	-2.39	1.45	1.50
30	11	308	CLA	CMC-C2C	-2.39	1.45	1.50
30	16	301	CLA	CMD-C2D	-2.39	1.45	1.50
30	32	312	CLA	CMC-C2C	-2.39	1.45	1.50
41	21	310	A86	O4-C34	-2.39	1.40	1.46
41	41	310	A86	O4-C34	-2.39	1.40	1.46
41	13	312	A86	C14-C15	2.39	1.57	1.52
30	36	309	CLA	C3B-CAB	-2.39	1.43	1.47
41	33	312	A86	C14-C15	2.39	1.57	1.52
30	B	607	CLA	CMC-C2C	-2.39	1.45	1.50
30	C	507	CLA	CMC-C2C	-2.39	1.45	1.50
30	35	304	CLA	CMB-C2B	-2.39	1.46	1.51
30	33	301	CLA	C3B-C2B	-2.39	1.37	1.40
41	32	314	A86	C14-C15	2.39	1.57	1.52
30	17	306	CLA	MG-ND	-2.39	2.01	2.05
41	41	311	A86	C-C1	2.39	1.55	1.50
30	c	505	CLA	CHC-C1C	2.39	1.41	1.35
30	39	307	CLA	CMD-C2D	-2.39	1.45	1.50
30	B	603	CLA	CMC-C2C	-2.39	1.45	1.50
40	V	201	HEM	C3D-C2D	-2.39	1.31	1.36
41	17	314	A86	C24-C1	2.39	1.51	1.45
30	D	402	CLA	CMD-C2D	-2.39	1.45	1.50
30	37	309	CLA	CMD-C2D	-2.39	1.45	1.50
30	c	511	CLA	CMC-C2C	-2.38	1.45	1.50
30	D	406	CLA	MG-ND	-2.38	2.01	2.05
30	40	203	CLA	C3B-C2B	-2.38	1.37	1.40
30	b	611	CLA	MG-ND	-2.38	2.01	2.05
30	B	601	CLA	CMD-C2D	-2.38	1.45	1.50
30	17	309	CLA	CMC-C2C	-2.38	1.45	1.50
41	38	313	A86	O4-C34	-2.38	1.40	1.46
30	19	306	CLA	CMD-C2D	-2.38	1.45	1.50
30	c	510	CLA	C3B-C2B	-2.38	1.37	1.40
30	33	308	CLA	C3B-C2B	-2.38	1.37	1.40
30	36	309	CLA	MG-ND	-2.38	2.01	2.05
30	C	505	CLA	C4B-CHC	-2.38	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	307	CLA	C3B-CAB	-2.38	1.43	1.47
30	18	310	CLA	C3B-C2B	-2.38	1.37	1.40
30	19	307	CLA	CMD-C2D	-2.38	1.45	1.50
41	16	313	A86	O4-C34	-2.38	1.40	1.46
30	17	303	CLA	C3B-CAB	-2.38	1.43	1.47
30	38	301	CLA	CMD-C2D	-2.38	1.45	1.50
30	37	303	CLA	C3B-C2B	-2.38	1.37	1.40
41	36	313	A86	O4-C34	-2.38	1.40	1.46
30	12	313	CLA	CMC-C2C	-2.38	1.45	1.50
30	39	306	CLA	CMD-C2D	-2.38	1.45	1.50
30	C	505	CLA	CHC-C1C	2.38	1.41	1.35
41	38	314	A86	C-C1	2.38	1.55	1.50
30	33	305	CLA	MG-ND	-2.38	2.01	2.05
30	13	308	CLA	C3B-CAB	-2.38	1.43	1.47
30	39	306	CLA	C3B-CAB	-2.38	1.43	1.47
30	12	306	CLA	CMD-C2D	-2.38	1.45	1.50
30	39	305	CLA	CMD-C2D	-2.38	1.45	1.50
30	C	520	CLA	MG-ND	-2.38	2.01	2.05
41	41	310	A86	C24-C1	2.38	1.51	1.45
36	d	410	LMG	O4-C4	-2.38	1.37	1.43
30	34	308	CLA	C3B-CAB	-2.38	1.43	1.47
30	C	514	CLA	CMD-C2D	-2.38	1.45	1.50
30	c	509	CLA	CHC-C1C	2.38	1.41	1.35
41	35	311	A86	C-C1	2.38	1.55	1.50
30	C	510	CLA	CMD-C2D	-2.38	1.45	1.50
30	20	203	CLA	C3B-C2B	-2.38	1.37	1.40
30	C	514	CLA	MG-ND	-2.37	2.01	2.05
30	31	301	CLA	CMD-C2D	-2.37	1.45	1.50
30	39	302	CLA	CMD-C2D	-2.37	1.45	1.50
41	33	312	A86	O4-C34	-2.37	1.40	1.46
30	B	602	CLA	C3B-CAB	-2.37	1.43	1.47
41	37	316	A86	C24-C1	2.37	1.51	1.45
30	17	303	CLA	CMD-C2D	-2.37	1.45	1.50
30	37	301	CLA	CMD-C2D	-2.37	1.45	1.50
30	d	402	CLA	MG-ND	-2.37	2.01	2.05
30	B	614	CLA	CMC-C2C	-2.37	1.45	1.50
31	d	404	PHO	CMD-C2D	-2.37	1.45	1.51
41	14	312	A86	C-C1	2.37	1.55	1.50
41	11	313	A86	C24-C1	2.37	1.51	1.45
41	13	311	A86	O4-C34	-2.37	1.40	1.46
30	c	522	CLA	C3B-C2B	-2.37	1.37	1.40
30	13	303	CLA	CMD-C2D	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	33	311	CLA	CMD-C2D	-2.37	1.45	1.50
41	21	310	A86	C24-C1	2.37	1.51	1.45
30	31	303	CLA	CMD-C2D	-2.37	1.45	1.50
30	16	309	CLA	MG-ND	-2.37	2.01	2.05
30	16	309	CLA	CMC-C2C	-2.37	1.45	1.50
41	13	315	A86	C14-C15	2.37	1.57	1.52
41	12	315	A86	O4-C34	-2.37	1.40	1.46
30	35	308	CLA	MG-ND	-2.37	2.01	2.05
32	f	101	BCR	C30-C25	-2.37	1.50	1.53
41	11	311	A86	C-C1	2.37	1.55	1.50
30	C	502	CLA	MG-ND	-2.37	2.01	2.05
30	12	307	CLA	CMD-C2D	-2.37	1.45	1.50
30	33	310	CLA	CMC-C2C	-2.37	1.45	1.50
30	37	303	CLA	CMC-C2C	-2.37	1.45	1.50
30	21	304	CLA	CMB-C2B	-2.37	1.46	1.51
30	b	604	CLA	CMC-C2C	-2.37	1.45	1.50
33	B	621	SQD	O2-C2	-2.37	1.37	1.43
30	C	511	CLA	CAA-C2A	-2.37	1.49	1.54
41	35	314	A86	C14-C15	2.37	1.57	1.52
30	14	310	CLA	CMD-C2D	-2.37	1.45	1.50
30	36	301	CLA	CMD-C2D	-2.36	1.45	1.50
30	A	402	CLA	MG-ND	-2.36	2.01	2.05
30	C	509	CLA	C1D-ND	2.36	1.40	1.37
41	21	311	A86	C-C1	2.36	1.55	1.50
41	13	317	A86	C24-C1	2.36	1.51	1.45
30	c	522	CLA	CMD-C2D	-2.36	1.45	1.50
30	16	309	CLA	C3B-CAB	-2.36	1.43	1.47
30	36	306	CLA	C3B-C2B	-2.36	1.37	1.40
30	36	303	CLA	MG-ND	-2.36	2.01	2.05
30	34	303	CLA	CMD-C2D	-2.36	1.45	1.50
30	34	307	CLA	CMD-C2D	-2.36	1.45	1.50
33	B	621	SQD	O4-C4	-2.36	1.37	1.43
30	c	504	CLA	C3B-CAB	-2.36	1.43	1.47
30	C	509	CLA	CHC-C1C	2.36	1.41	1.35
30	38	310	CLA	C3B-C2B	-2.36	1.37	1.40
41	34	311	A86	O4-C34	-2.36	1.40	1.46
41	35	310	A86	C14-C15	2.36	1.57	1.52
30	39	301	CLA	CMD-C2D	-2.36	1.45	1.50
30	C	505	CLA	CMC-C2C	-2.36	1.45	1.50
30	18	309	CLA	CMD-C2D	-2.36	1.45	1.50
41	33	302	A86	C14-C15	2.36	1.57	1.52
30	C	520	CLA	C3B-CAB	-2.36	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	37	307	CLA	C3B-C2B	-2.36	1.37	1.40
30	37	309	CLA	CMC-C2C	-2.36	1.45	1.50
41	31	311	A86	C24-C1	2.36	1.51	1.45
30	c	522	CLA	C3B-CAB	-2.36	1.43	1.47
30	b	607	CLA	C3B-C2B	-2.36	1.37	1.40
30	11	307	CLA	CMD-C2D	-2.36	1.45	1.50
41	15	310	A86	C14-C15	2.36	1.57	1.52
30	39	302	CLA	MG-ND	-2.36	2.01	2.05
41	37	312	A86	C-C1	2.36	1.55	1.50
30	c	505	CLA	C4B-CHC	-2.36	1.34	1.41
30	36	303	CLA	CMD-C2D	-2.36	1.45	1.50
30	31	306	CLA	C3B-C2B	-2.36	1.37	1.40
41	15	314	A86	C14-C15	2.36	1.57	1.52
30	31	307	CLA	MG-ND	-2.36	2.01	2.05
41	11	310	A86	C14-C15	2.35	1.57	1.52
30	14	308	CLA	C3B-CAB	-2.35	1.43	1.47
38	C	517	DGD	O1G-C1G	-2.35	1.39	1.45
38	c	517	DGD	O2E-C2E	-2.35	1.37	1.43
30	37	306	CLA	MG-ND	-2.35	2.01	2.05
41	12	316	A86	C24-C1	2.35	1.51	1.45
41	33	313	A86	C-C1	2.35	1.55	1.50
30	32	307	CLA	CMD-C2D	-2.35	1.45	1.50
30	B	611	CLA	MG-ND	-2.35	2.01	2.05
41	32	319	A86	C14-C15	2.35	1.57	1.52
30	19	302	CLA	CMD-C2D	-2.35	1.45	1.50
30	C	506	CLA	C3B-CAB	-2.35	1.43	1.47
41	36	310	A86	O4-C34	-2.35	1.40	1.46
30	16	307	CLA	MG-ND	-2.35	2.01	2.05
30	c	509	CLA	C1D-ND	2.35	1.40	1.37
41	12	315	A86	C14-C15	2.35	1.57	1.52
38	c	518	DGD	O1G-C1G	-2.35	1.39	1.45
30	c	514	CLA	CMD-C2D	-2.35	1.45	1.50
30	13	309	CLA	CMC-C2C	-2.35	1.45	1.50
30	38	309	CLA	CMD-C2D	-2.35	1.45	1.50
41	32	318	A86	O4-C34	-2.35	1.40	1.46
30	37	303	CLA	CMD-C2D	-2.35	1.45	1.50
41	11	311	A86	C24-C1	2.35	1.51	1.45
41	35	314	A86	O4-C34	-2.35	1.40	1.46
41	39	309	A86	C24-C1	2.35	1.51	1.45
30	36	302	CLA	C3B-CAB	-2.35	1.43	1.47
41	32	315	A86	C-C1	2.35	1.55	1.50
30	b	609	CLA	C3B-CAB	-2.35	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	33	308	CLA	CMD-C2D	-2.35	1.45	1.50
30	37	308	CLA	CMD-C2D	-2.35	1.45	1.50
41	38	313	A86	C14-C15	2.34	1.57	1.52
41	17	312	A86	C-C1	2.34	1.55	1.50
30	W	102	CLA	CMD-C2D	-2.34	1.45	1.50
41	12	319	A86	C14-C15	2.34	1.57	1.52
41	33	317	A86	C24-C1	2.34	1.51	1.45
30	35	304	CLA	CMD-C2D	-2.34	1.45	1.50
30	13	308	CLA	MG-ND	-2.34	2.01	2.05
30	31	306	CLA	CMD-C2D	-2.34	1.45	1.50
41	32	315	A86	C24-C1	2.34	1.51	1.45
30	c	513	CLA	C3B-C2B	-2.34	1.37	1.40
30	19	301	CLA	CMD-C2D	-2.34	1.45	1.50
41	11	314	A86	C24-C1	2.34	1.51	1.45
41	17	316	A86	C24-C1	2.34	1.51	1.45
41	13	312	A86	C-C1	2.34	1.55	1.50
30	C	508	CLA	CHC-C1C	2.34	1.41	1.35
41	34	312	A86	C-C1	2.34	1.55	1.50
31	d	404	PHO	CMB-C2B	-2.34	1.46	1.51
41	32	314	A86	O4-C34	-2.34	1.40	1.46
41	15	311	A86	C-C1	2.34	1.55	1.50
41	11	314	A86	C14-C15	2.34	1.57	1.52
30	32	303	CLA	C3B-C2B	-2.34	1.37	1.40
41	20	211	A86	C24-C1	2.34	1.51	1.45
30	31	303	CLA	C3B-CAB	-2.34	1.43	1.47
41	15	314	A86	C24-C1	2.34	1.51	1.45
36	12	301	LMG	O6-C5	-2.34	1.38	1.44
33	A	406	SQD	O3-C3	-2.34	1.37	1.43
30	c	504	CLA	CMC-C2C	-2.34	1.45	1.50
30	16	303	CLA	CMC-C2C	-2.34	1.45	1.50
41	35	314	A86	C24-C1	2.34	1.51	1.45
41	17	316	A86	C14-C15	2.34	1.57	1.52
41	18	313	A86	O4-C34	-2.34	1.40	1.46
41	12	316	A86	C-C1	2.34	1.55	1.50
31	D	403	PHO	CMD-C2D	-2.34	1.46	1.51
41	31	310	A86	O4-C34	-2.34	1.40	1.46
30	19	301	CLA	MG-ND	-2.34	2.01	2.05
30	C	520	CLA	CMD-C2D	-2.34	1.45	1.50
30	33	305	CLA	C3B-CAB	-2.34	1.43	1.47
30	32	305	CLA	CMD-C2D	-2.34	1.45	1.50
30	b	614	CLA	C3B-C2B	-2.34	1.37	1.40
38	J	101	DGD	O3D-C3D	-2.34	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	504	CLA	C3B-CAB	-2.34	1.43	1.47
30	11	307	CLA	MG-ND	-2.34	2.01	2.05
41	11	314	A86	O4-C34	-2.34	1.40	1.46
41	12	319	A86	O4-C34	-2.33	1.40	1.46
41	31	311	A86	C-C1	2.33	1.55	1.50
41	14	311	A86	C14-C15	2.33	1.57	1.52
41	18	313	A86	C14-C15	2.33	1.57	1.52
33	b	620	SQD	O2-C2	-2.33	1.37	1.43
36	D	408	LMG	O4-C4	-2.33	1.37	1.43
30	19	306	CLA	C3B-CAB	-2.33	1.43	1.47
41	14	311	A86	O4-C34	-2.33	1.40	1.46
30	C	512	CLA	CMC-C2C	-2.33	1.45	1.50
30	32	313	CLA	CMD-C2D	-2.33	1.45	1.50
30	19	301	CLA	C3B-CAB	-2.33	1.43	1.47
41	15	314	A86	O4-C34	-2.33	1.40	1.46
41	32	318	A86	C14-C15	2.33	1.57	1.52
38	J	101	DGD	O2E-C2E	-2.33	1.37	1.43
30	15	304	CLA	CMD-C2D	-2.33	1.45	1.50
30	32	303	CLA	CMC-C2C	-2.33	1.45	1.50
30	32	310	CLA	CMD-C2D	-2.33	1.45	1.50
33	B	621	SQD	O3-C3	-2.33	1.37	1.43
41	16	310	A86	O4-C34	-2.33	1.40	1.46
41	13	311	A86	C14-C15	2.33	1.57	1.52
41	31	314	A86	O4-C34	-2.33	1.40	1.46
30	32	306	CLA	MG-ND	-2.33	2.01	2.05
30	36	307	CLA	MG-ND	-2.33	2.01	2.05
30	16	302	CLA	C3B-CAB	-2.33	1.43	1.47
30	19	305	CLA	CMD-C2D	-2.33	1.45	1.50
30	14	302	CLA	C3B-CAB	-2.33	1.43	1.47
30	17	307	CLA	C3B-C2B	-2.33	1.37	1.40
30	20	209	CLA	C3B-C2B	-2.33	1.37	1.40
30	14	309	CLA	C3B-CAB	-2.33	1.43	1.47
30	d	402	CLA	CMD-C2D	-2.33	1.45	1.50
30	13	308	CLA	CMC-C2C	-2.33	1.45	1.50
30	39	308	CLA	CMD-C2D	-2.33	1.45	1.50
30	c	506	CLA	MG-ND	-2.33	2.01	2.05
41	31	314	A86	C24-C1	2.33	1.50	1.45
41	40	211	A86	C24-C1	2.33	1.50	1.45
41	13	315	A86	O4-C34	-2.33	1.40	1.46
41	32	319	A86	O4-C34	-2.33	1.40	1.46
30	19	302	CLA	MG-ND	-2.33	2.01	2.05
30	31	307	CLA	C3B-CAB	-2.33	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	303	CLA	CMD-C2D	-2.33	1.45	1.50
30	a	402	CLA	MG-ND	-2.33	2.01	2.05
41	11	310	A86	O4-C34	-2.33	1.40	1.46
41	36	313	A86	C14-C15	2.33	1.57	1.52
30	11	309	CLA	CMD-C2D	-2.33	1.45	1.50
30	11	306	CLA	CMD-C2D	-2.33	1.45	1.50
30	c	508	CLA	C3B-C2B	-2.32	1.37	1.40
30	16	303	CLA	CMD-C2D	-2.32	1.45	1.50
36	12	301	LMG	O7-C8	-2.32	1.40	1.46
30	33	303	CLA	C3B-CAB	-2.32	1.43	1.47
30	16	304	CLA	CMD-C2D	-2.32	1.45	1.50
41	18	302	A86	C14-C15	2.32	1.57	1.52
30	C	507	CLA	C1D-ND	2.32	1.40	1.37
41	12	319	A86	C24-C1	2.32	1.50	1.45
30	38	303	CLA	C3B-CAB	-2.32	1.43	1.47
30	36	303	CLA	CMC-C2C	-2.32	1.45	1.50
30	12	310	CLA	CMD-C2D	-2.32	1.45	1.50
30	C	520	CLA	C3B-C2B	-2.32	1.37	1.40
41	38	314	A86	C24-C1	2.32	1.50	1.45
30	11	303	CLA	CMD-C2D	-2.32	1.45	1.50
30	18	303	CLA	C3B-CAB	-2.32	1.43	1.47
38	j	101	DGD	O2E-C2E	-2.32	1.37	1.43
41	37	316	A86	C14-C15	2.32	1.57	1.52
30	17	308	CLA	CMD-C2D	-2.32	1.45	1.50
41	15	311	A86	C24-C1	2.32	1.50	1.45
30	b	602	CLA	CMD-C2D	-2.32	1.45	1.50
30	19	307	CLA	MG-ND	-2.32	2.01	2.05
30	15	308	CLA	MG-ND	-2.32	2.01	2.05
30	c	508	CLA	CAC-C3C	-2.32	1.45	1.51
30	36	304	CLA	CMD-C2D	-2.32	1.45	1.50
41	18	314	A86	C24-C1	2.31	1.50	1.45
30	b	607	CLA	CMC-C2C	-2.31	1.45	1.50
30	31	303	CLA	MG-ND	-2.31	2.01	2.05
33	A	406	SQD	O4-C4	-2.31	1.37	1.43
30	B	602	CLA	CMD-C2D	-2.31	1.45	1.50
41	13	316	A86	C14-C15	2.31	1.57	1.52
31	d	404	PHO	C3B-CAB	-2.31	1.43	1.47
30	c	523	CLA	CMD-C2D	-2.31	1.45	1.50
30	39	301	CLA	MG-ND	-2.31	2.01	2.05
30	37	305	CLA	MG-ND	-2.31	2.01	2.05
30	12	314	CLA	CMD-C2D	-2.31	1.45	1.50
41	35	310	A86	O4-C34	-2.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	601	CLA	CMC-C2C	-2.31	1.45	1.50
30	16	306	CLA	C3B-C2B	-2.31	1.37	1.40
30	31	315	CLA	MG-ND	-2.31	2.01	2.05
41	32	318	A86	C24-C1	2.31	1.50	1.45
30	17	303	CLA	CMC-C2C	-2.31	1.45	1.50
30	19	304	CLA	MG-ND	-2.31	2.01	2.05
41	32	319	A86	C24-C1	2.31	1.50	1.45
30	16	306	CLA	CMC-C2C	-2.31	1.45	1.50
41	31	314	A86	C14-C15	2.31	1.57	1.52
30	B	605	CLA	CMC-C2C	-2.31	1.45	1.50
30	13	310	CLA	CMD-C2D	-2.31	1.45	1.50
30	34	302	CLA	CMD-C2D	-2.31	1.45	1.50
30	16	308	CLA	CMC-C2C	-2.31	1.45	1.50
30	14	304	CLA	C3B-CAB	-2.31	1.43	1.47
38	j	101	DGD	O3D-C3D	-2.31	1.37	1.43
30	14	304	CLA	CMD-C2D	-2.31	1.45	1.50
41	20	211	A86	O4-C34	-2.31	1.40	1.46
41	38	302	A86	C14-C15	2.31	1.57	1.52
33	b	620	SQD	O3-C3	-2.31	1.37	1.43
30	M	101	CLA	CMC-C2C	-2.31	1.45	1.50
41	33	317	A86	C14-C15	2.31	1.57	1.52
41	35	316	A86	C14-C15	2.31	1.57	1.52
33	b	620	SQD	O4-C4	-2.31	1.37	1.43
41	40	211	A86	O4-C34	-2.31	1.40	1.46
30	C	502	CLA	CMC-C2C	-2.30	1.45	1.50
30	34	301	CLA	MG-ND	-2.30	2.01	2.05
41	15	310	A86	O4-C34	-2.30	1.40	1.46
30	b	606	CLA	CAC-C3C	-2.30	1.45	1.51
30	39	306	CLA	MG-ND	-2.30	2.01	2.05
30	c	506	CLA	C3B-CAB	-2.30	1.43	1.47
41	16	311	A86	C24-C1	2.30	1.50	1.45
41	33	316	A86	C14-C15	2.30	1.57	1.52
30	38	311	CLA	MG-ND	-2.30	2.01	2.05
30	39	301	CLA	CMC-C2C	-2.30	1.45	1.50
31	D	403	PHO	CMB-C2B	-2.30	1.46	1.51
30	C	521	CLA	CMD-C2D	-2.30	1.45	1.50
30	33	303	CLA	CMD-C2D	-2.30	1.45	1.50
41	13	301	A86	C14-C15	2.30	1.57	1.52
38	C	516	DGD	O2E-C2E	-2.30	1.37	1.43
30	34	303	CLA	MG-ND	-2.30	2.01	2.05
41	13	317	A86	O4-C34	-2.30	1.40	1.46
33	l	101	SQD	O2-C2	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	31	307	CLA	CMC-C2C	-2.30	1.45	1.50
30	11	308	CLA	C3B-CAB	-2.30	1.43	1.47
41	34	311	A86	C14-C15	2.30	1.57	1.52
30	B	604	CLA	CMC-C2C	-2.30	1.45	1.50
30	C	504	CLA	CMC-C2C	-2.30	1.45	1.50
30	b	601	CLA	MG-ND	-2.30	2.01	2.05
30	39	304	CLA	MG-ND	-2.30	2.01	2.05
30	13	302	CLA	C3B-CAB	-2.30	1.43	1.47
30	13	309	CLA	C3B-CAB	-2.30	1.43	1.47
30	31	309	CLA	CMD-C2D	-2.30	1.45	1.50
41	21	311	A86	C24-C1	2.30	1.50	1.45
41	16	313	A86	C14-C15	2.30	1.57	1.52
30	33	304	CLA	MG-ND	-2.30	2.01	2.05
41	31	316	A86	C14-C15	2.30	1.57	1.52
30	33	305	CLA	CMD-C2D	-2.30	1.45	1.50
30	36	308	CLA	CMD-C2D	-2.30	1.45	1.50
41	14	312	A86	C24-C1	2.29	1.50	1.45
41	33	317	A86	O4-C34	-2.29	1.40	1.46
30	34	304	CLA	C3B-CAB	-2.29	1.43	1.47
30	39	301	CLA	C3B-CAB	-2.29	1.43	1.47
30	18	311	CLA	MG-ND	-2.29	2.01	2.05
30	b	608	CLA	CMC-C2C	-2.29	1.45	1.50
41	31	310	A86	C14-C15	2.29	1.57	1.52
36	b	618	LMG	O1-C7	-2.29	1.39	1.43
30	34	301	CLA	C3B-C2B	-2.29	1.37	1.40
30	B	606	CLA	CAC-C3C	-2.29	1.45	1.51
30	34	304	CLA	CMD-C2D	-2.29	1.46	1.50
30	12	313	CLA	C3B-CAB	-2.29	1.43	1.47
30	39	307	CLA	MG-ND	-2.29	2.01	2.05
30	19	308	CLA	CMD-C2D	-2.29	1.46	1.50
30	20	203	CLA	CMD-C2D	-2.29	1.46	1.50
33	a	405	SQD	O3-C3	-2.29	1.37	1.43
38	C	516	DGD	O4D-C4D	-2.29	1.37	1.43
41	13	312	A86	C24-C1	2.29	1.50	1.45
30	W	102	CLA	MG-ND	-2.29	2.01	2.05
30	m	101	CLA	CMC-C2C	-2.29	1.46	1.50
30	d	407	CLA	MG-ND	-2.29	2.01	2.05
30	19	305	CLA	MG-ND	-2.29	2.01	2.05
30	18	311	CLA	CMC-C2C	-2.29	1.46	1.50
30	32	307	CLA	C3B-CAB	-2.29	1.43	1.47
41	17	316	A86	O4-C34	-2.29	1.40	1.46
30	40	203	CLA	CMD-C2D	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	17	308	CLA	C4B-CHC	-2.28	1.34	1.41
41	16	311	A86	C-C1	2.28	1.55	1.50
41	13	317	A86	C14-C15	2.28	1.57	1.52
30	32	306	CLA	C3B-C2B	-2.28	1.37	1.40
30	38	306	CLA	CMD-C2D	-2.28	1.46	1.50
30	19	306	CLA	MG-ND	-2.28	2.01	2.05
30	D	406	CLA	CMC-C2C	-2.28	1.46	1.50
30	36	306	CLA	CMC-C2C	-2.28	1.46	1.50
30	w	102	CLA	CMD-C2D	-2.28	1.46	1.50
30	13	304	CLA	CMD-C2D	-2.28	1.46	1.50
30	17	305	CLA	MG-ND	-2.28	2.01	2.05
41	15	315	A86	C14-C15	2.28	1.57	1.52
30	40	208	CLA	CMB-C2B	-2.28	1.46	1.51
30	14	308	CLA	MG-ND	-2.28	2.01	2.05
30	c	511	CLA	CAA-C2A	-2.28	1.49	1.54
30	C	506	CLA	MG-ND	-2.28	2.01	2.05
30	34	304	CLA	C3B-C2B	-2.28	1.37	1.40
41	36	311	A86	C24-C1	2.28	1.50	1.45
30	C	512	CLA	CMD-C2D	-2.28	1.46	1.50
30	13	307	CLA	CMD-C2D	-2.28	1.46	1.50
41	36	313	A86	C24-C1	2.28	1.50	1.45
30	12	311	CLA	CMC-C2C	-2.28	1.46	1.50
30	33	309	CLA	CMC-C2C	-2.28	1.46	1.50
41	12	315	A86	C24-C1	2.28	1.50	1.45
30	c	512	CLA	CMC-C2C	-2.28	1.46	1.50
30	33	301	CLA	MG-ND	-2.28	2.01	2.05
41	37	316	A86	O4-C34	-2.28	1.40	1.46
38	c	517	DGD	O4D-C4D	-2.28	1.37	1.43
38	j	101	DGD	O2D-C2D	-2.28	1.37	1.43
30	37	308	CLA	C4B-CHC	-2.28	1.34	1.41
30	C	508	CLA	C3B-C2B	-2.28	1.37	1.40
30	B	608	CLA	CMC-C2C	-2.28	1.46	1.50
30	36	308	CLA	CMC-C2C	-2.28	1.46	1.50
30	b	601	CLA	CMD-C2D	-2.28	1.46	1.50
30	b	609	CLA	CMC-C2C	-2.28	1.46	1.50
30	18	309	CLA	CMC-C2C	-2.28	1.46	1.50
30	c	513	CLA	MG-ND	-2.28	2.01	2.05
30	15	301	CLA	CMD-C2D	-2.27	1.46	1.50
30	31	302	CLA	MG-ND	-2.27	2.01	2.05
41	35	311	A86	C24-C1	2.27	1.50	1.45
30	19	301	CLA	CMC-C2C	-2.27	1.46	1.50
30	15	308	CLA	CMD-C2D	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	37	304	CLA	CMD-C2D	-2.27	1.46	1.50
33	a	405	SQD	O4-C4	-2.27	1.37	1.43
41	37	315	A86	O4-C34	-2.27	1.40	1.46
30	b	603	CLA	C4B-CHC	-2.27	1.34	1.41
30	39	303	CLA	CMD-C2D	-2.27	1.46	1.50
41	21	314	A86	O4-C34	-2.27	1.40	1.46
30	32	310	CLA	C3B-C2B	-2.27	1.37	1.40
30	20	206	CLA	CMD-C2D	-2.27	1.46	1.50
36	b	618	LMG	O8-C9	-2.27	1.40	1.45
39	d	405	PL9	C36-C34	-2.27	1.46	1.51
41	33	313	A86	C24-C1	2.27	1.50	1.45
30	16	305	CLA	MG-ND	-2.27	2.01	2.05
30	d	407	CLA	CMC-C2C	-2.27	1.46	1.50
30	20	208	CLA	CMB-C2B	-2.27	1.46	1.51
30	14	301	CLA	C3B-C2B	-2.27	1.37	1.40
30	17	304	CLA	CMD-C2D	-2.27	1.46	1.50
30	38	309	CLA	CMC-C2C	-2.27	1.46	1.50
41	11	316	A86	C14-C15	2.27	1.57	1.52
30	b	608	CLA	C3B-CAB	-2.27	1.43	1.47
30	14	308	CLA	CMC-C2C	-2.27	1.46	1.50
30	38	311	CLA	CMC-C2C	-2.27	1.46	1.50
30	16	301	CLA	C3B-C2B	-2.27	1.37	1.40
41	32	304	A86	C14-C15	2.27	1.57	1.52
30	C	519	CLA	C3B-CAB	-2.26	1.43	1.47
30	B	609	CLA	C3B-CAB	-2.26	1.43	1.47
30	39	305	CLA	MG-ND	-2.26	2.01	2.05
41	12	316	A86	O4-C34	-2.26	1.40	1.46
30	34	302	CLA	C3B-CAB	-2.26	1.43	1.47
30	16	308	CLA	CMD-C2D	-2.26	1.46	1.50
30	34	304	CLA	CMC-C2C	-2.26	1.46	1.50
30	35	308	CLA	CMD-C2D	-2.26	1.46	1.50
41	40	213	A86	O4-C34	-2.26	1.40	1.46
38	h	102	DGD	O4D-C4D	-2.26	1.37	1.43
30	B	601	CLA	MG-ND	-2.26	2.01	2.05
41	35	310	A86	C24-C1	2.26	1.50	1.45
41	41	311	A86	C24-C1	2.26	1.50	1.45
41	15	316	A86	C14-C15	2.26	1.57	1.52
30	32	307	CLA	CMC-C2C	-2.26	1.46	1.50
30	33	301	CLA	CMC-C2C	-2.26	1.46	1.50
30	z	101	CLA	C3B-CAB	-2.26	1.43	1.47
30	11	301	CLA	C3B-CAB	-2.26	1.43	1.47
30	31	301	CLA	C3B-CAB	-2.26	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	38	314	A86	O4-C34	-2.26	1.40	1.46
30	32	305	CLA	C3B-CAB	-2.26	1.43	1.47
41	20	213	A86	O4-C34	-2.26	1.40	1.46
30	B	609	CLA	MG-ND	-2.26	2.01	2.05
30	37	309	CLA	MG-ND	-2.26	2.01	2.05
30	20	208	CLA	CMC-C2C	-2.26	1.46	1.50
30	33	305	CLA	CMC-C2C	-2.26	1.46	1.50
30	C	508	CLA	CAC-C3C	-2.26	1.45	1.51
30	20	209	CLA	MG-ND	-2.26	2.01	2.05
41	32	315	A86	O4-C34	-2.26	1.41	1.46
30	34	304	CLA	MG-ND	-2.26	2.01	2.05
41	40	201	A86	O4-C34	-2.26	1.41	1.46
41	34	312	A86	C24-C1	2.26	1.50	1.45
41	34	312	A86	O4-C34	-2.26	1.41	1.46
30	14	307	CLA	CMD-C2D	-2.26	1.46	1.50
31	D	403	PHO	C3B-CAB	-2.26	1.43	1.47
41	41	314	A86	O4-C34	-2.25	1.41	1.46
30	14	304	CLA	CMC-C2C	-2.25	1.46	1.50
30	34	308	CLA	CMC-C2C	-2.25	1.46	1.50
30	39	308	CLA	MG-ND	-2.25	2.01	2.05
30	C	509	CLA	C4B-CHC	-2.25	1.34	1.41
30	18	306	CLA	CMD-C2D	-2.25	1.46	1.50
41	41	311	A86	O4-C34	-2.25	1.41	1.46
36	Q	301	LMG	O4-C4	-2.25	1.37	1.43
30	34	310	CLA	CMD-C2D	-2.25	1.46	1.50
30	C	521	CLA	MG-ND	-2.25	2.01	2.05
30	33	304	CLA	CMC-C2C	-2.25	1.46	1.50
30	40	206	CLA	CMD-C2D	-2.25	1.46	1.50
41	35	315	A86	C14-C15	2.25	1.57	1.52
30	19	308	CLA	MG-ND	-2.25	2.01	2.05
30	32	303	CLA	MG-ND	-2.25	2.01	2.05
30	b	601	CLA	CMC-C2C	-2.25	1.46	1.50
30	13	303	CLA	MG-ND	-2.25	2.01	2.05
41	32	314	A86	C24-C1	2.25	1.50	1.45
30	w	102	CLA	MG-ND	-2.25	2.01	2.05
41	17	312	A86	O4-C34	-2.25	1.41	1.46
36	b	619	LMG	O3-C3	-2.25	1.37	1.43
41	17	315	A86	O4-C34	-2.25	1.41	1.46
41	40	212	A86	C14-C15	2.25	1.57	1.52
30	40	209	CLA	C3B-C2B	-2.25	1.37	1.40
30	18	301	CLA	MG-ND	-2.25	2.01	2.05
41	12	304	A86	C14-C15	2.25	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	H	102	DGD	O4D-C4D	-2.24	1.37	1.43
41	36	311	A86	C-C1	2.24	1.55	1.50
38	j	101	DGD	O6D-C5D	-2.24	1.38	1.44
30	19	303	CLA	CMD-C2D	-2.24	1.46	1.50
30	34	307	CLA	C3B-C2B	-2.24	1.37	1.40
30	B	604	CLA	C3B-CAB	-2.24	1.43	1.47
30	12	307	CLA	CMC-C2C	-2.24	1.46	1.50
30	c	508	CLA	CHC-C1C	2.24	1.40	1.35
30	C	513	CLA	MG-ND	-2.24	2.01	2.05
36	b	619	LMG	O2-C2	-2.24	1.37	1.43
30	14	301	CLA	CMC-C2C	-2.24	1.46	1.50
36	B	619	LMG	O8-C9	-2.24	1.40	1.45
41	11	310	A86	C24-C1	2.24	1.50	1.45
41	31	310	A86	C24-C1	2.24	1.50	1.45
30	c	523	CLA	MG-ND	-2.24	2.01	2.05
30	B	603	CLA	C4B-CHC	-2.24	1.34	1.41
36	b	618	LMG	O4-C4	-2.24	1.37	1.43
30	D	405	CLA	C1D-ND	2.24	1.40	1.37
36	B	619	LMG	O1-C7	-2.24	1.39	1.43
30	12	305	CLA	C3B-CAB	-2.24	1.43	1.47
30	15	309	CLA	CMD-C2D	-2.24	1.46	1.50
30	13	307	CLA	C3B-C2B	-2.24	1.37	1.40
30	B	609	CLA	CMC-C2C	-2.24	1.46	1.50
30	B	608	CLA	C3B-CAB	-2.24	1.43	1.47
30	D	406	CLA	C3B-CAB	-2.24	1.43	1.47
41	13	312	A86	O4-C34	-2.24	1.41	1.46
41	17	311	A86	O4-C34	-2.24	1.41	1.46
30	b	605	CLA	CMC-C2C	-2.24	1.46	1.50
30	c	502	CLA	C4B-CHC	-2.24	1.34	1.41
30	31	301	CLA	MG-ND	-2.24	2.01	2.05
30	36	305	CLA	MG-ND	-2.24	2.01	2.05
30	17	310	CLA	CMD-C2D	-2.23	1.46	1.50
41	20	201	A86	O4-C34	-2.23	1.41	1.46
41	37	312	A86	O4-C34	-2.23	1.41	1.46
30	33	311	CLA	MG-ND	-2.23	2.01	2.05
30	17	305	CLA	CMC-C2C	-2.23	1.46	1.50
30	b	606	CLA	MG-ND	-2.23	2.01	2.05
30	b	614	CLA	MG-ND	-2.23	2.01	2.05
36	B	620	LMG	O2-C2	-2.23	1.37	1.43
41	18	314	A86	O4-C34	-2.23	1.41	1.46
30	12	310	CLA	C3B-C2B	-2.23	1.37	1.40
41	34	311	A86	C24-C1	2.23	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	12	307	CLA	C3B-CAB	-2.23	1.43	1.47
30	c	513	CLA	CMC-C2C	-2.23	1.46	1.50
30	11	307	CLA	CMC-C2C	-2.23	1.46	1.50
30	b	604	CLA	C3B-CAB	-2.23	1.43	1.47
41	31	311	A86	O4-C34	-2.23	1.41	1.46
41	16	313	A86	C24-C1	2.23	1.50	1.45
38	c	518	DGD	O2E-C2E	-2.23	1.37	1.43
30	17	309	CLA	O2A-CGA	2.23	1.38	1.30
30	36	301	CLA	C3B-C2B	-2.23	1.37	1.40
36	c	519	LMG	O4-C4	-2.23	1.37	1.43
30	18	304	CLA	CMD-C2D	-2.23	1.46	1.50
30	36	304	CLA	CMC-C2C	-2.23	1.46	1.50
30	39	307	CLA	CMC-C2C	-2.23	1.46	1.50
30	37	309	CLA	O2A-CGA	2.23	1.38	1.30
30	C	513	CLA	CMC-C2C	-2.23	1.46	1.50
41	13	315	A86	C24-C1	2.23	1.50	1.45
41	37	312	A86	C24-C1	2.23	1.50	1.45
41	11	311	A86	O4-C34	-2.23	1.41	1.46
30	11	302	CLA	MG-ND	-2.23	2.01	2.05
30	36	304	CLA	MG-ND	-2.23	2.01	2.05
30	16	301	CLA	C3B-CAB	-2.23	1.43	1.47
30	B	614	CLA	C4B-CHC	-2.23	1.34	1.41
30	C	511	CLA	C1D-ND	2.23	1.40	1.37
41	20	212	A86	C14-C15	2.23	1.57	1.52
30	11	301	CLA	CMD-C2D	-2.22	1.46	1.50
30	14	303	CLA	CMC-C2C	-2.22	1.46	1.50
41	16	311	A86	O4-C34	-2.22	1.41	1.46
30	20	206	CLA	MG-ND	-2.22	2.01	2.05
30	b	611	CLA	CAC-C3C	-2.22	1.45	1.51
30	18	312	CLA	CMD-C2D	-2.22	1.46	1.50
30	31	302	CLA	C3B-C2B	-2.22	1.37	1.40
41	14	312	A86	O4-C34	-2.22	1.41	1.46
30	35	309	CLA	CMD-C2D	-2.22	1.46	1.50
30	40	206	CLA	C3B-C2B	-2.22	1.37	1.40
30	M	101	CLA	C3B-CAB	-2.22	1.43	1.47
30	m	101	CLA	MG-ND	-2.22	2.01	2.05
32	F	101	BCR	C30-C25	-2.22	1.50	1.53
41	21	311	A86	O4-C34	-2.22	1.41	1.46
30	M	101	CLA	MG-ND	-2.22	2.01	2.05
41	17	312	A86	C24-C1	2.22	1.50	1.45
30	39	306	CLA	CMC-C2C	-2.22	1.46	1.50
30	37	310	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	38	304	CLA	CMD-C2D	-2.22	1.46	1.50
30	B	611	CLA	C3B-CAB	-2.22	1.43	1.47
30	11	303	CLA	C3B-CAB	-2.22	1.43	1.47
36	B	620	LMG	O3-C3	-2.22	1.37	1.43
30	35	308	CLA	CMC-C2C	-2.22	1.46	1.50
30	37	305	CLA	CMC-C2C	-2.22	1.46	1.50
38	J	101	DGD	O2D-C2D	-2.22	1.37	1.43
30	31	305	CLA	CMD-C2D	-2.22	1.46	1.50
30	35	301	CLA	CMD-C2D	-2.22	1.46	1.50
38	C	517	DGD	O2E-C2E	-2.22	1.37	1.43
30	33	304	CLA	C3B-C2B	-2.22	1.37	1.40
30	34	301	CLA	CMC-C2C	-2.22	1.46	1.50
30	14	302	CLA	CMD-C2D	-2.21	1.46	1.50
30	15	306	CLA	CMC-C2C	-2.21	1.46	1.50
30	18	303	CLA	CMD-C2D	-2.21	1.46	1.50
30	40	208	CLA	CMC-C2C	-2.21	1.46	1.50
30	d	406	CLA	CAA-C2A	-2.21	1.50	1.54
30	13	304	CLA	MG-ND	-2.21	2.01	2.05
30	38	301	CLA	MG-ND	-2.21	2.01	2.05
42	32	302	LMU	O3'-C3'	2.21	1.48	1.43
41	33	313	A86	O4-C34	-2.21	1.41	1.46
38	c	517	DGD	O2G-C2G	-2.21	1.41	1.46
41	37	311	A86	O4-C34	-2.21	1.41	1.46
30	11	305	CLA	CMD-C2D	-2.21	1.46	1.50
30	c	509	CLA	C4B-CHC	-2.21	1.34	1.41
41	36	311	A86	O4-C34	-2.21	1.41	1.46
30	b	622	CLA	CMC-C2C	-2.21	1.46	1.50
30	12	312	CLA	CMC-C2C	-2.21	1.46	1.50
38	c	517	DGD	O3D-C3D	-2.21	1.37	1.43
36	B	619	LMG	O4-C4	-2.21	1.37	1.43
39	D	404	PL9	C36-C34	-2.21	1.46	1.51
30	35	303	CLA	CMD-C2D	-2.21	1.46	1.50
30	17	309	CLA	MG-ND	-2.21	2.01	2.05
30	15	308	CLA	CMC-C2C	-2.21	1.46	1.50
41	15	310	A86	C24-C1	2.21	1.50	1.45
41	35	311	A86	O4-C34	-2.21	1.41	1.46
30	20	204	CLA	C3B-C2B	-2.21	1.37	1.40
30	11	302	CLA	CMC-C2C	-2.21	1.46	1.50
30	15	301	CLA	CMC-C2C	-2.21	1.46	1.50
30	34	310	CLA	CMC-C2C	-2.21	1.46	1.50
30	14	304	CLA	MG-ND	-2.21	2.01	2.05
30	15	303	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	17	304	CLA	CMC-C2C	-2.20	1.46	1.50
30	18	303	CLA	CMC-C2C	-2.20	1.46	1.50
33	L	103	SQD	O2-C2	-2.20	1.37	1.43
41	15	311	A86	O4-C34	-2.20	1.41	1.46
41	13	311	A86	C24-C1	2.20	1.50	1.45
32	f	101	BCR	C33-C5	-2.20	1.47	1.50
30	16	304	CLA	CMC-C2C	-2.20	1.46	1.50
30	37	305	CLA	CMD-C2D	-2.20	1.46	1.50
30	40	209	CLA	MG-ND	-2.20	2.01	2.05
30	15	302	CLA	CMD-C2D	-2.20	1.46	1.50
30	31	315	CLA	CMC-C2C	-2.20	1.46	1.50
30	32	311	CLA	CMC-C2C	-2.20	1.46	1.50
30	B	611	CLA	CAC-C3C	-2.20	1.45	1.51
30	36	301	CLA	MG-ND	-2.20	2.01	2.05
30	C	502	CLA	C4B-CHC	-2.20	1.34	1.41
30	b	614	CLA	C4B-CHC	-2.20	1.34	1.41
30	C	510	CLA	CMA-C3A	-2.20	1.48	1.53
30	d	402	CLA	CMC-C2C	-2.20	1.46	1.50
30	m	101	CLA	C3B-CAB	-2.20	1.43	1.47
30	19	307	CLA	CMC-C2C	-2.20	1.46	1.50
30	36	304	CLA	C3B-CAB	-2.20	1.43	1.47
30	16	304	CLA	C3B-CAB	-2.20	1.43	1.47
32	F	101	BCR	C33-C5	-2.20	1.47	1.50
30	14	307	CLA	C3B-C2B	-2.20	1.37	1.40
30	38	303	CLA	CMC-C2C	-2.20	1.46	1.50
30	38	303	CLA	CMD-C2D	-2.20	1.46	1.50
30	D	402	CLA	CMC-C2C	-2.20	1.46	1.50
30	13	302	CLA	CMD-C2D	-2.20	1.46	1.50
30	11	303	CLA	CMC-C2C	-2.20	1.46	1.50
30	B	615	CLA	C3B-CAB	-2.20	1.43	1.47
30	21	307	CLA	CMD-C2D	-2.20	1.46	1.50
30	34	303	CLA	CMC-C2C	-2.19	1.46	1.50
30	19	306	CLA	CMC-C2C	-2.19	1.46	1.50
30	14	301	CLA	MG-ND	-2.19	2.01	2.05
30	40	206	CLA	MG-ND	-2.19	2.01	2.05
30	c	512	CLA	CMD-C2D	-2.19	1.46	1.50
30	12	306	CLA	MG-ND	-2.19	2.01	2.05
30	36	302	CLA	CMD-C2D	-2.19	1.46	1.50
30	38	312	CLA	CMD-C2D	-2.19	1.46	1.50
30	B	607	CLA	C3B-C2B	-2.19	1.37	1.40
30	b	604	CLA	CHC-C1C	2.19	1.40	1.35
30	31	303	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	405	CLA	CAA-C2A	-2.19	1.50	1.54
41	18	313	A86	C24-C1	2.19	1.50	1.45
41	17	314	A86	O4-C34	-2.19	1.41	1.46
30	37	304	CLA	MG-ND	-2.19	2.01	2.05
41	33	312	A86	C24-C1	2.19	1.50	1.45
30	38	308	CLA	CMD-C2D	-2.19	1.46	1.50
30	34	302	CLA	MG-ND	-2.19	2.01	2.05
38	C	516	DGD	O2G-C2G	-2.19	1.41	1.46
30	b	615	CLA	C3B-CAB	-2.19	1.43	1.47
30	40	204	CLA	CMD-C2D	-2.19	1.46	1.50
30	17	304	CLA	MG-ND	-2.19	2.01	2.05
30	b	609	CLA	MG-ND	-2.19	2.01	2.05
30	18	310	CLA	MG-ND	-2.19	2.01	2.05
30	20	204	CLA	CMD-C2D	-2.19	1.46	1.50
30	13	304	CLA	CMC-C2C	-2.19	1.46	1.50
30	35	302	CLA	CMD-C2D	-2.19	1.46	1.50
30	35	306	CLA	CMC-C2C	-2.19	1.46	1.50
30	15	307	CLA	CMC-C2C	-2.19	1.46	1.50
30	40	207	CLA	CMD-C2D	-2.18	1.46	1.50
30	41	308	CLA	CMD-C2D	-2.18	1.46	1.50
30	11	303	CLA	MG-ND	-2.18	2.01	2.05
30	13	304	CLA	C3B-CAB	-2.18	1.43	1.47
30	d	407	CLA	C3B-CAB	-2.18	1.43	1.47
30	12	307	CLA	MG-ND	-2.18	2.01	2.05
30	B	606	CLA	MG-ND	-2.18	2.01	2.05
32	c	516	BCR	C38-C26	-2.18	1.47	1.50
30	11	302	CLA	C3B-C2B	-2.18	1.37	1.40
30	12	305	CLA	CMD-C2D	-2.18	1.46	1.50
30	17	305	CLA	CMD-C2D	-2.18	1.46	1.50
30	12	306	CLA	CMC-C2C	-2.18	1.46	1.50
41	14	311	A86	C24-C1	2.18	1.50	1.45
30	21	301	CLA	CMD-C2D	-2.18	1.46	1.50
30	12	303	CLA	C3B-C2B	-2.18	1.37	1.40
30	36	301	CLA	C3B-CAB	-2.18	1.43	1.47
30	18	301	CLA	CMC-C2C	-2.18	1.46	1.50
30	31	302	CLA	CMC-C2C	-2.18	1.46	1.50
30	c	506	CLA	C4B-CHC	-2.18	1.34	1.41
30	37	304	CLA	CMC-C2C	-2.18	1.46	1.50
30	b	603	CLA	C3B-CAB	-2.18	1.43	1.47
30	41	307	CLA	CMD-C2D	-2.18	1.46	1.50
30	b	611	CLA	C3B-CAB	-2.18	1.43	1.47
30	20	203	CLA	MG-ND	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	304	CLA	MG-ND	-2.18	2.01	2.05
30	B	603	CLA	C3B-CAB	-2.18	1.43	1.47
30	41	301	CLA	C3B-C2B	-2.17	1.37	1.40
30	38	308	CLA	MG-ND	-2.17	2.01	2.05
30	40	203	CLA	MG-ND	-2.17	2.01	2.05
30	32	307	CLA	C3B-C2B	-2.17	1.37	1.40
30	C	521	CLA	CMC-C2C	-2.17	1.46	1.50
30	16	301	CLA	MG-ND	-2.17	2.01	2.05
30	21	301	CLA	C3B-C2B	-2.17	1.37	1.40
30	B	614	CLA	MG-ND	-2.17	2.01	2.05
30	16	302	CLA	CMD-C2D	-2.17	1.46	1.50
30	21	302	CLA	CMD-C2D	-2.17	1.46	1.50
30	19	303	CLA	CMC-C2C	-2.17	1.46	1.50
30	21	308	CLA	CMD-C2D	-2.17	1.46	1.50
30	38	301	CLA	CMC-C2C	-2.17	1.46	1.50
41	39	309	A86	O4-C34	-2.17	1.41	1.46
41	19	309	A86	O4-C34	-2.17	1.41	1.46
30	38	305	CLA	C3B-C2B	-2.17	1.37	1.40
38	C	516	DGD	O3D-C3D	-2.17	1.37	1.43
41	37	314	A86	O4-C34	-2.17	1.41	1.46
30	38	310	CLA	MG-ND	-2.17	2.01	2.05
38	c	517	DGD	O4E-C4E	-2.16	1.37	1.43
30	34	306	CLA	CMC-C2C	-2.16	1.46	1.50
30	34	303	CLA	C3B-CAB	-2.16	1.43	1.47
30	35	301	CLA	CMC-C2C	-2.16	1.46	1.50
30	11	306	CLA	C3B-C2B	-2.16	1.37	1.40
41	37	302	A86	O4-C34	-2.16	1.41	1.46
30	12	312	CLA	MG-ND	-2.16	2.01	2.05
30	32	313	CLA	MG-ND	-2.16	2.01	2.05
30	18	308	CLA	CMD-C2D	-2.16	1.46	1.50
36	B	620	LMG	O7-C8	-2.16	1.41	1.46
41	18	302	A86	O4-C34	-2.16	1.41	1.46
30	20	207	CLA	CMD-C2D	-2.16	1.46	1.50
30	39	303	CLA	CMC-C2C	-2.16	1.46	1.50
30	c	511	CLA	C1D-ND	2.16	1.40	1.37
30	20	205	CLA	C3B-C2B	-2.16	1.37	1.40
30	34	306	CLA	CMD-C2D	-2.16	1.46	1.50
41	38	302	A86	O4-C34	-2.16	1.41	1.46
30	C	506	CLA	C4B-CHC	-2.16	1.35	1.41
30	B	623	CLA	CMC-C2C	-2.16	1.46	1.50
41	38	313	A86	C24-C1	2.16	1.50	1.45
30	17	303	CLA	MG-ND	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	31	309	CLA	MG-ND	-2.16	2.01	2.05
38	J	101	DGD	O6D-C5D	-2.16	1.39	1.44
41	17	302	A86	O4-C34	-2.16	1.41	1.46
30	32	309	CLA	CMD-C2D	-2.16	1.46	1.50
30	13	303	CLA	CMC-C2C	-2.16	1.46	1.50
31	D	403	PHO	C3B-C2B	-2.16	1.37	1.40
30	20	205	CLA	MG-ND	-2.15	2.01	2.05
30	19	305	CLA	C3B-CAB	-2.15	1.43	1.47
30	31	306	CLA	C3B-CAB	-2.15	1.43	1.47
30	18	305	CLA	CMD-C2D	-2.15	1.46	1.50
30	41	302	CLA	CMD-C2D	-2.15	1.46	1.50
30	20	207	CLA	MG-ND	-2.15	2.01	2.05
30	20	206	CLA	C3B-C2B	-2.15	1.37	1.40
41	13	316	A86	O4-C34	-2.15	1.41	1.46
32	c	520	BCR	C33-C5	-2.15	1.47	1.50
30	12	312	CLA	C3B-C2B	-2.15	1.37	1.40
30	35	307	CLA	C3B-CAB	-2.15	1.43	1.47
30	37	303	CLA	MG-ND	-2.15	2.01	2.05
31	A	403	PHO	CAA-C2A	-2.15	1.49	1.54
30	18	308	CLA	MG-ND	-2.15	2.01	2.05
30	d	406	CLA	C1D-ND	2.15	1.40	1.37
31	d	404	PHO	C1C-NC	-2.15	1.31	1.38
30	11	315	CLA	CMC-C2C	-2.15	1.46	1.50
41	21	313	A86	O4-C34	-2.15	1.41	1.46
30	40	209	CLA	CMD-C2D	-2.15	1.46	1.50
30	C	502	CLA	CAC-C3C	-2.15	1.45	1.51
30	36	304	CLA	C3B-C2B	-2.15	1.37	1.40
30	13	304	CLA	C3B-C2B	-2.15	1.37	1.40
30	40	205	CLA	MG-ND	-2.15	2.01	2.05
30	41	301	CLA	CMD-C2D	-2.15	1.46	1.50
41	40	210	A86	O4-C34	-2.15	1.41	1.46
41	13	314	A86	O4-C34	-2.15	1.41	1.46
30	35	308	CLA	C3B-CAB	-2.15	1.43	1.47
30	b	611	CLA	C4B-CHC	-2.15	1.35	1.41
38	C	517	DGD	O2D-C2D	-2.15	1.37	1.43
38	J	101	DGD	O3G-C3G	-2.15	1.39	1.43
30	17	305	CLA	C3B-CAB	-2.15	1.43	1.47
30	32	305	CLA	MG-ND	-2.14	2.01	2.05
30	40	204	CLA	C3B-C2B	-2.14	1.37	1.40
30	20	209	CLA	CMD-C2D	-2.14	1.46	1.50
30	19	305	CLA	CMC-C2C	-2.14	1.46	1.50
30	31	305	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	33	315	A86	O4-C34	-2.14	1.41	1.46
41	33	316	A86	O4-C34	-2.14	1.41	1.46
30	13	310	CLA	MG-ND	-2.14	2.01	2.05
30	14	303	CLA	MG-ND	-2.14	2.01	2.05
30	39	305	CLA	C3B-CAB	-2.14	1.43	1.47
30	33	307	CLA	CMC-C2C	-2.14	1.46	1.50
30	35	307	CLA	CMC-C2C	-2.14	1.46	1.50
30	31	303	CLA	C3B-C2B	-2.14	1.37	1.40
30	C	503	CLA	CHC-C1C	2.14	1.40	1.35
30	38	312	CLA	MG-ND	-2.14	2.01	2.05
41	20	210	A86	C14-C15	2.14	1.56	1.52
41	20	210	A86	O4-C34	-2.14	1.41	1.46
30	C	519	CLA	CMD-C2D	-2.14	1.46	1.50
30	15	303	CLA	CMC-C2C	-2.14	1.46	1.50
30	c	522	CLA	CMC-C2C	-2.14	1.46	1.50
30	17	310	CLA	CMC-C2C	-2.14	1.46	1.50
30	33	307	CLA	CMD-C2D	-2.14	1.46	1.50
30	13	303	CLA	C3B-C2B	-2.14	1.37	1.40
30	20	205	CLA	C4B-CHC	-2.14	1.35	1.41
38	j	101	DGD	O4D-C4D	-2.14	1.37	1.43
30	11	315	CLA	C3B-C2B	-2.14	1.37	1.40
38	h	102	DGD	O3D-C3D	-2.14	1.37	1.43
36	32	301	LMG	O6-C5	-2.14	1.39	1.44
30	38	305	CLA	CMD-C2D	-2.14	1.46	1.50
41	14	314	A86	O4-C34	-2.14	1.41	1.46
41	34	314	A86	O4-C34	-2.14	1.41	1.46
30	c	523	CLA	CMC-C2C	-2.14	1.46	1.50
30	12	303	CLA	CMC-C2C	-2.14	1.46	1.50
30	38	305	CLA	CMC-C2C	-2.14	1.46	1.50
30	37	305	CLA	C3B-CAB	-2.14	1.43	1.47
31	d	403	PHO	CAA-C2A	-2.13	1.49	1.54
30	11	305	CLA	CMC-C2C	-2.13	1.46	1.50
30	32	309	CLA	CMC-C2C	-2.13	1.46	1.50
30	40	207	CLA	CMC-C2C	-2.13	1.46	1.50
30	21	306	CLA	CMD-C2D	-2.13	1.46	1.50
30	33	311	CLA	CMC-C2C	-2.13	1.46	1.50
30	39	305	CLA	CMC-C2C	-2.13	1.46	1.50
30	B	607	CLA	C3B-CAB	-2.13	1.43	1.47
30	33	304	CLA	C4B-CHC	-2.13	1.35	1.41
31	d	403	PHO	C1C-NC	-2.13	1.31	1.38
30	33	303	CLA	MG-ND	-2.13	2.01	2.05
30	14	305	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	37	305	CLA	C3B-C2B	-2.13	1.37	1.40
30	15	307	CLA	C3B-CAB	-2.13	1.43	1.47
30	35	301	CLA	C3B-CAB	-2.13	1.43	1.47
30	b	610	CLA	CAC-C3C	-2.13	1.45	1.51
31	d	404	PHO	C3B-C2B	-2.13	1.37	1.40
30	35	303	CLA	CMC-C2C	-2.13	1.46	1.50
30	c	502	CLA	CAC-C3C	-2.13	1.45	1.51
41	12	318	A86	O4-C34	-2.13	1.41	1.46
31	D	403	PHO	C1C-NC	-2.13	1.31	1.38
32	C	515	BCR	C38-C26	-2.13	1.47	1.50
30	40	207	CLA	C3B-C2B	-2.13	1.37	1.40
41	41	313	A86	O4-C34	-2.13	1.41	1.46
30	18	305	CLA	CMC-C2C	-2.13	1.46	1.50
30	17	305	CLA	C3B-C2B	-2.13	1.37	1.40
30	35	307	CLA	CMD-C2D	-2.13	1.46	1.50
30	35	309	CLA	MG-ND	-2.13	2.01	2.05
30	32	306	CLA	C4B-CHC	-2.13	1.35	1.41
30	21	301	CLA	CMC-C2C	-2.13	1.46	1.50
30	41	301	CLA	CMC-C2C	-2.13	1.46	1.50
30	19	302	CLA	CMC-C2C	-2.13	1.46	1.50
30	37	310	CLA	CMC-C2C	-2.13	1.46	1.50
30	38	311	CLA	C3B-C2B	-2.13	1.37	1.40
40	E	101	HEM	CAA-C2A	2.13	1.55	1.52
30	40	205	CLA	C3B-C2B	-2.13	1.37	1.40
41	31	313	A86	O4-C34	-2.13	1.41	1.46
30	41	306	CLA	CMD-C2D	-2.13	1.46	1.50
41	11	313	A86	O4-C34	-2.13	1.41	1.46
31	A	403	PHO	C1C-NC	-2.13	1.32	1.38
30	15	308	CLA	C3B-CAB	-2.13	1.43	1.47
30	15	307	CLA	CMD-C2D	-2.12	1.46	1.50
30	15	304	CLA	CMC-C2C	-2.12	1.46	1.50
30	B	607	CLA	C4B-CHC	-2.12	1.35	1.41
30	31	302	CLA	C4B-CHC	-2.12	1.35	1.41
30	37	301	CLA	CMC-C2C	-2.12	1.46	1.50
30	40	205	CLA	CMD-C2D	-2.12	1.46	1.50
30	20	207	CLA	CMC-C2C	-2.12	1.46	1.50
30	19	306	CLA	C4B-CHC	-2.12	1.35	1.41
30	39	306	CLA	C4B-CHC	-2.12	1.35	1.41
30	21	305	CLA	CMD-C2D	-2.12	1.46	1.50
30	33	305	CLA	C3B-C2B	-2.12	1.37	1.40
41	15	315	A86	O4-C34	-2.12	1.41	1.46
30	B	611	CLA	C4B-CHC	-2.12	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	515	BCR	C33-C5	-2.12	1.47	1.50
41	15	313	A86	O4-C34	-2.12	1.41	1.46
38	j	101	DGD	O4E-C4E	-2.12	1.38	1.43
30	c	511	CLA	C3B-C2B	-2.12	1.37	1.40
30	18	305	CLA	C3B-C2B	-2.12	1.37	1.40
30	B	606	CLA	C5-C3	-2.12	1.46	1.51
30	c	510	CLA	CMA-C3A	-2.12	1.48	1.53
30	c	523	CLA	C3B-C2B	-2.12	1.37	1.40
30	18	312	CLA	MG-ND	-2.12	2.01	2.05
30	B	623	CLA	C1D-ND	2.12	1.40	1.37
30	C	519	CLA	CMC-C2C	-2.12	1.46	1.50
30	B	604	CLA	CHC-C1C	2.12	1.40	1.35
33	L	103	SQD	O3-C3	-2.12	1.38	1.43
30	C	508	CLA	C3B-CAB	-2.12	1.43	1.47
30	11	315	CLA	MG-ND	-2.12	2.01	2.05
30	34	306	CLA	MG-ND	-2.12	2.01	2.05
30	21	303	CLA	MG-ND	-2.11	2.01	2.05
38	c	518	DGD	O2D-C2D	-2.11	1.38	1.43
30	c	503	CLA	CHC-C1C	2.11	1.40	1.35
30	C	507	CLA	C3B-CAB	-2.11	1.43	1.47
36	M	102	LMG	O8-C9	-2.11	1.40	1.45
30	18	306	CLA	MG-ND	-2.11	2.01	2.05
30	40	204	CLA	MG-ND	-2.11	2.01	2.05
30	40	207	CLA	MG-ND	-2.11	2.01	2.05
30	D	401	CLA	CAC-C3C	-2.11	1.45	1.51
30	12	303	CLA	MG-ND	-2.11	2.01	2.05
30	13	306	CLA	CMC-C2C	-2.11	1.46	1.50
30	C	521	CLA	C3B-C2B	-2.11	1.37	1.40
36	m	102	LMG	O8-C9	-2.11	1.40	1.45
30	32	310	CLA	C3B-CAB	-2.11	1.43	1.47
41	18	315	A86	O4-C34	-2.11	1.41	1.46
32	Y	101	BCR	C33-C5	-2.11	1.47	1.50
30	b	612	CLA	C3B-CAB	-2.11	1.43	1.47
30	B	615	CLA	C4B-CHC	-2.11	1.35	1.41
30	C	510	CLA	C3B-CAB	-2.11	1.43	1.47
30	20	207	CLA	C3B-C2B	-2.11	1.37	1.40
30	37	310	CLA	MG-ND	-2.11	2.01	2.05
30	20	205	CLA	CMD-C2D	-2.11	1.46	1.50
30	40	205	CLA	C4B-CHC	-2.11	1.35	1.41
30	41	305	CLA	CMD-C2D	-2.11	1.46	1.50
30	33	303	CLA	C3B-C2B	-2.11	1.37	1.40
30	b	615	CLA	C4B-CHC	-2.11	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	306	CLA	MG-ND	-2.11	2.01	2.05
30	d	401	CLA	CAC-C3C	-2.11	1.45	1.51
30	14	303	CLA	C3B-C2B	-2.11	1.37	1.40
30	16	304	CLA	C3B-C2B	-2.11	1.37	1.40
30	34	302	CLA	C3B-C2B	-2.11	1.37	1.40
30	15	309	CLA	MG-ND	-2.11	2.01	2.05
30	b	607	CLA	C3B-CAB	-2.10	1.43	1.47
30	39	302	CLA	CMC-C2C	-2.10	1.46	1.50
30	B	612	CLA	C3B-CAB	-2.10	1.43	1.47
30	b	606	CLA	C5-C3	-2.10	1.46	1.51
30	32	305	CLA	C3B-C2B	-2.10	1.37	1.40
30	34	303	CLA	C3B-C2B	-2.10	1.37	1.40
30	12	314	CLA	MG-ND	-2.10	2.01	2.05
33	B	621	SQD	O47-C45	-2.10	1.41	1.46
41	33	302	A86	O4-C34	-2.10	1.41	1.46
30	B	613	CLA	C3B-CAB	-2.10	1.43	1.47
30	d	401	CLA	C4B-CHC	-2.10	1.35	1.41
30	40	204	CLA	C3B-CAB	-2.10	1.43	1.47
30	32	306	CLA	CMC-C2C	-2.10	1.46	1.50
30	20	204	CLA	C3B-CAB	-2.10	1.43	1.47
30	20	204	CLA	MG-ND	-2.10	2.01	2.05
41	13	301	A86	O4-C34	-2.10	1.41	1.46
30	41	302	CLA	CMC-C2C	-2.10	1.46	1.50
30	a	403	CLA	C1D-ND	2.10	1.40	1.37
39	d	408	PL9	C15-C14	-2.10	1.45	1.50
33	b	620	SQD	O47-C45	-2.10	1.41	1.46
30	20	204	CLA	CMC-C2C	-2.10	1.46	1.50
30	C	519	CLA	C3B-C2B	-2.10	1.37	1.40
38	J	101	DGD	O4E-C4E	-2.10	1.38	1.43
41	41	311	A86	C14-C15	2.10	1.56	1.52
41	40	210	A86	C14-C15	2.10	1.56	1.52
30	35	307	CLA	MG-ND	-2.09	2.01	2.05
30	z	101	CLA	CMC-C2C	-2.09	1.46	1.50
41	39	309	A86	C14-C15	2.09	1.56	1.52
41	32	304	A86	O4-C34	-2.09	1.41	1.46
41	32	317	A86	O4-C34	-2.09	1.41	1.46
30	17	310	CLA	MG-ND	-2.09	2.01	2.05
30	15	301	CLA	C3B-CAB	-2.09	1.43	1.47
32	b	623	BCR	C33-C5	-2.09	1.47	1.50
38	C	516	DGD	O4E-C4E	-2.09	1.38	1.43
30	C	511	CLA	CAC-C3C	-2.09	1.45	1.51
32	c	516	BCR	C33-C5	-2.09	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	37	302	A86	C35-C34	2.09	1.55	1.51
30	C	502	CLA	C3B-CAB	-2.09	1.43	1.47
30	33	310	CLA	C4B-CHC	-2.09	1.35	1.41
30	34	310	CLA	MG-ND	-2.09	2.01	2.05
39	D	407	PL9	C15-C14	-2.09	1.45	1.50
30	15	307	CLA	MG-ND	-2.09	2.01	2.05
30	11	309	CLA	MG-ND	-2.09	2.01	2.05
30	b	607	CLA	C4B-CHC	-2.09	1.35	1.41
36	b	619	LMG	O7-C8	-2.09	1.41	1.46
30	34	307	CLA	C3B-CAB	-2.09	1.43	1.47
41	35	315	A86	O4-C34	-2.09	1.41	1.46
30	D	401	CLA	C4B-CHC	-2.09	1.35	1.41
30	37	304	CLA	C4B-CHC	-2.09	1.35	1.41
32	B	624	BCR	C33-C5	-2.09	1.47	1.50
30	12	309	CLA	CMC-C2C	-2.09	1.46	1.50
30	17	301	CLA	CMC-C2C	-2.09	1.46	1.50
33	l	101	SQD	O4-C4	-2.09	1.38	1.43
41	11	316	A86	O4-C34	-2.09	1.41	1.46
30	20	203	CLA	C4B-CHC	-2.09	1.35	1.41
30	11	303	CLA	C3B-C2B	-2.09	1.37	1.40
30	b	605	CLA	CAC-C3C	-2.08	1.45	1.51
33	l	101	SQD	O3-C3	-2.08	1.38	1.43
30	14	310	CLA	MG-ND	-2.08	2.01	2.05
41	35	313	A86	O4-C34	-2.08	1.41	1.46
30	35	309	CLA	C3B-CAB	-2.08	1.43	1.47
30	c	502	CLA	C3B-CAB	-2.08	1.43	1.47
30	35	304	CLA	CMC-C2C	-2.08	1.46	1.50
30	A	404	CLA	C1D-ND	2.08	1.40	1.37
30	21	304	CLA	MG-ND	-2.08	2.01	2.05
38	j	101	DGD	O3G-C3G	-2.08	1.39	1.43
30	c	510	CLA	C3B-CAB	-2.08	1.43	1.47
30	c	511	CLA	CAC-C3C	-2.08	1.45	1.51
30	12	306	CLA	C4B-CHC	-2.08	1.35	1.41
30	b	602	CLA	CAC-C3C	-2.08	1.45	1.51
30	B	606	CLA	C4B-CHC	-2.08	1.35	1.41
30	18	311	CLA	C3B-C2B	-2.08	1.37	1.40
30	Z	102	CLA	CMD-C2D	-2.08	1.46	1.50
30	B	608	CLA	MG-ND	-2.08	2.01	2.05
30	13	305	CLA	CMC-C2C	-2.08	1.46	1.50
30	13	303	CLA	C4B-CHC	-2.08	1.35	1.41
30	17	307	CLA	MG-ND	-2.08	2.01	2.05
30	35	302	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	31	316	A86	O4-C34	-2.08	1.41	1.46
41	41	314	A86	C14-C15	2.08	1.56	1.52
30	16	305	CLA	C4B-CHC	-2.08	1.35	1.41
36	M	102	LMG	O2-C2	-2.08	1.38	1.43
32	c	515	BCR	C33-C5	-2.08	1.47	1.50
30	B	605	CLA	CAC-C3C	-2.08	1.45	1.51
30	41	304	CLA	CMD-C2D	-2.08	1.46	1.50
30	b	608	CLA	MG-ND	-2.08	2.01	2.05
30	11	304	CLA	CMC-C2C	-2.08	1.46	1.50
30	40	205	CLA	CMC-C2C	-2.07	1.46	1.50
30	40	204	CLA	CMC-C2C	-2.07	1.46	1.50
30	31	302	CLA	C3B-CAB	-2.07	1.43	1.47
30	32	312	CLA	C4B-CHC	-2.07	1.35	1.41
30	11	302	CLA	C4B-CHC	-2.07	1.35	1.41
30	C	520	CLA	CMC-C2C	-2.07	1.46	1.50
30	20	208	CLA	CMD-C2D	-2.07	1.46	1.50
30	12	307	CLA	C3B-C2B	-2.07	1.37	1.40
30	41	304	CLA	MG-ND	-2.07	2.01	2.05
30	14	306	CLA	CMD-C2D	-2.07	1.46	1.50
30	38	301	CLA	C3B-CAB	-2.07	1.43	1.47
30	C	507	CLA	C4B-CHC	-2.07	1.35	1.41
40	v	201	HEM	CHC-C4B	-2.07	1.35	1.41
33	L	103	SQD	O4-C4	-2.07	1.38	1.43
33	A	406	SQD	O47-C45	-2.07	1.41	1.46
41	38	315	A86	O4-C34	-2.07	1.41	1.46
30	b	613	CLA	C4B-CHC	-2.07	1.35	1.41
30	21	302	CLA	CMC-C2C	-2.07	1.46	1.50
41	41	313	A86	C14-C15	2.07	1.56	1.52
30	B	613	CLA	C4B-CHC	-2.07	1.35	1.41
30	17	304	CLA	C4B-CHC	-2.07	1.35	1.41
30	13	310	CLA	CMC-C2C	-2.07	1.46	1.50
41	16	310	A86	C14-C15	2.07	1.56	1.52
30	34	303	CLA	C4B-CHC	-2.07	1.35	1.41
30	C	510	CLA	C4B-CHC	-2.07	1.35	1.41
30	18	301	CLA	C3B-CAB	-2.07	1.43	1.47
30	36	305	CLA	C4B-CHC	-2.07	1.35	1.41
30	18	303	CLA	C3B-C2B	-2.06	1.37	1.40
30	37	304	CLA	C3B-C2B	-2.06	1.37	1.40
30	40	203	CLA	C4B-CHC	-2.06	1.35	1.41
30	33	307	CLA	MG-ND	-2.06	2.01	2.05
30	41	303	CLA	C3B-CAB	-2.06	1.43	1.47
30	20	202	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	19	309	A86	C14-C15	2.06	1.56	1.52
30	33	304	CLA	C3B-CAB	-2.06	1.43	1.47
30	B	610	CLA	CAC-C3C	-2.06	1.45	1.51
41	40	211	A86	C14-C15	2.06	1.56	1.52
41	12	304	A86	O4-C34	-2.06	1.41	1.46
30	11	309	CLA	CMC-C2C	-2.06	1.46	1.50
30	31	309	CLA	CMC-C2C	-2.06	1.46	1.50
41	35	316	A86	O4-C34	-2.06	1.41	1.46
30	38	303	CLA	C3B-C2B	-2.06	1.37	1.40
30	18	312	CLA	C3B-CAB	-2.06	1.43	1.47
30	18	304	CLA	C4B-CHC	-2.06	1.35	1.41
30	15	302	CLA	CMC-C2C	-2.06	1.46	1.50
30	34	305	CLA	CMC-C2C	-2.06	1.46	1.50
30	32	306	CLA	C3B-CAB	-2.06	1.43	1.47
30	41	309	CLA	O2A-CGA	2.06	1.37	1.30
41	17	302	A86	C35-C34	2.06	1.55	1.51
30	41	303	CLA	MG-ND	-2.06	2.01	2.05
30	34	309	CLA	C4B-CHC	-2.06	1.35	1.41
40	e	101	HEM	CAA-C2A	2.06	1.55	1.52
30	40	202	CLA	CMC-C2C	-2.06	1.46	1.50
30	14	303	CLA	C4B-CHC	-2.06	1.35	1.41
30	c	507	CLA	C3B-CAB	-2.06	1.43	1.47
30	37	307	CLA	MG-ND	-2.06	2.01	2.05
30	21	309	CLA	O2A-CGA	2.06	1.37	1.30
30	b	615	CLA	CAC-C3C	-2.06	1.45	1.51
38	J	101	DGD	O4D-C4D	-2.06	1.38	1.43
30	32	313	CLA	CMC-C2C	-2.06	1.46	1.50
30	38	306	CLA	MG-ND	-2.06	2.01	2.05
30	35	305	CLA	CMD-C2D	-2.06	1.46	1.50
30	B	623	CLA	C3B-CAB	-2.06	1.43	1.47
30	13	306	CLA	CMD-C2D	-2.06	1.46	1.50
30	19	304	CLA	CMD-C2D	-2.06	1.46	1.50
30	12	309	CLA	CMD-C2D	-2.06	1.46	1.50
30	20	202	CLA	CMD-C2D	-2.06	1.46	1.50
38	c	517	DGD	O3G-C1D	-2.06	1.36	1.40
30	c	510	CLA	C4B-CHC	-2.06	1.35	1.41
30	34	304	CLA	C4B-CHC	-2.06	1.35	1.41
41	15	316	A86	O4-C34	-2.06	1.41	1.46
30	b	606	CLA	C4B-CHC	-2.06	1.35	1.41
30	15	305	CLA	CMD-C2D	-2.06	1.46	1.50
30	16	306	CLA	C4B-CHC	-2.06	1.35	1.41
30	z	101	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	511	CLA	C3B-C2B	-2.05	1.37	1.40
30	14	304	CLA	C3B-C2B	-2.05	1.37	1.40
30	b	613	CLA	C3B-CAB	-2.05	1.43	1.47
39	D	404	PL9	C41-C39	-2.05	1.47	1.51
30	11	306	CLA	C3B-CAB	-2.05	1.43	1.47
30	39	304	CLA	C3B-C2B	-2.05	1.37	1.40
30	33	311	CLA	C3B-C2B	-2.05	1.37	1.40
30	15	306	CLA	CMD-C2D	-2.05	1.46	1.50
30	36	306	CLA	CMD-C2D	-2.05	1.46	1.50
30	d	402	CLA	C4B-CHC	-2.05	1.35	1.41
30	31	308	CLA	C4B-CHC	-2.05	1.35	1.41
30	21	303	CLA	C3B-CAB	-2.05	1.43	1.47
30	B	615	CLA	CAC-C3C	-2.05	1.45	1.51
30	40	206	CLA	C4B-CHC	-2.05	1.35	1.41
30	33	306	CLA	CMC-C2C	-2.05	1.46	1.50
30	14	309	CLA	C4B-CHC	-2.05	1.35	1.41
30	38	301	CLA	C4B-CHC	-2.05	1.35	1.41
30	21	306	CLA	C3B-C2B	-2.05	1.37	1.40
30	c	508	CLA	C3B-CAB	-2.05	1.43	1.47
30	32	309	CLA	C3B-CAB	-2.05	1.43	1.47
30	14	310	CLA	CMC-C2C	-2.05	1.46	1.50
30	37	301	CLA	C3B-C2B	-2.05	1.37	1.40
30	37	310	CLA	C3B-C2B	-2.05	1.37	1.40
38	H	102	DGD	O2D-C2D	-2.05	1.38	1.43
30	17	304	CLA	C3B-C2B	-2.05	1.37	1.40
38	h	102	DGD	O2D-C2D	-2.05	1.38	1.43
30	18	303	CLA	MG-ND	-2.05	2.01	2.05
30	18	301	CLA	C4B-CHC	-2.05	1.35	1.41
30	37	304	CLA	CAC-C3C	-2.05	1.45	1.51
41	21	311	A86	C14-C15	2.05	1.56	1.52
30	16	306	CLA	CMD-C2D	-2.05	1.46	1.50
30	B	602	CLA	CAC-C3C	-2.05	1.45	1.51
41	40	213	A86	C14-C15	2.04	1.56	1.52
30	13	302	CLA	MG-ND	-2.04	2.01	2.05
30	c	524	CLA	CMD-C2D	-2.04	1.46	1.50
39	D	407	PL9	C16-C14	-2.04	1.47	1.51
40	V	201	HEM	CHC-C4B	-2.04	1.35	1.41
30	39	304	CLA	CMD-C2D	-2.04	1.46	1.50
30	D	405	CLA	C3B-CAB	-2.04	1.43	1.47
30	32	307	CLA	C4B-CHC	-2.04	1.35	1.41
38	H	102	DGD	O3D-C3D	-2.04	1.38	1.43
30	14	306	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	20	205	CLA	CMC-C2C	-2.04	1.46	1.50
30	35	307	CLA	C3B-C2B	-2.04	1.37	1.40
30	c	507	CLA	C4B-CHC	-2.04	1.35	1.41
30	12	313	CLA	C4B-CHC	-2.04	1.35	1.41
36	m	102	LMG	O2-C2	-2.04	1.38	1.43
32	h	101	BCR	C33-C5	-2.04	1.47	1.50
30	38	303	CLA	MG-ND	-2.04	2.01	2.05
30	12	314	CLA	CMC-C2C	-2.04	1.46	1.50
41	36	310	A86	C14-C15	2.04	1.56	1.52
30	17	304	CLA	CAC-C3C	-2.04	1.45	1.51
30	21	304	CLA	CMD-C2D	-2.04	1.46	1.50
36	c	519	LMG	O2-C2	-2.04	1.38	1.43
30	38	307	CLA	CMD-C2D	-2.04	1.46	1.50
30	40	202	CLA	CMD-C2D	-2.04	1.46	1.50
30	11	302	CLA	C3B-CAB	-2.04	1.43	1.47
30	33	305	CLA	C4B-CHC	-2.04	1.35	1.41
30	35	306	CLA	CMD-C2D	-2.04	1.46	1.50
30	15	307	CLA	C3B-C2B	-2.04	1.37	1.40
30	20	206	CLA	C4B-CHC	-2.03	1.35	1.41
35	A	408	LHG	C8-C7	-2.03	1.44	1.50
30	C	519	CLA	C4B-CHC	-2.03	1.35	1.41
30	40	208	CLA	CMD-C2D	-2.03	1.46	1.50
41	21	314	A86	C14-C15	2.03	1.56	1.52
30	38	312	CLA	C3B-CAB	-2.03	1.43	1.47
30	15	309	CLA	C3B-CAB	-2.03	1.43	1.47
30	13	309	CLA	C4B-CHC	-2.03	1.35	1.41
30	33	307	CLA	C3B-C2B	-2.03	1.37	1.40
30	31	306	CLA	MG-ND	-2.03	2.01	2.05
30	39	303	CLA	MG-ND	-2.03	2.01	2.05
30	31	306	CLA	CMC-C2C	-2.03	1.46	1.50
41	20	211	A86	C14-C15	2.03	1.56	1.52
32	H	101	BCR	C38-C26	-2.03	1.47	1.50
30	34	307	CLA	MG-ND	-2.03	2.01	2.05
30	12	308	CLA	CMC-C2C	-2.03	1.46	1.50
30	11	305	CLA	MG-ND	-2.03	2.01	2.05
30	17	301	CLA	C4B-CHC	-2.03	1.35	1.41
30	41	304	CLA	CMC-C2C	-2.03	1.46	1.50
30	15	302	CLA	C3B-C2B	-2.03	1.37	1.40
41	20	213	A86	C14-C15	2.03	1.56	1.52
41	13	313	A86	C35-C34	2.03	1.55	1.51
30	38	304	CLA	C4B-CHC	-2.03	1.35	1.41
32	h	101	BCR	C38-C26	-2.03	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	40	209	CLA	CMC-C2C	-2.03	1.46	1.50
30	c	522	CLA	C4B-CHC	-2.03	1.35	1.41
30	41	306	CLA	C3B-C2B	-2.03	1.37	1.40
30	C	504	CLA	C4B-CHC	-2.03	1.35	1.41
41	21	313	A86	C14-C15	2.03	1.56	1.52
36	w	101	LMG	O4-C4	-2.02	1.38	1.43
30	18	304	CLA	CMC-C2C	-2.02	1.46	1.50
30	38	312	CLA	C3B-C2B	-2.02	1.37	1.40
30	12	306	CLA	C3B-CAB	-2.02	1.43	1.47
30	19	302	CLA	C4B-CHC	-2.02	1.35	1.41
30	37	301	CLA	C4B-CHC	-2.02	1.35	1.41
30	33	308	CLA	MG-ND	-2.02	2.01	2.05
32	Y	101	BCR	C34-C9	-2.02	1.46	1.50
41	11	312	A86	C33-C34	2.02	1.55	1.51
30	b	612	CLA	C4B-CHC	-2.02	1.35	1.41
30	19	304	CLA	C3B-C2B	-2.02	1.37	1.40
30	36	307	CLA	C3B-C2B	-2.02	1.37	1.40
41	17	313	A86	C33-C34	2.02	1.55	1.51
30	11	308	CLA	C4B-CHC	-2.02	1.35	1.41
30	m	101	CLA	CAC-C3C	-2.02	1.45	1.51
30	15	309	CLA	O2A-CGA	2.02	1.37	1.30
30	d	407	CLA	C4B-CHC	-2.02	1.35	1.41
41	35	312	A86	C33-C34	2.02	1.55	1.51
30	36	306	CLA	C4B-CHC	-2.02	1.35	1.41
30	39	302	CLA	C4B-CHC	-2.02	1.35	1.41
30	33	306	CLA	C4B-CHC	-2.02	1.35	1.41
30	12	305	CLA	MG-ND	-2.02	2.01	2.05
30	18	310	CLA	CMC-C2C	-2.02	1.46	1.50
30	32	310	CLA	CMC-C2C	-2.02	1.46	1.50
30	c	514	CLA	C4B-CHC	-2.02	1.35	1.41
32	c	516	BCR	C27-C26	-2.02	1.47	1.51
30	b	601	CLA	C4B-CHC	-2.02	1.35	1.41
30	12	314	CLA	C3B-CAB	-2.02	1.43	1.47
30	15	301	CLA	MG-ND	-2.02	2.01	2.05
40	e	101	HEM	C3D-C2D	-2.02	1.32	1.36
30	C	520	CLA	C4B-CHC	-2.02	1.35	1.41
30	31	301	CLA	C3B-C2B	-2.01	1.37	1.40
41	39	310	A86	C14-C15	2.01	1.56	1.52
41	31	312	A86	C33-C34	2.01	1.55	1.51
33	b	620	SQD	C4-C5	-2.01	1.48	1.53
30	b	622	CLA	C3B-CAB	-2.01	1.43	1.47
30	31	303	CLA	C4B-CHC	-2.01	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	36	305	CLA	CMC-C2C	-2.01	1.46	1.50
30	34	306	CLA	C3B-CAB	-2.01	1.43	1.47
30	13	302	CLA	C3B-C2B	-2.01	1.37	1.40
30	15	306	CLA	C3B-C2B	-2.01	1.37	1.40
30	c	504	CLA	C4B-CHC	-2.01	1.35	1.41
30	35	302	CLA	C3B-C2B	-2.01	1.37	1.40
31	A	403	PHO	C3B-CAB	-2.01	1.43	1.47
30	B	601	CLA	C4B-CHC	-2.01	1.35	1.41
30	12	306	CLA	C3B-C2B	-2.01	1.37	1.40
35	a	407	LHG	C8-C7	-2.01	1.44	1.50
30	18	307	CLA	CMD-C2D	-2.01	1.46	1.50
30	32	308	CLA	CMC-C2C	-2.01	1.46	1.50
30	21	303	CLA	C3B-C2B	-2.01	1.37	1.40
30	39	307	CLA	C4B-CHC	-2.01	1.35	1.41
30	38	305	CLA	C3B-CAB	-2.01	1.43	1.47
30	40	209	CLA	C3B-CAB	-2.01	1.43	1.47
32	Z	101	BCR	C33-C5	-2.01	1.47	1.50
41	21	312	A86	C14-C15	2.01	1.56	1.52
41	35	312	A86	C35-C34	2.01	1.55	1.51
30	21	304	CLA	CMC-C2C	-2.01	1.46	1.50
30	a	403	CLA	C4B-CHC	-2.01	1.35	1.41
30	34	305	CLA	C4B-CHC	-2.01	1.35	1.41
41	13	313	A86	C33-C34	2.01	1.55	1.51
41	15	312	A86	C35-C34	2.01	1.55	1.51
30	31	305	CLA	C3B-C2B	-2.01	1.37	1.40
30	12	310	CLA	C3B-CAB	-2.01	1.43	1.47
39	d	405	PL9	C41-C39	-2.01	1.47	1.51
30	38	307	CLA	CMC-C2C	-2.01	1.46	1.50
41	37	313	A86	C35-C34	2.00	1.55	1.51
30	13	306	CLA	MG-ND	-2.00	2.01	2.05
30	21	309	CLA	CMC-C2C	-2.00	1.46	1.50
30	14	307	CLA	C3B-CAB	-2.00	1.43	1.47
30	18	310	CLA	C4B-CHC	-2.00	1.35	1.41
30	13	310	CLA	C3B-C2B	-2.00	1.37	1.40
30	16	307	CLA	C3B-C2B	-2.00	1.37	1.40
30	35	301	CLA	MG-ND	-2.00	2.01	2.05
30	38	304	CLA	MG-ND	-2.00	2.01	2.05
41	15	312	A86	C33-C34	2.00	1.55	1.51
30	14	310	CLA	C3B-C2B	-2.00	1.37	1.40
30	39	303	CLA	C3B-CAB	-2.00	1.43	1.47
30	D	406	CLA	C4B-CHC	-2.00	1.35	1.41
30	20	208	CLA	MG-ND	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	32	313	CLA	C3B-C2B	-2.00	1.37	1.40
30	36	302	CLA	C4B-CHC	-2.00	1.35	1.41

All (5504) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	37	315	A86	O1-C20-C19	55.34	154.96	113.38
41	17	311	A86	O1-C20-C19	55.33	154.95	113.38
41	17	315	A86	O1-C20-C19	55.33	154.95	113.38
41	37	311	A86	O1-C20-C19	55.30	154.93	113.38
41	18	313	A86	O1-C20-C19	55.09	154.76	113.38
41	38	313	A86	O1-C20-C19	55.07	154.75	113.38
41	40	210	A86	O1-C20-C19	55.05	154.74	113.38
41	11	310	A86	O1-C20-C19	55.03	154.72	113.38
41	20	210	A86	O1-C20-C19	55.01	154.70	113.38
41	35	310	A86	O1-C20-C19	55.01	154.70	113.38
41	34	311	A86	O1-C20-C19	55.00	154.70	113.38
41	31	310	A86	O1-C20-C19	55.00	154.70	113.38
41	12	315	A86	O1-C20-C19	55.00	154.69	113.38
41	33	312	A86	O1-C20-C19	54.98	154.69	113.38
41	15	310	A86	O1-C20-C19	54.98	154.69	113.38
41	14	311	A86	O1-C20-C19	54.97	154.68	113.38
41	13	311	A86	O1-C20-C19	54.95	154.66	113.38
41	32	314	A86	O1-C20-C19	54.95	154.66	113.38
41	17	314	A86	O1-C20-C19	54.29	154.17	113.38
41	31	313	A86	O1-C20-C19	54.29	154.17	113.38
41	38	315	A86	O1-C20-C19	54.27	154.15	113.38
41	14	314	A86	O1-C20-C19	54.26	154.14	113.38
41	32	317	A86	O1-C20-C19	54.24	154.13	113.38
41	34	314	A86	O1-C20-C19	54.23	154.12	113.38
41	12	318	A86	O1-C20-C19	54.22	154.12	113.38
41	37	314	A86	O1-C20-C19	54.21	154.11	113.38
41	35	313	A86	O1-C20-C19	54.20	154.10	113.38
41	33	315	A86	O1-C20-C19	54.20	154.10	113.38
41	18	315	A86	O1-C20-C19	54.20	154.10	113.38
41	15	313	A86	O1-C20-C19	54.19	154.09	113.38
41	11	313	A86	O1-C20-C19	54.18	154.09	113.38
41	13	314	A86	O1-C20-C19	54.16	154.07	113.38
41	40	212	A86	O1-C20-C19	54.09	154.02	113.38
41	20	212	A86	O1-C20-C19	54.09	154.01	113.38
41	19	311	A86	O1-C20-C19	53.42	153.51	113.38
41	39	311	A86	O1-C20-C19	53.39	153.49	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	16	310	A86	O1-C20-C19	53.38	153.48	113.38
41	36	310	A86	O1-C20-C19	53.34	153.45	113.38
41	17	302	A86	O1-C20-C19	52.73	152.99	113.38
41	37	302	A86	O1-C20-C19	52.71	152.98	113.38
41	37	316	A86	O1-C20-C19	52.62	152.91	113.38
41	32	318	A86	O1-C20-C19	52.60	152.90	113.38
41	12	319	A86	O1-C20-C19	52.59	152.89	113.38
41	17	316	A86	O1-C20-C19	52.59	152.88	113.38
41	15	314	A86	O1-C20-C19	52.55	152.86	113.38
41	31	314	A86	O1-C20-C19	52.52	152.84	113.38
41	33	317	A86	O1-C20-C19	52.52	152.84	113.38
41	13	317	A86	O1-C20-C19	52.51	152.83	113.38
41	11	314	A86	O1-C20-C19	52.49	152.81	113.38
41	35	314	A86	O1-C20-C19	52.45	152.78	113.38
41	16	313	A86	O1-C20-C19	52.44	152.78	113.38
41	13	315	A86	O1-C20-C19	52.43	152.77	113.38
41	32	319	A86	O1-C20-C19	52.42	152.76	113.38
41	36	313	A86	O1-C20-C19	52.40	152.74	113.38
41	37	312	A86	O1-C20-C19	52.04	152.47	113.38
41	32	315	A86	O1-C20-C19	52.01	152.45	113.38
41	34	312	A86	O1-C20-C19	52.01	152.45	113.38
41	17	312	A86	O1-C20-C19	52.00	152.44	113.38
41	14	312	A86	O1-C20-C19	51.99	152.44	113.38
41	18	314	A86	O1-C20-C19	51.96	152.42	113.38
41	12	316	A86	O1-C20-C19	51.94	152.40	113.38
41	36	311	A86	O1-C20-C19	51.93	152.39	113.38
41	11	311	A86	O1-C20-C19	51.92	152.39	113.38
41	33	313	A86	O1-C20-C19	51.92	152.38	113.38
41	13	312	A86	O1-C20-C19	51.91	152.38	113.38
41	31	311	A86	O1-C20-C19	51.90	152.37	113.38
41	38	314	A86	O1-C20-C19	51.90	152.37	113.38
41	16	311	A86	O1-C20-C19	51.84	152.33	113.38
41	35	311	A86	O1-C20-C19	51.83	152.31	113.38
41	15	311	A86	O1-C20-C19	51.82	152.31	113.38
41	20	201	A86	O1-C20-C19	51.63	152.17	113.38
41	40	201	A86	O1-C20-C19	51.58	152.13	113.38
41	40	213	A86	O1-C20-C19	51.57	152.12	113.38
41	20	213	A86	O1-C20-C19	51.53	152.09	113.38
41	21	314	A86	O1-C20-C19	51.51	152.08	113.38
41	41	314	A86	O1-C20-C19	51.49	152.06	113.38
41	19	309	A86	O1-C20-C19	50.71	151.47	113.38
41	11	312	A86	O1-C20-C19	50.69	151.46	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	39	309	A86	O1-C20-C19	50.66	151.44	113.38
41	31	312	A86	O1-C20-C19	50.65	151.43	113.38
41	15	312	A86	O1-C20-C19	50.64	151.42	113.38
41	17	313	A86	O1-C20-C19	50.60	151.40	113.38
41	35	312	A86	O1-C20-C19	50.58	151.38	113.38
41	36	312	A86	O1-C20-C19	50.58	151.38	113.38
41	13	313	A86	O1-C20-C19	50.57	151.37	113.38
41	14	313	A86	O1-C20-C19	50.57	151.37	113.38
41	32	316	A86	O1-C20-C19	50.56	151.36	113.38
41	16	312	A86	O1-C20-C19	50.56	151.36	113.38
41	37	313	A86	O1-C20-C19	50.54	151.35	113.38
41	12	317	A86	O1-C20-C19	50.52	151.34	113.38
41	33	314	A86	O1-C20-C19	50.51	151.32	113.38
41	34	313	A86	O1-C20-C19	50.49	151.31	113.38
41	21	311	A86	O1-C20-C19	49.09	150.26	113.38
41	41	311	A86	O1-C20-C19	49.09	150.26	113.38
41	40	211	A86	O1-C20-C19	49.05	150.23	113.38
41	20	211	A86	O1-C20-C19	48.95	150.16	113.38
41	41	313	A86	O1-C20-C19	48.90	150.11	113.38
41	21	313	A86	O1-C20-C19	48.86	150.09	113.38
41	21	310	A86	O1-C20-C19	48.59	149.89	113.38
41	41	310	A86	O1-C20-C19	48.58	149.88	113.38
41	38	302	A86	O1-C20-C19	48.03	149.46	113.38
41	11	316	A86	O1-C20-C19	48.02	149.45	113.38
41	12	304	A86	O1-C20-C19	48.01	149.45	113.38
41	15	315	A86	O1-C20-C19	47.99	149.43	113.38
41	32	304	A86	O1-C20-C19	47.98	149.43	113.38
41	13	301	A86	O1-C20-C19	47.97	149.42	113.38
41	15	316	A86	O1-C20-C19	47.97	149.42	113.38
41	33	302	A86	O1-C20-C19	47.97	149.41	113.38
41	33	316	A86	O1-C20-C19	47.96	149.41	113.38
41	18	302	A86	O1-C20-C19	47.96	149.41	113.38
41	31	316	A86	O1-C20-C19	47.95	149.41	113.38
41	13	316	A86	O1-C20-C19	47.93	149.39	113.38
41	35	316	A86	O1-C20-C19	47.93	149.39	113.38
41	35	315	A86	O1-C20-C19	47.91	149.38	113.38
41	19	310	A86	O1-C20-C19	46.13	148.03	113.38
41	39	310	A86	O1-C20-C19	46.12	148.03	113.38
41	41	312	A86	O1-C20-C19	45.26	147.38	113.38
41	21	312	A86	O1-C20-C19	45.24	147.37	113.38
41	12	304	A86	C17-C16-C15	11.89	121.30	109.16
41	33	302	A86	C17-C16-C15	11.87	121.27	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	38	302	A86	C17-C16-C15	11.87	121.27	109.16
41	32	304	A86	C17-C16-C15	11.86	121.27	109.16
41	11	316	A86	C17-C16-C15	11.86	121.26	109.16
41	35	315	A86	C17-C16-C15	11.86	121.26	109.16
41	15	315	A86	C17-C16-C15	11.85	121.25	109.16
41	18	302	A86	C17-C16-C15	11.84	121.24	109.16
41	13	316	A86	C17-C16-C15	11.84	121.24	109.16
41	31	316	A86	C17-C16-C15	11.83	121.23	109.16
41	13	301	A86	C17-C16-C15	11.83	121.23	109.16
41	33	316	A86	C17-C16-C15	11.81	121.21	109.16
41	35	316	A86	C17-C16-C15	11.79	121.19	109.16
41	15	316	A86	C17-C16-C15	11.77	121.17	109.16
41	17	315	A86	C21-C20-C19	-11.52	101.32	114.28
41	37	315	A86	C21-C20-C19	-11.49	101.36	114.28
41	40	210	A86	O1-C20-C21	-11.37	101.43	115.06
41	20	210	A86	O1-C20-C21	-11.33	101.48	115.06
41	31	313	A86	O1-C20-C21	-11.27	101.56	115.06
41	17	314	A86	O1-C20-C21	-11.26	101.56	115.06
41	37	314	A86	O1-C20-C21	-11.25	101.57	115.06
41	35	313	A86	O1-C20-C21	-11.25	101.58	115.06
41	38	315	A86	O1-C20-C21	-11.25	101.58	115.06
41	15	313	A86	O1-C20-C21	-11.24	101.59	115.06
41	11	313	A86	O1-C20-C21	-11.23	101.59	115.06
41	18	315	A86	O1-C20-C21	-11.23	101.59	115.06
41	32	317	A86	O1-C20-C21	-11.23	101.60	115.06
41	12	318	A86	O1-C20-C21	-11.21	101.62	115.06
41	17	311	A86	O1-C20-C21	-11.20	101.63	115.06
41	33	315	A86	O1-C20-C21	-11.20	101.64	115.06
41	34	314	A86	O1-C20-C21	-11.20	101.64	115.06
41	13	314	A86	O1-C20-C21	-11.19	101.64	115.06
41	14	314	A86	O1-C20-C21	-11.19	101.65	115.06
41	37	311	A86	O1-C20-C21	-11.16	101.68	115.06
41	37	315	A86	O1-C20-C21	-11.06	101.81	115.06
41	17	315	A86	O1-C20-C21	-11.04	101.83	115.06
41	40	212	A86	O1-C20-C21	-10.97	101.91	115.06
41	20	212	A86	O1-C20-C21	-10.96	101.93	115.06
41	18	313	A86	O1-C20-C21	-10.93	101.95	115.06
41	38	313	A86	O1-C20-C21	-10.93	101.95	115.06
41	12	315	A86	O1-C20-C21	-10.93	101.96	115.06
41	34	311	A86	O1-C20-C21	-10.92	101.97	115.06
41	17	316	A86	C21-C20-C19	-10.91	102.01	114.28
41	37	316	A86	C21-C20-C19	-10.91	102.01	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	11	310	A86	O1-C20-C21	-10.90	101.99	115.06
41	31	310	A86	O1-C20-C21	-10.90	101.99	115.06
41	13	311	A86	O1-C20-C21	-10.89	102.01	115.06
41	17	302	A86	C21-C20-C19	-10.88	102.03	114.28
41	14	311	A86	O1-C20-C21	-10.88	102.02	115.06
41	32	318	A86	C21-C20-C19	-10.88	102.04	114.28
41	12	319	A86	C21-C20-C19	-10.87	102.05	114.28
41	32	314	A86	O1-C20-C21	-10.87	102.03	115.06
41	16	313	A86	C21-C20-C19	-10.87	102.06	114.28
41	33	317	A86	C21-C20-C19	-10.86	102.06	114.28
41	13	317	A86	C21-C20-C19	-10.86	102.07	114.28
41	16	310	A86	O1-C20-C21	-10.85	102.06	115.06
41	35	310	A86	O1-C20-C21	-10.85	102.06	115.06
41	32	319	A86	C21-C20-C19	-10.84	102.08	114.28
41	33	312	A86	O1-C20-C21	-10.84	102.07	115.06
41	13	315	A86	C21-C20-C19	-10.84	102.08	114.28
41	36	313	A86	C21-C20-C19	-10.84	102.08	114.28
41	15	310	A86	O1-C20-C21	-10.83	102.07	115.06
41	15	314	A86	C21-C20-C19	-10.83	102.10	114.28
41	11	314	A86	C21-C20-C19	-10.82	102.10	114.28
41	37	302	A86	C21-C20-C19	-10.82	102.11	114.28
41	31	314	A86	C21-C20-C19	-10.82	102.11	114.28
41	36	310	A86	O1-C20-C21	-10.81	102.10	115.06
41	35	314	A86	C21-C20-C19	-10.80	102.13	114.28
41	19	309	A86	C21-C20-C19	-10.73	102.21	114.28
41	39	309	A86	C21-C20-C19	-10.71	102.24	114.28
41	15	310	A86	C21-C20-C19	-10.64	102.31	114.28
41	35	310	A86	C21-C20-C19	-10.64	102.31	114.28
41	33	312	A86	C21-C20-C19	-10.63	102.32	114.28
41	37	311	A86	C21-C20-C19	-10.62	102.33	114.28
41	32	314	A86	C21-C20-C19	-10.60	102.36	114.28
41	17	311	A86	C21-C20-C19	-10.59	102.36	114.28
41	11	310	A86	C21-C20-C19	-10.59	102.37	114.28
41	18	313	A86	C21-C20-C19	-10.58	102.38	114.28
41	38	313	A86	C21-C20-C19	-10.57	102.39	114.28
41	14	311	A86	C21-C20-C19	-10.57	102.39	114.28
41	11	312	A86	C21-C20-C19	-10.57	102.39	114.28
41	12	315	A86	C21-C20-C19	-10.56	102.40	114.28
41	34	311	A86	C21-C20-C19	-10.56	102.40	114.28
41	35	312	A86	C21-C20-C19	-10.56	102.40	114.28
41	13	313	A86	C21-C20-C19	-10.56	102.40	114.28
41	20	212	A86	C36-C31-C32	-10.56	109.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	13	311	A86	C21-C20-C19	-10.55	102.41	114.28
41	31	310	A86	C21-C20-C19	-10.55	102.41	114.28
41	15	312	A86	C21-C20-C19	-10.55	102.41	114.28
41	17	313	A86	C21-C20-C19	-10.54	102.42	114.28
41	40	212	A86	C36-C31-C32	-10.53	109.25	119.70
41	16	312	A86	C21-C20-C19	-10.52	102.45	114.28
41	36	312	A86	C21-C20-C19	-10.51	102.45	114.28
41	37	313	A86	C21-C20-C19	-10.51	102.45	114.28
41	31	312	A86	C21-C20-C19	-10.51	102.46	114.28
41	34	313	A86	C21-C20-C19	-10.51	102.46	114.28
41	33	314	A86	C21-C20-C19	-10.50	102.47	114.28
41	14	313	A86	C21-C20-C19	-10.49	102.48	114.28
41	32	316	A86	C21-C20-C19	-10.47	102.50	114.28
41	12	317	A86	C21-C20-C19	-10.46	102.51	114.28
41	19	311	A86	O1-C20-C21	-10.36	102.64	115.06
41	39	311	A86	O1-C20-C21	-10.34	102.67	115.06
41	39	311	A86	C21-C20-C19	-10.31	102.69	114.28
41	19	311	A86	C21-C20-C19	-10.28	102.72	114.28
41	15	315	A86	C21-C20-C19	-10.17	102.83	114.28
41	32	304	A86	C21-C20-C19	-10.15	102.86	114.28
41	33	316	A86	C21-C20-C19	-10.15	102.86	114.28
41	34	312	A86	O1-C20-C21	-10.15	102.90	115.06
41	37	312	A86	O1-C20-C21	-10.15	102.90	115.06
41	38	314	A86	O1-C20-C21	-10.14	102.90	115.06
41	13	301	A86	C21-C20-C19	-10.14	102.87	114.28
41	20	210	A86	C21-C20-C19	-10.14	102.87	114.28
41	13	316	A86	C21-C20-C19	-10.13	102.88	114.28
41	18	314	A86	O1-C20-C21	-10.13	102.92	115.06
41	32	315	A86	O1-C20-C21	-10.13	102.92	115.06
41	40	210	A86	C21-C20-C19	-10.13	102.89	114.28
41	35	315	A86	C21-C20-C19	-10.12	102.89	114.28
41	12	304	A86	C21-C20-C19	-10.12	102.89	114.28
41	36	311	A86	O1-C20-C21	-10.12	102.94	115.06
41	12	316	A86	O1-C20-C21	-10.11	102.94	115.06
41	11	316	A86	C21-C20-C19	-10.11	102.90	114.28
41	13	312	A86	O1-C20-C21	-10.11	102.94	115.06
41	33	302	A86	C21-C20-C19	-10.11	102.91	114.28
41	31	316	A86	C21-C20-C19	-10.10	102.92	114.28
41	33	313	A86	O1-C20-C21	-10.10	102.96	115.06
41	14	312	A86	O1-C20-C21	-10.09	102.97	115.06
41	18	302	A86	C21-C20-C19	-10.09	102.93	114.28
41	17	312	A86	O1-C20-C21	-10.08	102.97	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	16	311	A86	O1-C20-C21	-10.08	102.98	115.06
41	38	302	A86	C21-C20-C19	-10.08	102.94	114.28
41	20	212	A86	C21-C20-C19	-10.07	102.95	114.28
41	35	316	A86	C21-C20-C19	-10.07	102.95	114.28
41	15	316	A86	C21-C20-C19	-10.07	102.95	114.28
41	11	311	A86	O1-C20-C21	-10.06	103.00	115.06
41	31	311	A86	O1-C20-C21	-10.06	103.01	115.06
41	40	212	A86	C21-C20-C19	-10.05	102.97	114.28
41	15	311	A86	O1-C20-C21	-10.03	103.04	115.06
41	35	311	A86	O1-C20-C21	-10.02	103.05	115.06
41	40	213	A86	O1-C20-C21	-10.02	103.06	115.06
41	41	314	A86	O1-C20-C21	-9.97	103.11	115.06
41	21	314	A86	O1-C20-C21	-9.97	103.11	115.06
41	20	213	A86	O1-C20-C21	-9.96	103.12	115.06
30	B	612	CLA	C4A-NA-C1A	9.96	111.18	106.71
41	19	310	A86	C36-C31-C32	-9.94	109.84	119.70
41	34	314	A86	C21-C20-C19	-9.91	103.13	114.28
41	14	314	A86	C21-C20-C19	-9.91	103.13	114.28
41	17	312	A86	C21-C20-C19	-9.89	103.15	114.28
41	33	315	A86	C21-C20-C19	-9.89	103.15	114.28
30	b	612	CLA	C4A-NA-C1A	9.89	111.15	106.71
41	12	318	A86	C21-C20-C19	-9.88	103.16	114.28
41	14	312	A86	C21-C20-C19	-9.88	103.16	114.28
41	11	311	A86	C21-C20-C19	-9.88	103.16	114.28
41	37	312	A86	C21-C20-C19	-9.87	103.17	114.28
41	39	310	A86	C36-C31-C32	-9.87	109.90	119.70
41	13	314	A86	C21-C20-C19	-9.87	103.18	114.28
41	32	315	A86	C21-C20-C19	-9.87	103.18	114.28
41	32	317	A86	C21-C20-C19	-9.87	103.18	114.28
41	38	315	A86	C21-C20-C19	-9.86	103.18	114.28
41	31	311	A86	C21-C20-C19	-9.86	103.19	114.28
41	34	312	A86	C21-C20-C19	-9.86	103.19	114.28
41	31	313	A86	C21-C20-C19	-9.85	103.19	114.28
41	17	314	A86	C21-C20-C19	-9.85	103.19	114.28
41	35	311	A86	C21-C20-C19	-9.85	103.20	114.28
41	15	311	A86	C21-C20-C19	-9.85	103.20	114.28
41	18	315	A86	C21-C20-C19	-9.84	103.21	114.28
41	15	313	A86	C21-C20-C19	-9.83	103.22	114.28
41	35	313	A86	C21-C20-C19	-9.83	103.22	114.28
41	11	313	A86	C21-C20-C19	-9.83	103.22	114.28
41	33	313	A86	C21-C20-C19	-9.83	103.22	114.28
41	18	314	A86	C21-C20-C19	-9.82	103.23	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	13	312	A86	C21-C20-C19	-9.82	103.23	114.28
41	37	314	A86	C21-C20-C19	-9.82	103.23	114.28
41	12	316	A86	C21-C20-C19	-9.81	103.24	114.28
41	36	310	A86	C21-C20-C19	-9.81	103.24	114.28
41	36	311	A86	C21-C20-C19	-9.81	103.25	114.28
41	16	311	A86	C21-C20-C19	-9.80	103.26	114.28
41	16	310	A86	C21-C20-C19	-9.79	103.27	114.28
41	40	201	A86	C21-C20-C19	-9.78	103.28	114.28
41	38	314	A86	C21-C20-C19	-9.78	103.28	114.28
41	20	201	A86	C21-C20-C19	-9.76	103.30	114.28
41	37	302	A86	O1-C20-C21	-9.70	103.44	115.06
41	17	302	A86	O1-C20-C21	-9.65	103.49	115.06
41	20	213	A86	C21-C20-C19	-9.65	103.43	114.28
41	40	213	A86	C21-C20-C19	-9.61	103.47	114.28
41	21	314	A86	C21-C20-C19	-9.60	103.48	114.28
41	41	314	A86	C21-C20-C19	-9.59	103.50	114.28
41	21	310	A86	C21-C20-C19	-9.52	103.57	114.28
41	41	310	A86	C21-C20-C19	-9.52	103.58	114.28
41	17	315	A86	C36-C31-C32	-9.45	110.32	119.70
41	37	315	A86	C36-C31-C32	-9.43	110.34	119.70
41	20	201	A86	O1-C20-C21	-9.42	103.76	115.06
41	32	318	A86	O1-C20-C21	-9.41	103.78	115.06
41	15	314	A86	O1-C20-C21	-9.40	103.79	115.06
41	12	319	A86	O1-C20-C21	-9.40	103.79	115.06
41	31	314	A86	O1-C20-C21	-9.39	103.81	115.06
41	33	317	A86	O1-C20-C21	-9.38	103.82	115.06
41	35	314	A86	O1-C20-C21	-9.37	103.83	115.06
41	40	201	A86	O1-C20-C21	-9.37	103.83	115.06
41	11	314	A86	O1-C20-C21	-9.37	103.83	115.06
41	13	317	A86	O1-C20-C21	-9.35	103.85	115.06
41	37	316	A86	O1-C20-C21	-9.35	103.85	115.06
41	17	316	A86	O1-C20-C21	-9.34	103.87	115.06
41	32	319	A86	O1-C20-C21	-9.31	103.90	115.06
41	16	313	A86	O1-C20-C21	-9.31	103.91	115.06
41	36	313	A86	O1-C20-C21	-9.30	103.91	115.06
41	39	311	A86	C36-C31-C32	-9.30	110.47	119.70
41	21	311	A86	O1-C20-C21	-9.30	103.92	115.06
41	13	315	A86	O1-C20-C21	-9.30	103.92	115.06
41	19	311	A86	C36-C31-C32	-9.29	110.48	119.70
41	41	311	A86	O1-C20-C21	-9.28	103.94	115.06
41	40	211	A86	O1-C20-C21	-9.25	103.98	115.06
41	41	313	A86	C21-C20-C19	-9.24	103.88	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	20	211	A86	O1-C20-C21	-9.22	104.00	115.06
41	21	313	A86	C21-C20-C19	-9.22	103.91	114.28
41	41	311	A86	C21-C20-C19	-9.17	103.96	114.28
41	40	211	A86	C21-C20-C19	-9.17	103.97	114.28
41	21	314	A86	C36-C31-C32	-9.16	110.60	119.70
41	40	213	A86	C36-C31-C32	-9.16	110.61	119.70
41	21	311	A86	C21-C20-C19	-9.15	103.98	114.28
41	19	309	A86	O1-C20-C21	-9.15	104.09	115.06
41	20	211	A86	C21-C20-C19	-9.13	104.01	114.28
30	14	302	CLA	C4A-NA-C1A	9.13	110.81	106.71
41	20	213	A86	C36-C31-C32	-9.13	110.64	119.70
41	39	309	A86	O1-C20-C21	-9.13	104.12	115.06
41	37	302	A86	C36-C31-C32	-9.13	110.64	119.70
41	41	314	A86	C36-C31-C32	-9.12	110.64	119.70
41	17	302	A86	C36-C31-C32	-9.12	110.65	119.70
41	12	304	A86	C33-C32-C31	9.12	118.07	109.21
41	32	304	A86	C33-C32-C31	9.08	118.04	109.21
30	13	302	CLA	C4A-NA-C1A	9.07	110.78	106.71
41	15	315	A86	C33-C32-C31	9.06	118.02	109.21
41	13	316	A86	C33-C32-C31	9.04	118.00	109.21
30	33	303	CLA	C4A-NA-C1A	9.04	110.77	106.71
41	35	315	A86	C33-C32-C31	9.04	117.99	109.21
41	39	310	A86	C21-C20-C19	-9.03	104.12	114.28
41	15	316	A86	C33-C32-C31	9.03	117.98	109.21
30	36	302	CLA	C4A-NA-C1A	9.02	110.76	106.71
41	35	316	A86	C33-C32-C31	9.01	117.97	109.21
41	19	310	A86	C21-C20-C19	-9.01	104.14	114.28
30	11	301	CLA	C4A-NA-C1A	9.00	110.75	106.71
41	21	313	A86	O1-C20-C21	-9.00	104.27	115.06
41	41	313	A86	O1-C20-C21	-9.00	104.27	115.06
41	33	316	A86	C33-C32-C31	9.00	117.96	109.21
41	13	301	A86	C33-C32-C31	9.00	117.96	109.21
41	38	302	A86	C33-C32-C31	8.99	117.95	109.21
41	18	302	A86	C33-C32-C31	8.99	117.95	109.21
41	11	316	A86	C33-C32-C31	8.98	117.94	109.21
30	16	302	CLA	C4A-NA-C1A	8.98	110.74	106.71
30	12	305	CLA	C4A-NA-C1A	8.96	110.73	106.71
41	31	316	A86	C33-C32-C31	8.95	117.91	109.21
41	33	302	A86	C33-C32-C31	8.95	117.91	109.21
30	34	302	CLA	C4A-NA-C1A	8.94	110.72	106.71
30	c	510	CLA	C4A-NA-C1A	8.93	110.72	106.71
41	31	312	A86	O1-C20-C21	-8.89	104.40	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	36	312	A86	O1-C20-C21	-8.88	104.42	115.06
30	31	301	CLA	C4A-NA-C1A	8.88	110.70	106.71
30	32	305	CLA	C4A-NA-C1A	8.87	110.69	106.71
41	16	312	A86	O1-C20-C21	-8.87	104.43	115.06
41	14	313	A86	O1-C20-C21	-8.86	104.44	115.06
41	11	312	A86	O1-C20-C21	-8.85	104.45	115.06
41	32	316	A86	O1-C20-C21	-8.85	104.45	115.06
41	12	317	A86	O1-C20-C21	-8.85	104.45	115.06
41	15	312	A86	O1-C20-C21	-8.84	104.47	115.06
41	37	313	A86	O1-C20-C21	-8.82	104.48	115.06
41	17	313	A86	O1-C20-C21	-8.82	104.49	115.06
41	33	314	A86	O1-C20-C21	-8.81	104.50	115.06
41	34	313	A86	O1-C20-C21	-8.80	104.52	115.06
41	35	312	A86	O1-C20-C21	-8.79	104.52	115.06
41	13	313	A86	O1-C20-C21	-8.79	104.52	115.06
30	C	510	CLA	C4A-NA-C1A	8.76	110.64	106.71
41	21	310	A86	O1-C20-C21	-8.71	104.61	115.06
41	41	310	A86	O1-C20-C21	-8.69	104.64	115.06
41	13	313	A86	C33-C32-C31	8.62	117.59	109.21
41	37	313	A86	C33-C32-C31	8.59	117.56	109.21
30	C	521	CLA	C4A-NA-C1A	8.57	110.56	106.71
41	34	313	A86	C33-C32-C31	8.57	117.54	109.21
41	17	313	A86	C33-C32-C31	8.56	117.53	109.21
41	33	314	A86	C33-C32-C31	8.56	117.53	109.21
41	14	313	A86	C33-C32-C31	8.54	117.51	109.21
41	15	312	A86	C33-C32-C31	8.53	117.50	109.21
41	21	312	A86	C17-C16-C15	8.53	117.86	109.16
41	41	312	A86	C17-C16-C15	8.53	117.86	109.16
41	32	316	A86	C33-C32-C31	8.52	117.49	109.21
41	36	312	A86	C33-C32-C31	8.51	117.48	109.21
41	12	317	A86	C33-C32-C31	8.51	117.48	109.21
41	31	312	A86	C33-C32-C31	8.49	117.46	109.21
41	16	312	A86	C33-C32-C31	8.48	117.45	109.21
30	c	523	CLA	C4A-NA-C1A	8.48	110.52	106.71
41	35	312	A86	C33-C32-C31	8.46	117.44	109.21
30	17	303	CLA	C4A-NA-C1A	8.44	110.50	106.71
41	11	312	A86	C33-C32-C31	8.44	117.42	109.21
30	c	505	CLA	C4A-NA-C1A	8.41	110.49	106.71
41	40	201	A86	C36-C31-C32	-8.41	111.35	119.70
30	37	303	CLA	C4A-NA-C1A	8.39	110.48	106.71
41	33	316	A86	C4-C5-C6	-8.38	115.35	127.31
41	12	304	A86	C4-C5-C6	-8.37	115.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	20	201	A86	C36-C31-C32	-8.37	111.39	119.70
41	33	302	A86	C4-C5-C6	-8.36	115.38	127.31
41	35	315	A86	C4-C5-C6	-8.36	115.38	127.31
41	13	301	A86	C4-C5-C6	-8.36	115.38	127.31
41	13	316	A86	C4-C5-C6	-8.36	115.38	127.31
41	15	315	A86	C4-C5-C6	-8.35	115.39	127.31
30	35	302	CLA	C4A-NA-C1A	8.35	110.46	106.71
41	11	312	A86	C17-C16-C15	8.34	117.67	109.16
41	32	304	A86	C4-C5-C6	-8.34	115.41	127.31
41	35	316	A86	C4-C5-C6	-8.34	115.41	127.31
41	15	316	A86	C4-C5-C6	-8.33	115.42	127.31
41	11	316	A86	C4-C5-C6	-8.33	115.43	127.31
41	15	312	A86	C17-C16-C15	8.32	117.66	109.16
41	18	302	A86	C4-C5-C6	-8.32	115.44	127.31
30	15	302	CLA	C4A-NA-C1A	8.32	110.45	106.71
41	38	302	A86	C4-C5-C6	-8.32	115.44	127.31
41	31	316	A86	C4-C5-C6	-8.31	115.45	127.31
41	35	312	A86	C17-C16-C15	8.30	117.63	109.16
41	34	313	A86	C17-C16-C15	8.30	117.63	109.16
41	31	312	A86	C17-C16-C15	8.29	117.62	109.16
41	14	313	A86	C17-C16-C15	8.28	117.61	109.16
30	D	406	CLA	C4A-NA-C1A	8.27	110.43	106.71
41	37	302	A86	C4-C5-C6	-8.27	115.50	127.31
41	37	313	A86	C17-C16-C15	8.27	117.60	109.16
41	12	317	A86	C17-C16-C15	8.27	117.60	109.16
41	17	302	A86	C4-C5-C6	-8.27	115.51	127.31
41	16	312	A86	C17-C16-C15	8.24	117.57	109.16
30	32	310	CLA	C4A-NA-C1A	8.24	110.41	106.71
41	17	313	A86	C17-C16-C15	8.24	117.57	109.16
30	A	402	CLA	C4A-NA-C1A	8.23	110.41	106.71
30	13	307	CLA	C4A-NA-C1A	8.23	110.40	106.71
41	33	314	A86	C17-C16-C15	8.22	117.54	109.16
41	36	312	A86	C17-C16-C15	8.21	117.54	109.16
41	32	316	A86	C17-C16-C15	8.20	117.53	109.16
41	13	313	A86	C17-C16-C15	8.19	117.52	109.16
30	33	308	CLA	C4A-NA-C1A	8.19	110.39	106.71
30	C	505	CLA	C4A-NA-C1A	8.18	110.38	106.71
30	31	306	CLA	C4A-NA-C1A	8.18	110.38	106.71
30	11	306	CLA	C4A-NA-C1A	8.17	110.38	106.71
30	d	407	CLA	C4A-NA-C1A	8.16	110.38	106.71
30	15	301	CLA	C4A-NA-C1A	8.16	110.38	106.71
30	39	303	CLA	C4A-NA-C1A	8.15	110.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	609	CLA	C4A-NA-C1A	8.14	110.36	106.71
30	19	303	CLA	C4A-NA-C1A	8.14	110.36	106.71
30	34	307	CLA	C4A-NA-C1A	8.12	110.36	106.71
30	35	301	CLA	C4A-NA-C1A	8.09	110.34	106.71
30	14	307	CLA	C4A-NA-C1A	8.08	110.34	106.71
41	21	313	A86	C36-C31-C32	-8.08	111.68	119.70
41	41	313	A86	C36-C31-C32	-8.05	111.70	119.70
30	12	310	CLA	C4A-NA-C1A	8.03	110.31	106.71
30	C	502	CLA	C4A-NA-C1A	7.99	110.30	106.71
30	36	306	CLA	C4A-NA-C1A	7.99	110.30	106.71
41	41	312	A86	O1-C20-C21	-7.99	105.49	115.06
41	21	312	A86	C21-C20-C19	-7.98	105.30	114.28
41	21	312	A86	O1-C20-C21	-7.98	105.50	115.06
41	41	312	A86	C21-C20-C19	-7.97	105.31	114.28
41	41	311	A86	C36-C31-C32	-7.96	111.80	119.70
41	20	211	A86	C36-C31-C32	-7.95	111.81	119.70
41	40	211	A86	C36-C31-C32	-7.95	111.81	119.70
41	21	311	A86	C36-C31-C32	-7.94	111.82	119.70
30	16	306	CLA	C4A-NA-C1A	7.93	110.27	106.71
30	B	609	CLA	C4A-NA-C1A	7.93	110.27	106.71
30	38	304	CLA	C4A-NA-C1A	7.92	110.27	106.71
41	11	310	A86	C33-C32-C31	7.92	116.91	109.21
41	31	310	A86	C33-C32-C31	7.92	116.90	109.21
30	15	307	CLA	C4A-NA-C1A	7.91	110.26	106.71
30	a	402	CLA	C4A-NA-C1A	7.91	110.26	106.71
41	33	312	A86	C33-C32-C31	7.90	116.89	109.21
41	13	311	A86	C33-C32-C31	7.89	116.88	109.21
41	35	310	A86	C33-C32-C31	7.88	116.87	109.21
30	c	502	CLA	C4A-NA-C1A	7.87	110.24	106.71
41	15	310	A86	C33-C32-C31	7.85	116.84	109.21
30	C	514	CLA	C4A-NA-C1A	7.84	110.23	106.71
41	14	311	A86	C33-C32-C31	7.84	116.83	109.21
30	35	307	CLA	C4A-NA-C1A	7.83	110.23	106.71
30	15	306	CLA	C4A-NA-C1A	7.83	110.23	106.71
30	36	303	CLA	C4A-NA-C1A	7.83	110.22	106.71
30	35	306	CLA	C4A-NA-C1A	7.82	110.22	106.71
30	18	304	CLA	C4A-NA-C1A	7.81	110.22	106.71
41	34	311	A86	C33-C32-C31	7.81	116.80	109.21
30	c	514	CLA	C4A-NA-C1A	7.80	110.21	106.71
41	38	313	A86	C33-C32-C31	7.79	116.78	109.21
30	20	206	CLA	C4A-NA-C1A	7.79	110.21	106.71
30	16	303	CLA	C4A-NA-C1A	7.79	110.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	18	313	A86	C33-C32-C31	7.78	116.78	109.21
41	12	315	A86	C33-C32-C31	7.77	116.76	109.21
41	32	314	A86	C33-C32-C31	7.77	116.76	109.21
30	14	304	CLA	C4A-NA-C1A	7.77	110.20	106.71
30	33	305	CLA	C4A-NA-C1A	7.76	110.20	106.71
41	41	312	A86	C33-C32-C31	7.76	116.75	109.21
41	21	312	A86	C33-C32-C31	7.74	116.74	109.21
30	18	311	CLA	C4A-NA-C1A	7.74	110.19	106.71
30	38	305	CLA	C4A-NA-C1A	7.74	110.19	106.71
30	32	307	CLA	C4A-NA-C1A	7.73	110.18	106.71
30	11	303	CLA	C4A-NA-C1A	7.73	110.18	106.71
30	b	601	CLA	C4A-NA-C1A	7.72	110.18	106.71
30	C	504	CLA	C4A-NA-C1A	7.72	110.18	106.71
30	39	307	CLA	C4A-NA-C1A	7.70	110.17	106.71
41	20	201	A86	C17-C16-C15	7.67	116.99	109.16
30	37	305	CLA	C4A-NA-C1A	7.66	110.15	106.71
41	40	201	A86	C17-C16-C15	7.65	116.97	109.16
30	12	307	CLA	C4A-NA-C1A	7.65	110.14	106.71
30	19	307	CLA	C4A-NA-C1A	7.63	110.14	106.71
30	38	311	CLA	C4A-NA-C1A	7.63	110.14	106.71
30	40	206	CLA	C4A-NA-C1A	7.63	110.14	106.71
30	17	305	CLA	C4A-NA-C1A	7.61	110.13	106.71
30	B	601	CLA	C4A-NA-C1A	7.60	110.12	106.71
30	b	613	CLA	C4A-NA-C1A	7.60	110.12	106.71
30	14	305	CLA	C4A-NA-C1A	7.59	110.12	106.71
30	13	304	CLA	C4A-NA-C1A	7.58	110.11	106.71
41	17	315	A86	C4-C5-C6	-7.57	116.50	127.31
41	37	315	A86	C4-C5-C6	-7.57	116.50	127.31
30	20	204	CLA	C4A-NA-C1A	7.55	110.10	106.71
30	C	512	CLA	C4A-NA-C1A	7.54	110.09	106.71
30	b	608	CLA	C4A-NA-C1A	7.54	110.09	106.71
30	13	303	CLA	C4A-NA-C1A	7.53	110.09	106.71
30	14	303	CLA	C4A-NA-C1A	7.53	110.09	106.71
30	34	304	CLA	C4A-NA-C1A	7.53	110.09	106.71
30	37	301	CLA	C4A-NA-C1A	7.52	110.09	106.71
30	15	303	CLA	C4A-NA-C1A	7.51	110.08	106.71
30	17	301	CLA	C4A-NA-C1A	7.51	110.08	106.71
30	31	302	CLA	C4A-NA-C1A	7.51	110.08	106.71
30	33	307	CLA	C4A-NA-C1A	7.50	110.08	106.71
30	18	305	CLA	C4A-NA-C1A	7.50	110.08	106.71
30	c	504	CLA	C4A-NA-C1A	7.49	110.07	106.71
30	31	303	CLA	C4A-NA-C1A	7.47	110.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	34	303	CLA	C4A-NA-C1A	7.47	110.06	106.71
41	19	310	A86	O1-C20-C21	-7.47	106.11	115.06
30	35	303	CLA	C4A-NA-C1A	7.44	110.05	106.71
41	39	310	A86	O1-C20-C21	-7.44	106.14	115.06
30	33	304	CLA	C4A-NA-C1A	7.44	110.05	106.71
30	40	204	CLA	C4A-NA-C1A	7.43	110.05	106.71
30	32	306	CLA	C4A-NA-C1A	7.43	110.05	106.71
41	31	314	A86	C17-C16-C15	7.43	116.74	109.16
30	B	603	CLA	C4A-NA-C1A	7.42	110.04	106.71
30	11	302	CLA	C4A-NA-C1A	7.42	110.04	106.71
41	11	314	A86	C17-C16-C15	7.41	116.72	109.16
41	12	319	A86	C17-C16-C15	7.41	116.72	109.16
30	18	308	CLA	C4A-NA-C1A	7.40	110.03	106.71
30	12	306	CLA	C4A-NA-C1A	7.40	110.03	106.71
41	32	319	A86	C17-C16-C15	7.39	116.71	109.16
30	38	308	CLA	C4A-NA-C1A	7.39	110.03	106.71
41	38	302	A86	O1-C20-C21	-7.39	106.21	115.06
30	b	603	CLA	C4A-NA-C1A	7.38	110.03	106.71
41	15	316	A86	O1-C20-C21	-7.38	106.22	115.06
41	13	315	A86	C17-C16-C15	7.37	116.69	109.16
41	13	317	A86	C17-C16-C15	7.37	116.68	109.16
41	32	318	A86	C17-C16-C15	7.37	116.68	109.16
30	B	608	CLA	C4A-NA-C1A	7.36	110.02	106.71
30	11	305	CLA	C4A-NA-C1A	7.36	110.02	106.71
30	38	309	CLA	C4A-NA-C1A	7.36	110.02	106.71
41	11	316	A86	O1-C20-C21	-7.36	106.24	115.06
41	33	317	A86	C17-C16-C15	7.36	116.67	109.16
41	12	304	A86	O1-C20-C21	-7.35	106.25	115.06
30	20	203	CLA	C4A-NA-C1A	7.35	110.01	106.71
41	16	313	A86	C17-C16-C15	7.34	116.65	109.16
41	33	302	A86	O1-C20-C21	-7.34	106.26	115.06
41	35	314	A86	C17-C16-C15	7.34	116.65	109.16
41	37	316	A86	C17-C16-C15	7.34	116.65	109.16
41	36	313	A86	C17-C16-C15	7.34	116.65	109.16
30	b	611	CLA	C4A-NA-C1A	7.33	110.00	106.71
41	18	302	A86	O1-C20-C21	-7.33	106.27	115.06
41	35	316	A86	O1-C20-C21	-7.33	106.27	115.06
30	40	203	CLA	C4A-NA-C1A	7.33	110.00	106.71
30	B	607	CLA	C4A-NA-C1A	7.33	110.00	106.71
41	15	314	A86	C17-C16-C15	7.32	116.63	109.16
30	33	306	CLA	C4A-NA-C1A	7.32	110.00	106.71
41	31	316	A86	O1-C20-C21	-7.32	106.28	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	16	311	A86	C33-C32-C31	7.31	116.32	109.21
30	z	101	CLA	C4A-NA-C1A	7.31	109.99	106.71
41	36	311	A86	C33-C32-C31	7.30	116.31	109.21
30	12	308	CLA	C4A-NA-C1A	7.30	109.99	106.71
30	C	509	CLA	C4A-NA-C1A	7.30	109.99	106.71
41	13	301	A86	O1-C20-C21	-7.30	106.31	115.06
41	32	304	A86	O1-C20-C21	-7.29	106.32	115.06
41	33	316	A86	O1-C20-C21	-7.29	106.32	115.06
30	18	309	CLA	C4A-NA-C1A	7.29	109.98	106.71
30	21	307	CLA	C4A-NA-C1A	7.29	109.98	106.71
41	13	316	A86	O1-C20-C21	-7.29	106.32	115.06
30	B	613	CLA	C4A-NA-C1A	7.28	109.98	106.71
41	13	312	A86	C33-C32-C31	7.28	116.29	109.21
41	15	315	A86	O1-C20-C21	-7.28	106.33	115.06
41	35	315	A86	O1-C20-C21	-7.28	106.34	115.06
41	14	312	A86	C33-C32-C31	7.27	116.28	109.21
41	17	316	A86	C17-C16-C15	7.27	116.58	109.16
30	B	611	CLA	C4A-NA-C1A	7.27	109.97	106.71
30	Z	102	CLA	C4A-NA-C1A	7.27	109.97	106.71
30	16	305	CLA	C4A-NA-C1A	7.26	109.97	106.71
30	31	305	CLA	C4A-NA-C1A	7.26	109.97	106.71
41	13	314	A86	C33-C32-C31	7.26	116.26	109.21
41	31	313	A86	C33-C32-C31	7.26	116.26	109.21
41	33	313	A86	C33-C32-C31	7.25	116.26	109.21
41	11	313	A86	C33-C32-C31	7.25	116.25	109.21
30	16	304	CLA	C4A-NA-C1A	7.24	109.96	106.71
41	11	311	A86	C33-C32-C31	7.24	116.25	109.21
41	17	312	A86	C33-C32-C31	7.24	116.25	109.21
41	20	210	A86	C36-C31-C32	-7.24	112.51	119.70
30	c	509	CLA	C4A-NA-C1A	7.24	109.96	106.71
30	40	207	CLA	C4A-NA-C1A	7.24	109.96	106.71
41	34	312	A86	C33-C32-C31	7.24	116.25	109.21
41	39	311	A86	C4-C5-C6	-7.24	116.98	127.31
41	19	311	A86	C4-C5-C6	-7.23	116.99	127.31
41	31	311	A86	C33-C32-C31	7.22	116.23	109.21
41	18	314	A86	C33-C32-C31	7.22	116.23	109.21
41	37	312	A86	C33-C32-C31	7.21	116.22	109.21
30	C	508	CLA	C4A-NA-C1A	7.21	109.95	106.71
30	31	304	CLA	C4A-NA-C1A	7.21	109.95	106.71
41	35	311	A86	C33-C32-C31	7.21	116.22	109.21
41	40	210	A86	C36-C31-C32	-7.21	112.54	119.70
41	35	313	A86	C33-C32-C31	7.21	116.22	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	32	315	A86	C33-C32-C31	7.21	116.22	109.21
41	15	311	A86	C33-C32-C31	7.21	116.21	109.21
41	18	315	A86	C33-C32-C31	7.21	116.21	109.21
41	12	316	A86	C33-C32-C31	7.20	116.21	109.21
30	11	315	CLA	C4A-NA-C1A	7.20	109.94	106.71
41	33	315	A86	C33-C32-C31	7.19	116.20	109.21
41	38	314	A86	C33-C32-C31	7.19	116.20	109.21
30	13	306	CLA	C4A-NA-C1A	7.19	109.94	106.71
30	12	309	CLA	C4A-NA-C1A	7.19	109.94	106.71
30	36	304	CLA	C4A-NA-C1A	7.19	109.94	106.71
41	17	314	A86	C33-C32-C31	7.19	116.20	109.21
41	38	315	A86	C33-C32-C31	7.19	116.19	109.21
41	34	314	A86	C33-C32-C31	7.19	116.19	109.21
30	36	305	CLA	C4A-NA-C1A	7.18	109.94	106.71
30	C	503	CLA	C4A-NA-C1A	7.18	109.93	106.71
30	c	524	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	b	614	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	c	513	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	15	305	CLA	C4A-NA-C1A	7.17	109.93	106.71
30	c	512	CLA	C4A-NA-C1A	7.17	109.93	106.71
41	15	313	A86	C33-C32-C31	7.17	116.17	109.21
30	11	304	CLA	C4A-NA-C1A	7.16	109.92	106.71
41	32	317	A86	C33-C32-C31	7.16	116.17	109.21
41	12	318	A86	C33-C32-C31	7.15	116.16	109.21
30	35	305	CLA	C4A-NA-C1A	7.15	109.92	106.71
30	20	207	CLA	C4A-NA-C1A	7.15	109.92	106.71
41	37	314	A86	C33-C32-C31	7.14	116.15	109.21
30	21	302	CLA	C4A-NA-C1A	7.14	109.92	106.71
30	d	406	CLA	C4A-NA-C1A	7.14	109.92	106.71
41	14	314	A86	C33-C32-C31	7.14	116.15	109.21
30	12	312	CLA	C4A-NA-C1A	7.13	109.91	106.71
30	B	606	CLA	C4A-NA-C1A	7.13	109.91	106.71
30	41	307	CLA	C4A-NA-C1A	7.13	109.91	106.71
30	a	403	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	C	519	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	D	405	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	31	315	CLA	C4A-NA-C1A	7.11	109.90	106.71
30	C	513	CLA	C4A-NA-C1A	7.10	109.90	106.71
30	d	402	CLA	C4A-NA-C1A	7.10	109.90	106.71
41	13	312	A86	C17-C16-C15	7.10	116.40	109.16
30	32	309	CLA	C4A-NA-C1A	7.10	109.90	106.71
30	A	404	CLA	C4A-NA-C1A	7.09	109.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	14	312	A86	C17-C16-C15	7.09	116.39	109.16
30	17	304	CLA	C4A-NA-C1A	7.08	109.89	106.71
41	31	311	A86	C17-C16-C15	7.08	116.39	109.16
30	12	303	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	33	301	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	13	305	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	14	306	CLA	C4A-NA-C1A	7.08	109.89	106.71
30	19	305	CLA	C4A-NA-C1A	7.07	109.89	106.71
41	35	311	A86	C17-C16-C15	7.07	116.38	109.16
30	B	623	CLA	C4A-NA-C1A	7.07	109.88	106.71
41	16	311	A86	C17-C16-C15	7.07	116.37	109.16
30	41	306	CLA	C4A-NA-C1A	7.06	109.88	106.71
41	33	313	A86	C17-C16-C15	7.06	116.37	109.16
30	34	306	CLA	C4A-NA-C1A	7.06	109.88	106.71
30	D	402	CLA	C4A-NA-C1A	7.06	109.88	106.71
30	38	303	CLA	C4A-NA-C1A	7.05	109.88	106.71
41	32	315	A86	C17-C16-C15	7.05	116.35	109.16
41	37	312	A86	C17-C16-C15	7.04	116.35	109.16
30	37	307	CLA	C4A-NA-C1A	7.04	109.87	106.71
41	36	311	A86	C17-C16-C15	7.04	116.35	109.16
41	12	316	A86	C17-C16-C15	7.04	116.35	109.16
30	b	607	CLA	C4A-NA-C1A	7.04	109.87	106.71
41	17	312	A86	C17-C16-C15	7.04	116.34	109.16
41	11	311	A86	C17-C16-C15	7.03	116.34	109.16
30	41	301	CLA	C4A-NA-C1A	7.03	109.87	106.71
30	39	305	CLA	C4A-NA-C1A	7.02	109.86	106.71
41	34	312	A86	C17-C16-C15	7.02	116.32	109.16
30	B	614	CLA	C4A-NA-C1A	7.02	109.86	106.71
30	37	309	CLA	C4A-NA-C1A	7.02	109.86	106.71
30	b	606	CLA	C4A-NA-C1A	7.01	109.86	106.71
41	15	311	A86	C17-C16-C15	7.01	116.32	109.16
30	18	303	CLA	C4A-NA-C1A	7.01	109.86	106.71
30	35	308	CLA	C4A-NA-C1A	7.00	109.85	106.71
41	38	314	A86	C17-C16-C15	7.00	116.30	109.16
30	17	309	CLA	C4A-NA-C1A	6.99	109.85	106.71
30	21	301	CLA	C4A-NA-C1A	6.99	109.85	106.71
30	21	306	CLA	C4A-NA-C1A	6.99	109.85	106.71
30	34	305	CLA	C4A-NA-C1A	6.99	109.85	106.71
41	18	314	A86	C17-C16-C15	6.98	116.28	109.16
30	B	610	CLA	C4A-NA-C1A	6.98	109.84	106.71
30	32	308	CLA	C4A-NA-C1A	6.98	109.84	106.71
30	41	302	CLA	C4A-NA-C1A	6.98	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	41	308	CLA	C4A-NA-C1A	6.98	109.84	106.71
30	21	308	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	14	301	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	32	303	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	18	310	CLA	C4A-NA-C1A	6.94	109.83	106.71
30	34	301	CLA	C4A-NA-C1A	6.94	109.83	106.71
30	15	308	CLA	C4A-NA-C1A	6.94	109.83	106.71
30	c	503	CLA	C4A-NA-C1A	6.94	109.83	106.71
30	37	304	CLA	C4A-NA-C1A	6.92	109.82	106.71
41	37	311	A86	C33-C32-C31	6.91	115.92	109.21
30	39	302	CLA	C4A-NA-C1A	6.90	109.81	106.71
30	17	307	CLA	C4A-NA-C1A	6.89	109.81	106.71
30	38	306	CLA	C4A-NA-C1A	6.89	109.81	106.71
30	38	310	CLA	C4A-NA-C1A	6.89	109.80	106.71
41	21	312	A86	C25-C26-C27	-6.88	117.48	127.31
30	B	605	CLA	C4A-NA-C1A	6.87	109.80	106.71
30	18	306	CLA	C4A-NA-C1A	6.87	109.79	106.71
30	19	302	CLA	C4A-NA-C1A	6.87	109.79	106.71
30	C	520	CLA	C4A-NA-C1A	6.86	109.79	106.71
41	21	310	A86	C3-C2-C1	-6.86	117.52	127.31
41	41	312	A86	C25-C26-C27	-6.86	117.52	127.31
30	41	303	CLA	C4A-NA-C1A	6.86	109.79	106.71
30	c	508	CLA	C4A-NA-C1A	6.85	109.79	106.71
41	17	311	A86	C33-C32-C31	6.85	115.87	109.21
41	41	310	A86	C3-C2-C1	-6.85	117.54	127.31
30	15	304	CLA	C4A-NA-C1A	6.84	109.78	106.71
30	b	610	CLA	C4A-NA-C1A	6.83	109.78	106.71
30	39	304	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	19	304	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	21	303	CLA	C4A-NA-C1A	6.80	109.76	106.71
30	D	401	CLA	C4A-NA-C1A	6.79	109.76	106.71
30	36	301	CLA	C4A-NA-C1A	6.79	109.76	106.71
41	39	309	A86	C36-C31-C32	-6.78	112.96	119.70
30	40	208	CLA	C4A-NA-C1A	6.78	109.75	106.71
41	39	310	A86	C17-C16-C15	6.78	116.08	109.16
30	40	202	CLA	C4A-NA-C1A	6.78	109.75	106.71
30	b	605	CLA	C4A-NA-C1A	6.77	109.75	106.71
41	19	310	A86	C17-C16-C15	6.77	116.07	109.16
41	19	309	A86	C36-C31-C32	-6.77	112.98	119.70
30	16	301	CLA	C4A-NA-C1A	6.76	109.75	106.71
30	36	308	CLA	C4A-NA-C1A	6.76	109.75	106.71
30	B	602	CLA	C4A-NA-C1A	6.75	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	308	CLA	C4A-NA-C1A	6.74	109.74	106.71
30	18	307	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	41	309	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	20	208	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	38	307	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	c	522	CLA	C4A-NA-C1A	6.70	109.72	106.71
30	d	401	CLA	C4A-NA-C1A	6.69	109.72	106.71
30	c	506	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	18	301	CLA	C4A-NA-C1A	6.67	109.71	106.71
41	41	313	A86	C25-C26-C27	-6.67	117.79	127.31
30	C	506	CLA	C4A-NA-C1A	6.67	109.70	106.71
30	21	309	CLA	C4A-NA-C1A	6.66	109.70	106.71
30	35	304	CLA	C4A-NA-C1A	6.66	109.70	106.71
30	b	604	CLA	C4A-NA-C1A	6.66	109.70	106.71
41	21	313	A86	C25-C26-C27	-6.65	117.81	127.31
30	33	310	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	20	202	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	b	602	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	B	604	CLA	C4A-NA-C1A	6.61	109.68	106.71
30	41	305	CLA	C4A-NA-C1A	6.58	109.66	106.71
30	11	308	CLA	C4A-NA-C1A	6.58	109.66	106.71
30	17	306	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	12	313	CLA	C4A-NA-C1A	6.56	109.65	106.71
30	38	301	CLA	C4A-NA-C1A	6.55	109.65	106.71
30	b	622	CLA	C4A-NA-C1A	6.55	109.65	106.71
30	31	308	CLA	C4A-NA-C1A	6.55	109.65	106.71
41	19	309	A86	C3-C2-C1	-6.55	117.97	127.31
30	14	309	CLA	C4A-NA-C1A	6.54	109.64	106.71
30	37	306	CLA	C4A-NA-C1A	6.53	109.64	106.71
30	21	305	CLA	C4A-NA-C1A	6.53	109.64	106.71
41	39	309	A86	C3-C2-C1	-6.53	117.99	127.31
41	21	311	A86	C3-C2-C1	-6.52	118.00	127.31
30	34	309	CLA	C4A-NA-C1A	6.52	109.64	106.71
41	41	311	A86	C3-C2-C1	-6.51	118.01	127.31
41	20	211	A86	C3-C2-C1	-6.51	118.03	127.31
30	13	309	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	13	308	CLA	C4A-NA-C1A	6.49	109.63	106.71
30	w	103	CLA	C4A-NA-C1A	6.49	109.62	106.71
41	40	211	A86	C3-C2-C1	-6.48	118.06	127.31
30	11	307	CLA	C4A-NA-C1A	6.45	109.61	106.71
41	34	313	A86	C4-C5-C6	-6.44	118.13	127.31
30	19	306	CLA	C4A-NA-C1A	6.43	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	33	314	A86	C4-C5-C6	-6.43	118.13	127.31
30	40	209	CLA	C4A-NA-C1A	6.43	109.60	106.71
41	32	316	A86	C4-C5-C6	-6.43	118.13	127.31
41	13	313	A86	C4-C5-C6	-6.42	118.15	127.31
41	14	313	A86	C4-C5-C6	-6.41	118.16	127.31
30	20	205	CLA	C4A-NA-C1A	6.41	109.59	106.71
41	17	313	A86	C4-C5-C6	-6.39	118.19	127.31
41	40	212	A86	C3-C2-C1	-6.38	118.20	127.31
41	20	212	A86	C3-C2-C1	-6.38	118.20	127.31
41	12	317	A86	C4-C5-C6	-6.38	118.21	127.31
41	36	312	A86	C4-C5-C6	-6.38	118.21	127.31
41	16	312	A86	C4-C5-C6	-6.37	118.21	127.31
41	17	302	A86	C33-C32-C31	6.37	115.40	109.21
41	15	312	A86	C4-C5-C6	-6.37	118.22	127.31
41	37	302	A86	C33-C32-C31	6.37	115.40	109.21
30	32	312	CLA	C4A-NA-C1A	6.37	109.57	106.71
41	37	313	A86	C4-C5-C6	-6.37	118.22	127.31
30	16	307	CLA	CMB-C2B-C1B	-6.36	118.69	128.46
30	36	307	CLA	CMB-C2B-C1B	-6.36	118.69	128.46
41	35	312	A86	C4-C5-C6	-6.35	118.25	127.31
30	20	209	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	12	311	CLA	C4A-NA-C1A	6.33	109.55	106.71
30	14	308	CLA	C4A-NA-C1A	6.33	109.55	106.71
30	19	308	CLA	C4A-NA-C1A	6.33	109.55	106.71
30	W	103	CLA	C4A-NA-C1A	6.32	109.55	106.71
41	11	312	A86	C4-C5-C6	-6.32	118.30	127.31
41	31	312	A86	C4-C5-C6	-6.29	118.33	127.31
30	41	304	CLA	C4A-NA-C1A	6.29	109.53	106.71
30	40	205	CLA	C4A-NA-C1A	6.28	109.53	106.71
30	34	308	CLA	C4A-NA-C1A	6.23	109.51	106.71
41	36	310	A86	C33-C32-C31	6.22	115.26	109.21
30	16	307	CLA	C4A-NA-C1A	6.21	109.50	106.71
41	20	210	A86	C4-C5-C6	-6.21	118.45	127.31
30	31	307	CLA	C4A-NA-C1A	6.21	109.50	106.71
30	17	310	CLA	C4A-NA-C1A	6.20	109.50	106.71
30	14	310	CLA	C4A-NA-C1A	6.19	109.49	106.71
41	40	210	A86	C4-C5-C6	-6.19	118.48	127.31
30	37	310	CLA	C4A-NA-C1A	6.18	109.49	106.71
30	32	311	CLA	C4A-NA-C1A	6.18	109.48	106.71
41	16	310	A86	C33-C32-C31	6.17	115.21	109.21
30	W	102	CLA	C4A-NA-C1A	6.17	109.48	106.71
30	39	308	CLA	C4A-NA-C1A	6.17	109.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	314	CLA	C4A-NA-C1A	6.17	109.48	106.71
30	33	311	CLA	C4A-NA-C1A	6.17	109.48	106.71
30	39	306	CLA	C4A-NA-C1A	6.16	109.47	106.71
30	37	306	CLA	CMB-C2B-C1B	-6.14	119.02	128.46
30	17	306	CLA	CMB-C2B-C1B	-6.13	119.05	128.46
30	21	304	CLA	C4A-NA-C1A	6.12	109.46	106.71
30	11	309	CLA	C4A-NA-C1A	6.11	109.45	106.71
30	13	310	CLA	C4A-NA-C1A	6.11	109.45	106.71
30	36	307	CLA	C4A-NA-C1A	6.11	109.45	106.71
30	32	313	CLA	C4A-NA-C1A	6.10	109.45	106.71
41	38	314	A86	C3-C2-C1	-6.10	118.60	127.31
41	15	311	A86	C3-C2-C1	-6.10	118.61	127.31
30	31	309	CLA	C4A-NA-C1A	6.09	109.45	106.71
41	32	315	A86	C3-C2-C1	-6.09	118.61	127.31
41	36	310	A86	C36-C31-C32	-6.09	113.65	119.70
41	18	314	A86	C3-C2-C1	-6.09	118.62	127.31
41	21	311	A86	C25-C26-C27	-6.09	118.62	127.31
41	39	310	A86	C4-C5-C6	-6.09	118.62	127.31
30	34	310	CLA	C4A-NA-C1A	6.08	109.44	106.71
41	35	311	A86	C3-C2-C1	-6.08	118.63	127.31
41	12	316	A86	C3-C2-C1	-6.08	118.63	127.31
41	16	311	A86	C3-C2-C1	-6.08	118.64	127.31
41	36	311	A86	C3-C2-C1	-6.07	118.64	127.31
41	11	311	A86	C3-C2-C1	-6.07	118.64	127.31
30	35	309	CLA	C4A-NA-C1A	6.06	109.43	106.71
41	41	311	A86	C25-C26-C27	-6.06	118.67	127.31
41	34	312	A86	C3-C2-C1	-6.05	118.67	127.31
30	38	312	CLA	C4A-NA-C1A	6.05	109.42	106.71
41	14	312	A86	C3-C2-C1	-6.05	118.68	127.31
41	19	310	A86	C4-C5-C6	-6.04	118.68	127.31
41	31	311	A86	C3-C2-C1	-6.04	118.69	127.31
41	40	211	A86	C25-C26-C27	-6.04	118.70	127.31
41	17	312	A86	C3-C2-C1	-6.03	118.70	127.31
41	16	310	A86	C36-C31-C32	-6.03	113.71	119.70
41	20	211	A86	C25-C26-C27	-6.02	118.72	127.31
41	33	313	A86	C3-C2-C1	-6.02	118.72	127.31
41	37	312	A86	C3-C2-C1	-6.02	118.72	127.31
41	13	312	A86	C3-C2-C1	-6.00	118.75	127.31
30	w	102	CLA	C4A-NA-C1A	5.99	109.40	106.71
30	18	312	CLA	C4A-NA-C1A	5.98	109.39	106.71
30	19	301	CLA	C4A-NA-C1A	5.97	109.39	106.71
30	39	301	CLA	C4A-NA-C1A	5.97	109.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	33	309	CLA	C4A-NA-C1A	5.95	109.38	106.71
41	39	311	A86	C25-C26-C27	-5.94	118.83	127.31
30	15	309	CLA	C4A-NA-C1A	5.91	109.36	106.71
41	19	311	A86	C25-C26-C27	-5.90	118.89	127.31
41	21	312	A86	C4-C5-C6	-5.88	118.92	127.31
30	32	308	CLA	CMB-C2B-C1B	-5.87	119.44	128.46
30	33	306	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
41	41	312	A86	C4-C5-C6	-5.85	118.97	127.31
41	15	313	A86	C17-C16-C15	5.83	115.11	109.16
30	31	304	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
41	18	315	A86	C17-C16-C15	5.83	115.11	109.16
30	34	305	CLA	CMB-C2B-C1B	-5.83	119.51	128.46
41	38	315	A86	C17-C16-C15	5.82	115.10	109.16
41	32	317	A86	C17-C16-C15	5.81	115.09	109.16
41	35	313	A86	C17-C16-C15	5.81	115.09	109.16
41	13	314	A86	C17-C16-C15	5.80	115.08	109.16
41	11	313	A86	C17-C16-C15	5.80	115.08	109.16
41	31	313	A86	C17-C16-C15	5.79	115.07	109.16
41	12	318	A86	C17-C16-C15	5.79	115.07	109.16
41	41	312	A86	C36-C31-C32	-5.78	113.96	119.70
41	33	315	A86	C17-C16-C15	5.77	115.05	109.16
41	34	314	A86	C17-C16-C15	5.77	115.05	109.16
41	21	310	A86	C17-C16-C15	5.76	115.04	109.16
41	41	310	A86	C17-C16-C15	5.76	115.04	109.16
41	14	314	A86	C17-C16-C15	5.76	115.04	109.16
41	37	316	A86	C3-C2-C1	-5.75	119.10	127.31
41	21	312	A86	C36-C31-C32	-5.75	113.99	119.70
41	15	314	A86	C3-C2-C1	-5.75	119.11	127.31
41	37	314	A86	C17-C16-C15	5.74	115.02	109.16
41	17	314	A86	C17-C16-C15	5.74	115.02	109.16
41	11	314	A86	C3-C2-C1	-5.73	119.13	127.31
41	31	314	A86	C3-C2-C1	-5.73	119.13	127.31
41	35	314	A86	C3-C2-C1	-5.72	119.14	127.31
30	C	509	CLA	CMB-C2B-C1B	-5.72	119.67	128.46
30	13	305	CLA	CMB-C2B-C1B	-5.72	119.67	128.46
30	c	509	CLA	CMB-C2B-C1B	-5.71	119.69	128.46
41	33	317	A86	C3-C2-C1	-5.71	119.16	127.31
41	40	211	A86	C17-C16-C15	5.71	114.98	109.16
30	C	511	CLA	CMB-C2B-C1B	-5.70	119.70	128.46
30	m	101	CLA	C4A-NA-C1A	5.70	109.27	106.71
41	21	310	A86	C33-C32-C31	5.70	114.75	109.21
41	17	316	A86	C3-C2-C1	-5.70	119.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	511	CLA	CMB-C2B-C1B	-5.70	119.71	128.46
30	M	101	CLA	C4A-NA-C1A	5.69	109.26	106.71
30	18	306	CLA	CMB-C2B-C1B	-5.69	119.72	128.46
30	12	308	CLA	CMB-C2B-C1B	-5.69	119.72	128.46
41	41	310	A86	C33-C32-C31	5.69	114.74	109.21
41	13	317	A86	C3-C2-C1	-5.69	119.19	127.31
41	13	315	A86	C3-C2-C1	-5.69	119.20	127.31
41	36	313	A86	C3-C2-C1	-5.68	119.20	127.31
41	12	319	A86	C3-C2-C1	-5.68	119.20	127.31
30	11	304	CLA	CMB-C2B-C1B	-5.68	119.73	128.46
41	16	313	A86	C3-C2-C1	-5.68	119.21	127.31
30	38	306	CLA	CMB-C2B-C1B	-5.68	119.74	128.46
41	32	318	A86	C3-C2-C1	-5.67	119.22	127.31
41	32	319	A86	C3-C2-C1	-5.66	119.23	127.31
30	14	305	CLA	CMB-C2B-C1B	-5.64	119.80	128.46
41	20	211	A86	C17-C16-C15	5.64	114.92	109.16
41	37	311	A86	C4-C5-C6	-5.64	119.27	127.31
41	41	311	A86	C17-C16-C15	5.63	114.90	109.16
41	21	311	A86	C17-C16-C15	5.62	114.89	109.16
41	17	311	A86	C4-C5-C6	-5.61	119.30	127.31
30	16	305	CLA	CMB-C2B-C1B	-5.60	119.86	128.46
41	39	310	A86	C3-C2-C1	-5.60	119.32	127.31
30	36	305	CLA	CMB-C2B-C1B	-5.59	119.88	128.46
41	19	310	A86	C3-C2-C1	-5.58	119.35	127.31
41	21	313	A86	C17-C16-C15	5.55	114.82	109.16
41	41	313	A86	C17-C16-C15	5.50	114.77	109.16
41	37	312	A86	C4-C5-C6	-5.48	119.49	127.31
41	18	314	A86	C4-C5-C6	-5.47	119.51	127.31
41	20	212	A86	C33-C32-C31	5.46	114.52	109.21
41	21	313	A86	C3-C2-C1	-5.46	119.52	127.31
41	40	212	A86	C33-C32-C31	5.46	114.51	109.21
41	15	311	A86	C4-C5-C6	-5.45	119.53	127.31
41	41	313	A86	C3-C2-C1	-5.45	119.53	127.31
41	38	314	A86	C4-C5-C6	-5.45	119.53	127.31
41	21	312	A86	C3-C2-C1	-5.45	119.53	127.31
41	41	312	A86	C3-C2-C1	-5.45	119.53	127.31
41	13	312	A86	C4-C5-C6	-5.45	119.53	127.31
41	35	311	A86	C4-C5-C6	-5.44	119.55	127.31
41	36	311	A86	C4-C5-C6	-5.44	119.55	127.31
41	33	313	A86	C4-C5-C6	-5.44	119.55	127.31
41	12	316	A86	C4-C5-C6	-5.44	119.55	127.31
41	34	312	A86	C4-C5-C6	-5.43	119.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	17	312	A86	C4-C5-C6	-5.43	119.56	127.31
30	38	309	CLA	CMB-C2B-C1B	-5.43	120.12	128.46
41	16	311	A86	C4-C5-C6	-5.42	119.58	127.31
30	18	309	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
41	11	311	A86	C4-C5-C6	-5.41	119.59	127.31
41	38	302	A86	C25-C26-C27	-5.41	119.59	127.31
30	39	302	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
41	32	315	A86	C4-C5-C6	-5.41	119.60	127.31
41	31	311	A86	C4-C5-C6	-5.40	119.60	127.31
41	14	312	A86	C4-C5-C6	-5.40	119.60	127.31
41	33	316	A86	C25-C26-C27	-5.40	119.60	127.31
41	15	315	A86	C25-C26-C27	-5.40	119.61	127.31
41	32	304	A86	C25-C26-C27	-5.40	119.61	127.31
30	C	511	CLA	CMB-C2B-C3B	5.39	134.76	124.68
41	12	304	A86	C25-C26-C27	-5.39	119.62	127.31
41	15	316	A86	C25-C26-C27	-5.38	119.63	127.31
41	35	316	A86	C25-C26-C27	-5.38	119.63	127.31
30	19	302	CLA	CMB-C2B-C1B	-5.38	120.20	128.46
30	37	309	CLA	C2A-C1A-CHA	5.37	133.25	123.86
41	18	302	A86	C25-C26-C27	-5.37	119.64	127.31
41	31	316	A86	C25-C26-C27	-5.37	119.65	127.31
41	35	315	A86	C25-C26-C27	-5.37	119.65	127.31
41	11	316	A86	C25-C26-C27	-5.37	119.65	127.31
30	17	309	CLA	C2A-C1A-CHA	5.36	133.23	123.86
41	16	313	A86	C33-C32-C31	5.36	114.42	109.21
41	13	301	A86	C25-C26-C27	-5.36	119.67	127.31
41	13	316	A86	C25-C26-C27	-5.36	119.67	127.31
30	c	511	CLA	CMB-C2B-C3B	5.35	134.68	124.68
41	13	315	A86	C33-C32-C31	5.35	114.41	109.21
41	36	313	A86	C33-C32-C31	5.35	114.41	109.21
41	33	302	A86	C25-C26-C27	-5.34	119.69	127.31
41	37	316	A86	C33-C32-C31	5.34	114.40	109.21
30	36	309	CLA	C4A-NA-C1A	5.34	109.11	106.71
30	b	613	CLA	CMB-C2B-C1B	-5.34	120.26	128.46
41	13	317	A86	C33-C32-C31	5.34	114.40	109.21
41	12	319	A86	C33-C32-C31	5.33	114.39	109.21
41	17	316	A86	C33-C32-C31	5.32	114.39	109.21
41	32	319	A86	C33-C32-C31	5.32	114.38	109.21
41	31	314	A86	C33-C32-C31	5.32	114.38	109.21
41	21	312	A86	C20-C19-C18	-5.31	102.24	112.75
41	11	314	A86	C33-C32-C31	5.31	114.37	109.21
41	33	317	A86	C33-C32-C31	5.31	114.37	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	41	312	A86	C20-C19-C18	-5.30	102.26	112.75
41	32	318	A86	C33-C32-C31	5.30	114.36	109.21
41	15	314	A86	C33-C32-C31	5.30	114.36	109.21
30	B	613	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
30	21	305	CLA	CMB-C2B-C1B	-5.29	120.34	128.46
30	41	305	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
30	16	309	CLA	C4A-NA-C1A	5.28	109.08	106.71
41	40	210	A86	O4-C38-C39	5.27	120.79	111.09
33	l	101	SQD	O7-S-C6	5.27	113.20	106.94
41	20	210	A86	O4-C38-C39	5.27	120.78	111.09
41	35	314	A86	C33-C32-C31	5.27	114.33	109.21
41	37	314	A86	C3-C2-C1	-5.26	119.81	127.31
41	17	314	A86	C3-C2-C1	-5.25	119.82	127.31
41	13	314	A86	C3-C2-C1	-5.24	119.83	127.31
41	33	312	A86	C3-C2-C1	-5.23	119.84	127.31
41	15	310	A86	C3-C2-C1	-5.23	119.84	127.31
41	12	315	A86	C3-C2-C1	-5.23	119.85	127.31
41	13	311	A86	C3-C2-C1	-5.23	119.85	127.31
41	32	314	A86	C3-C2-C1	-5.22	119.86	127.31
30	C	507	CLA	CMB-C2B-C1B	-5.22	120.44	128.46
41	33	315	A86	C3-C2-C1	-5.22	119.86	127.31
41	35	310	A86	C3-C2-C1	-5.22	119.86	127.31
41	11	310	A86	C3-C2-C1	-5.21	119.87	127.31
30	36	307	CLA	CMB-C2B-C3B	5.21	134.42	124.68
30	16	307	CLA	CMB-C2B-C3B	5.21	134.42	124.68
30	C	507	CLA	CAA-C2A-C3A	-5.21	98.52	112.78
41	34	314	A86	C3-C2-C1	-5.20	119.89	127.31
30	37	306	CLA	CMB-C2B-C3B	5.20	134.41	124.68
41	18	313	A86	C3-C2-C1	-5.20	119.89	127.31
30	c	507	CLA	CAA-C2A-C3A	-5.20	98.55	112.78
41	31	310	A86	C3-C2-C1	-5.20	119.89	127.31
41	38	313	A86	C3-C2-C1	-5.19	119.90	127.31
30	C	514	CLA	CMB-C2B-C1B	-5.19	120.49	128.46
41	35	313	A86	C3-C2-C1	-5.19	119.91	127.31
30	17	306	CLA	CMB-C2B-C3B	5.19	134.38	124.68
41	32	317	A86	C3-C2-C1	-5.19	119.91	127.31
41	34	311	A86	C3-C2-C1	-5.18	119.91	127.31
30	16	303	CLA	CMB-C2B-C1B	-5.18	120.50	128.46
30	c	507	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
41	14	314	A86	C3-C2-C1	-5.17	119.93	127.31
41	12	318	A86	C3-C2-C1	-5.17	119.94	127.31
41	38	315	A86	C3-C2-C1	-5.17	119.94	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	18	315	A86	C3-C2-C1	-5.16	119.95	127.31
41	14	311	A86	C3-C2-C1	-5.16	119.95	127.31
30	b	607	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
30	36	303	CLA	CMB-C2B-C1B	-5.15	120.54	128.46
41	11	313	A86	C3-C2-C1	-5.15	119.97	127.31
30	b	615	CLA	C4A-NA-C1A	5.14	109.02	106.71
33	L	103	SQD	O7-S-C6	5.14	113.04	106.94
30	37	308	CLA	C4A-NA-C1A	5.14	109.02	106.71
41	31	313	A86	C3-C2-C1	-5.13	119.98	127.31
41	15	313	A86	C3-C2-C1	-5.13	119.98	127.31
30	15	304	CLA	CMB-C2B-C1B	-5.12	120.59	128.46
30	c	514	CLA	CMB-C2B-C1B	-5.12	120.59	128.46
30	B	607	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
41	38	314	A86	O4-C38-C39	5.11	120.49	111.09
30	35	304	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
41	16	310	A86	C25-C26-C27	-5.11	120.02	127.31
41	20	213	A86	O4-C38-C39	5.11	120.48	111.09
41	41	314	A86	O4-C38-C39	5.11	120.48	111.09
41	32	315	A86	O4-C38-C39	5.10	120.48	111.09
41	34	312	A86	O4-C38-C39	5.10	120.48	111.09
41	21	314	A86	O4-C38-C39	5.10	120.47	111.09
41	18	314	A86	O4-C38-C39	5.10	120.47	111.09
41	36	310	A86	C25-C26-C27	-5.10	120.04	127.31
41	12	316	A86	O4-C38-C39	5.09	120.45	111.09
41	40	213	A86	O4-C38-C39	5.08	120.44	111.09
41	14	312	A86	O4-C38-C39	5.08	120.44	111.09
41	13	312	A86	O4-C38-C39	5.07	120.42	111.09
41	11	311	A86	O4-C38-C39	5.07	120.42	111.09
41	15	311	A86	O4-C38-C39	5.07	120.42	111.09
41	37	312	A86	O4-C38-C39	5.07	120.42	111.09
41	16	311	A86	O4-C38-C39	5.07	120.42	111.09
41	31	311	A86	O4-C38-C39	5.07	120.41	111.09
30	B	615	CLA	C4A-NA-C1A	5.06	108.98	106.71
41	33	313	A86	O4-C38-C39	5.06	120.41	111.09
30	17	308	CLA	C4A-NA-C1A	5.06	108.98	106.71
41	40	201	A86	C12-C11-C13	5.05	124.50	116.02
41	35	311	A86	O4-C38-C39	5.05	120.38	111.09
30	C	510	CLA	CMB-C2B-C1B	-5.05	120.71	128.46
41	36	310	A86	C3-C2-C1	-5.04	120.11	127.31
41	36	311	A86	O4-C38-C39	5.04	120.36	111.09
41	17	312	A86	O4-C38-C39	5.03	120.35	111.09
41	19	309	A86	O4-C38-C39	5.03	120.33	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	20	201	A86	C12-C11-C13	5.03	124.46	116.02
41	16	310	A86	C3-C2-C1	-5.02	120.14	127.31
41	39	309	A86	O4-C38-C39	5.02	120.33	111.09
41	40	210	A86	C25-C26-C27	-5.01	120.16	127.31
41	20	210	A86	C25-C26-C27	-5.01	120.16	127.31
33	L	103	SQD	O6-C1-C2	5.01	116.12	108.30
30	20	208	CLA	CMB-C2B-C1B	-5.01	120.77	128.46
41	15	316	A86	O4-C38-C39	5.01	120.30	111.09
41	20	201	A86	C3-C2-C1	-5.00	120.17	127.31
30	40	208	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
41	20	201	A86	O4-C38-C39	4.99	120.28	111.09
41	33	302	A86	O4-C38-C39	4.99	120.26	111.09
30	c	510	CLA	CMB-C2B-C1B	-4.99	120.80	128.46
41	40	201	A86	C3-C2-C1	-4.98	120.20	127.31
41	40	201	A86	O4-C38-C39	4.98	120.25	111.09
41	33	312	A86	C17-C16-C15	4.98	114.24	109.16
30	37	309	CLA	CAA-C2A-C1A	4.98	128.29	111.97
41	31	316	A86	O4-C38-C39	4.98	120.25	111.09
41	38	302	A86	O4-C38-C39	4.98	120.25	111.09
33	l	101	SQD	O6-C1-C2	4.98	116.07	108.30
41	13	301	A86	O4-C38-C39	4.98	120.25	111.09
41	35	316	A86	O4-C38-C39	4.98	120.24	111.09
30	c	511	CLA	C4A-NA-C1A	4.98	108.94	106.71
30	17	309	CLA	CAA-C2A-C1A	4.97	128.28	111.97
41	18	302	A86	O4-C38-C39	4.97	120.24	111.09
41	11	316	A86	O4-C38-C39	4.97	120.23	111.09
41	33	316	A86	O4-C38-C39	4.97	120.23	111.09
41	13	316	A86	O4-C38-C39	4.97	120.23	111.09
41	32	304	A86	O4-C38-C39	4.96	120.22	111.09
30	c	507	CLA	C4A-NA-C1A	4.96	108.94	106.71
41	35	315	A86	O4-C38-C39	4.96	120.22	111.09
41	32	314	A86	C17-C16-C15	4.96	114.22	109.16
41	12	304	A86	O4-C38-C39	4.95	120.20	111.09
41	15	315	A86	O4-C38-C39	4.95	120.20	111.09
41	35	310	A86	C17-C16-C15	4.95	114.21	109.16
41	13	311	A86	C17-C16-C15	4.95	114.21	109.16
30	32	308	CLA	CMB-C2B-C3B	4.94	133.93	124.68
41	37	315	A86	O4-C38-C39	4.94	120.17	111.09
30	C	507	CLA	C4A-NA-C1A	4.94	108.92	106.71
41	15	310	A86	C17-C16-C15	4.92	114.19	109.16
41	12	315	A86	C17-C16-C15	4.91	114.18	109.16
41	14	311	A86	C17-C16-C15	4.91	114.18	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	40	212	A86	O4-C38-C39	4.91	120.13	111.09
41	20	212	A86	O4-C38-C39	4.91	120.12	111.09
41	21	314	A86	C3-C2-C1	-4.91	120.31	127.31
41	41	314	A86	C3-C2-C1	-4.90	120.32	127.31
30	34	305	CLA	CMB-C2B-C3B	4.90	133.84	124.68
41	31	310	A86	C17-C16-C15	4.90	114.16	109.16
41	17	315	A86	O4-C38-C39	4.89	120.09	111.09
30	31	304	CLA	CMB-C2B-C3B	4.89	133.83	124.68
41	34	311	A86	C17-C16-C15	4.89	114.15	109.16
30	C	511	CLA	C4A-NA-C1A	4.88	108.90	106.71
41	18	313	A86	C17-C16-C15	4.88	114.14	109.16
41	39	309	A86	C17-C16-C15	4.88	114.14	109.16
30	33	306	CLA	CMB-C2B-C3B	4.88	133.80	124.68
41	20	213	A86	C3-C2-C1	-4.87	120.36	127.31
41	11	312	A86	O4-C38-C39	4.86	120.04	111.09
41	11	310	A86	C17-C16-C15	4.86	114.12	109.16
41	17	302	A86	O4-C38-C39	4.86	120.03	111.09
30	D	405	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
41	40	213	A86	C3-C2-C1	-4.86	120.38	127.31
41	38	313	A86	C17-C16-C15	4.85	114.11	109.16
30	b	613	CLA	CMB-C2B-C3B	4.85	133.75	124.68
41	31	312	A86	O4-C38-C39	4.85	120.01	111.09
30	12	308	CLA	CMB-C2B-C3B	4.84	133.74	124.68
41	19	309	A86	C17-C16-C15	4.84	114.10	109.16
41	35	312	A86	O4-C38-C39	4.84	119.99	111.09
30	11	304	CLA	CMB-C2B-C3B	4.84	133.72	124.68
41	17	314	A86	O4-C38-C39	4.83	119.98	111.09
41	16	312	A86	O4-C38-C39	4.83	119.98	111.09
41	16	310	A86	O4-C38-C39	4.83	119.97	111.09
41	37	302	A86	O4-C38-C39	4.83	119.97	111.09
41	32	316	A86	O4-C38-C39	4.83	119.97	111.09
41	14	314	A86	O4-C38-C39	4.82	119.97	111.09
41	14	313	A86	O4-C38-C39	4.82	119.96	111.09
41	41	313	A86	O4-C38-C39	4.82	119.96	111.09
41	12	317	A86	O4-C38-C39	4.82	119.96	111.09
41	36	312	A86	O4-C38-C39	4.82	119.95	111.09
41	15	312	A86	O4-C38-C39	4.81	119.94	111.09
30	13	305	CLA	CMB-C2B-C3B	4.81	133.68	124.68
41	12	318	A86	O4-C38-C39	4.81	119.94	111.09
41	37	314	A86	O4-C38-C39	4.81	119.94	111.09
41	36	310	A86	O4-C38-C39	4.81	119.93	111.09
41	13	313	A86	O4-C38-C39	4.80	119.93	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	18	315	A86	O4-C38-C39	4.80	119.92	111.09
41	34	313	A86	O4-C38-C39	4.80	119.92	111.09
41	37	311	A86	O4-C38-C39	4.80	119.92	111.09
41	11	313	A86	O4-C38-C39	4.80	119.91	111.09
41	21	313	A86	O4-C38-C39	4.80	119.91	111.09
41	33	315	A86	O4-C38-C39	4.79	119.91	111.09
41	13	314	A86	O4-C38-C39	4.79	119.91	111.09
41	17	313	A86	O4-C38-C39	4.79	119.91	111.09
30	B	613	CLA	CMB-C2B-C3B	4.79	133.64	124.68
41	32	317	A86	O4-C38-C39	4.79	119.90	111.09
41	33	314	A86	O4-C38-C39	4.79	119.90	111.09
41	34	314	A86	O4-C38-C39	4.79	119.90	111.09
41	17	311	A86	O4-C38-C39	4.78	119.89	111.09
41	31	313	A86	O4-C38-C39	4.78	119.89	111.09
30	14	305	CLA	CMB-C2B-C3B	4.78	133.62	124.68
41	35	313	A86	O4-C38-C39	4.78	119.89	111.09
41	37	313	A86	O4-C38-C39	4.78	119.88	111.09
38	C	516	DGD	O3G-C3G-C2G	-4.77	99.39	110.90
30	d	406	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
41	13	315	A86	O4-C38-C39	4.77	119.86	111.09
41	37	316	A86	O4-C38-C39	4.76	119.84	111.09
41	38	315	A86	O4-C38-C39	4.76	119.84	111.09
41	17	316	A86	O4-C38-C39	4.76	119.84	111.09
41	11	314	A86	O4-C38-C39	4.76	119.84	111.09
41	16	313	A86	O4-C38-C39	4.76	119.84	111.09
41	31	314	A86	O4-C38-C39	4.76	119.84	111.09
41	12	319	A86	O4-C38-C39	4.76	119.84	111.09
41	15	313	A86	O4-C38-C39	4.76	119.84	111.09
41	32	318	A86	O4-C38-C39	4.75	119.83	111.09
41	19	310	A86	O4-C38-C39	4.75	119.83	111.09
30	a	402	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
41	32	319	A86	O4-C38-C39	4.74	119.81	111.09
41	13	317	A86	O4-C38-C39	4.74	119.81	111.09
30	20	205	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
41	36	313	A86	O4-C38-C39	4.74	119.80	111.09
30	C	502	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
30	16	303	CLA	CMB-C2B-C3B	4.73	133.53	124.68
38	c	517	DGD	O3G-C3G-C2G	-4.73	99.48	110.90
30	18	306	CLA	CMB-C2B-C3B	4.73	133.53	124.68
30	35	307	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
41	33	317	A86	O4-C38-C39	4.72	119.78	111.09
30	c	502	CLA	CMB-C2B-C1B	-4.72	121.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	39	310	A86	O4-C38-C39	4.72	119.77	111.09
30	34	308	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
34	a	406	BCT	O2-C-O1	4.71	131.77	119.55
30	38	306	CLA	CMB-C2B-C3B	4.71	133.49	124.68
30	40	205	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
41	15	314	A86	O4-C38-C39	4.71	119.75	111.09
30	16	305	CLA	CMB-C2B-C3B	4.71	133.49	124.68
41	19	311	A86	O4-C38-C39	4.71	119.75	111.09
30	36	305	CLA	CMB-C2B-C3B	4.71	133.48	124.68
41	39	311	A86	O4-C38-C39	4.70	119.74	111.09
30	36	303	CLA	CMB-C2B-C3B	4.70	133.47	124.68
41	36	312	A86	C41-C32-C31	-4.69	106.27	110.47
30	A	402	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
41	36	310	A86	C17-C16-C15	4.69	113.94	109.16
41	16	312	A86	C41-C32-C31	-4.69	106.28	110.47
41	13	312	A86	C25-C26-C27	-4.69	120.62	127.31
41	35	314	A86	O4-C38-C39	4.69	119.71	111.09
30	16	302	CLA	CBA-CAA-C2A	4.68	127.68	113.86
30	36	302	CLA	CBA-CAA-C2A	4.68	127.68	113.86
30	15	307	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
34	A	407	BCT	O2-C-O1	4.68	131.68	119.55
30	20	209	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
41	16	310	A86	C17-C16-C15	4.68	113.94	109.16
41	17	311	A86	C3-C2-C1	-4.68	120.64	127.31
41	15	312	A86	C41-C32-C31	-4.67	106.29	110.47
41	11	311	A86	C25-C26-C27	-4.66	120.66	127.31
41	14	312	A86	C25-C26-C27	-4.66	120.66	127.31
41	33	313	A86	C25-C26-C27	-4.65	120.67	127.31
41	21	312	A86	O4-C38-C39	4.65	119.65	111.09
41	37	311	A86	C3-C2-C1	-4.65	120.67	127.31
41	34	312	A86	C25-C26-C27	-4.65	120.68	127.31
41	41	312	A86	O4-C38-C39	4.64	119.63	111.09
30	40	209	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
41	32	315	A86	C25-C26-C27	-4.63	120.70	127.31
41	31	311	A86	C25-C26-C27	-4.63	120.70	127.31
41	37	312	A86	C25-C26-C27	-4.63	120.71	127.31
30	33	309	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
30	39	307	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
41	12	316	A86	C25-C26-C27	-4.62	120.71	127.31
41	31	312	A86	C41-C32-C31	-4.62	106.34	110.47
41	17	312	A86	C25-C26-C27	-4.62	120.72	127.31
30	19	307	CLA	CMB-C2B-C1B	-4.62	121.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	35	311	A86	C25-C26-C27	-4.62	120.72	127.31
30	32	311	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
41	35	312	A86	C41-C32-C31	-4.61	106.35	110.47
30	B	612	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
30	31	307	CLA	CMB-C2B-C1B	-4.61	121.39	128.46
41	15	311	A86	C25-C26-C27	-4.60	120.74	127.31
41	11	312	A86	C41-C32-C31	-4.60	106.36	110.47
41	41	310	A86	O4-C38-C39	4.59	119.54	111.09
30	c	508	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
41	21	310	A86	O4-C38-C39	4.59	119.53	111.09
41	40	213	A86	C17-C16-C15	4.59	113.84	109.16
41	38	314	A86	C25-C26-C27	-4.59	120.77	127.31
30	b	612	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
41	20	213	A86	C17-C16-C15	4.58	113.83	109.16
41	32	316	A86	C41-C32-C31	-4.58	106.38	110.47
39	d	405	PL9	C7-C3-C4	4.58	120.60	116.88
30	b	603	CLA	O2D-CGD-O1D	-4.57	114.89	123.84
41	13	313	A86	C41-C32-C31	-4.57	106.38	110.47
30	39	302	CLA	CMB-C2B-C3B	4.57	133.23	124.68
41	34	313	A86	C41-C32-C31	-4.57	106.38	110.47
41	16	311	A86	C25-C26-C27	-4.57	120.78	127.31
41	18	314	A86	C25-C26-C27	-4.56	120.80	127.31
41	21	314	A86	C17-C16-C15	4.56	113.82	109.16
30	C	514	CLA	CMB-C2B-C3B	4.56	133.22	124.68
41	36	311	A86	C25-C26-C27	-4.56	120.80	127.31
30	C	508	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
41	12	317	A86	C41-C32-C31	-4.56	106.39	110.47
41	34	314	A86	C25-C26-C27	-4.56	120.81	127.31
30	c	514	CLA	CMB-C2B-C3B	4.56	133.20	124.68
41	41	314	A86	C17-C16-C15	4.56	113.81	109.16
41	14	314	A86	C25-C26-C27	-4.55	120.81	127.31
30	14	308	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
41	14	313	A86	C41-C32-C31	-4.55	106.40	110.47
41	35	310	A86	O4-C38-C39	4.54	119.44	111.09
41	32	317	A86	C25-C26-C27	-4.54	120.83	127.31
41	18	315	A86	C25-C26-C27	-4.54	120.83	127.31
41	17	314	A86	C25-C26-C27	-4.54	120.83	127.31
41	37	313	A86	C41-C32-C31	-4.54	106.41	110.47
30	19	302	CLA	CMB-C2B-C3B	4.53	133.16	124.68
41	11	313	A86	C25-C26-C27	-4.53	120.85	127.31
41	12	318	A86	C25-C26-C27	-4.53	120.85	127.31
30	B	603	CLA	O2D-CGD-O1D	-4.53	114.99	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	38	315	A86	C25-C26-C27	-4.52	120.86	127.31
41	17	313	A86	C41-C32-C31	-4.52	106.43	110.47
41	15	310	A86	O4-C38-C39	4.52	119.40	111.09
41	11	310	A86	O4-C38-C39	4.51	119.39	111.09
41	31	310	A86	O4-C38-C39	4.51	119.38	111.09
41	33	314	A86	C41-C32-C31	-4.51	106.44	110.47
41	12	315	A86	O4-C38-C39	4.50	119.38	111.09
41	32	314	A86	O4-C38-C39	4.50	119.37	111.09
41	17	315	A86	C33-C32-C31	4.50	113.58	109.21
41	37	314	A86	C25-C26-C27	-4.49	120.89	127.31
30	13	308	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
30	12	311	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
41	15	313	A86	C25-C26-C27	-4.49	120.91	127.31
41	20	211	A86	O4-C38-C39	4.48	119.33	111.09
41	14	311	A86	O4-C38-C39	4.48	119.33	111.09
41	31	313	A86	C25-C26-C27	-4.48	120.92	127.31
30	11	307	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
41	35	313	A86	C25-C26-C27	-4.47	120.93	127.31
41	13	311	A86	O4-C38-C39	4.47	119.31	111.09
41	33	312	A86	O4-C38-C39	4.47	119.31	111.09
41	40	211	A86	O4-C38-C39	4.46	119.30	111.09
41	34	311	A86	O4-C38-C39	4.46	119.30	111.09
41	18	313	A86	O4-C38-C39	4.46	119.29	111.09
41	21	311	A86	O4-C38-C39	4.46	119.29	111.09
41	13	314	A86	C25-C26-C27	-4.46	120.95	127.31
41	37	315	A86	C33-C32-C31	4.45	113.54	109.21
41	33	315	A86	C25-C26-C27	-4.45	120.96	127.31
30	B	611	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
41	38	313	A86	O4-C38-C39	4.44	119.27	111.09
41	20	212	A86	C4-C5-C6	-4.44	120.98	127.31
41	41	311	A86	O4-C38-C39	4.43	119.25	111.09
39	D	404	PL9	C7-C3-C4	4.43	120.48	116.88
30	40	202	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
30	20	202	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
30	D	401	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
41	40	212	A86	C4-C5-C6	-4.40	121.03	127.31
30	15	304	CLA	CMB-C2B-C3B	4.40	132.90	124.68
30	35	304	CLA	CMB-C2B-C3B	4.38	132.88	124.68
30	b	611	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
30	37	304	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
30	d	401	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
41	35	310	A86	C4-C5-C6	-4.35	121.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	521	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
30	m	101	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
30	c	523	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
41	15	310	A86	C4-C5-C6	-4.34	121.12	127.31
30	17	304	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
35	B	622	LHG	O4-P-O5	4.33	133.66	112.24
30	B	603	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
35	b	621	LHG	O4-P-O5	4.32	133.62	112.24
30	W	103	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
41	13	301	A86	C20-C19-C18	-4.32	104.20	112.75
41	31	310	A86	C4-C5-C6	-4.32	121.14	127.31
41	33	302	A86	C20-C19-C18	-4.32	104.21	112.75
41	11	310	A86	C4-C5-C6	-4.32	121.15	127.31
30	M	101	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
41	33	312	A86	C4-C5-C6	-4.31	121.16	127.31
41	32	304	A86	C20-C19-C18	-4.31	104.23	112.75
41	15	315	A86	C20-C19-C18	-4.30	104.23	112.75
41	38	302	A86	C20-C19-C18	-4.30	104.23	112.75
41	12	315	A86	C4-C5-C6	-4.30	121.17	127.31
41	12	304	A86	C20-C19-C18	-4.30	104.25	112.75
41	13	311	A86	C4-C5-C6	-4.30	121.18	127.31
41	18	302	A86	C20-C19-C18	-4.29	104.25	112.75
41	11	316	A86	C20-C19-C18	-4.29	104.25	112.75
41	13	316	A86	C20-C19-C18	-4.29	104.26	112.75
41	15	316	A86	C20-C19-C18	-4.29	104.26	112.75
35	a	407	LHG	O4-P-O5	4.29	133.44	112.24
30	B	607	CLA	CMB-C2B-C3B	4.29	132.70	124.68
35	A	408	LHG	O4-P-O5	4.28	133.42	112.24
41	18	313	A86	C4-C5-C6	-4.28	121.20	127.31
41	35	315	A86	C20-C19-C18	-4.28	104.28	112.75
41	33	316	A86	C20-C19-C18	-4.28	104.29	112.75
30	13	306	CLA	CMB-C2B-C1B	-4.27	121.89	128.46
41	35	316	A86	C20-C19-C18	-4.27	104.29	112.75
30	19	308	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
41	37	302	A86	C3-C2-C1	-4.27	121.22	127.31
30	b	603	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
30	39	308	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
30	14	306	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
41	17	315	A86	C25-C24-C1	-4.26	114.44	126.42
30	b	607	CLA	CMB-C2B-C3B	4.26	132.65	124.68
30	19	304	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
30	38	304	CLA	CMB-C2B-C1B	-4.26	121.92	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	37	315	A86	C25-C24-C1	-4.26	114.46	126.42
41	32	314	A86	C4-C5-C6	-4.25	121.24	127.31
30	w	103	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
41	31	316	A86	C20-C19-C18	-4.25	104.34	112.75
41	17	302	A86	C3-C2-C1	-4.25	121.24	127.31
41	14	311	A86	C4-C5-C6	-4.25	121.25	127.31
41	38	313	A86	C4-C5-C6	-4.24	121.25	127.31
41	34	311	A86	C4-C5-C6	-4.24	121.25	127.31
30	39	304	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
41	17	315	A86	C3-C2-C1	-4.24	121.26	127.31
41	19	311	A86	C33-C32-C31	4.24	113.33	109.21
30	18	304	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
30	11	305	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
30	B	612	CLA	CMB-C2B-C3B	4.23	132.60	124.68
30	b	612	CLA	CMB-C2B-C3B	4.23	132.60	124.68
30	33	307	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
30	12	309	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
30	33	303	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
30	20	205	CLA	CMB-C2B-C3B	4.22	132.58	124.68
30	20	208	CLA	CMB-C2B-C3B	4.22	132.58	124.68
30	D	405	CLA	CMB-C2B-C3B	4.22	132.57	124.68
41	37	315	A86	C3-C2-C1	-4.22	121.29	127.31
41	39	311	A86	C33-C32-C31	4.21	113.30	109.21
30	40	208	CLA	CMB-C2B-C3B	4.21	132.55	124.68
30	21	304	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
30	41	304	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
30	40	205	CLA	CMB-C2B-C3B	4.20	132.53	124.68
30	b	606	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
30	32	309	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
30	31	301	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
30	B	606	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
35	d	409	LHG	O4-P-O5	4.18	132.91	112.24
35	L	101	LHG	O4-P-O5	4.17	132.85	112.24
30	32	305	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
30	c	502	CLA	CMB-C2B-C3B	4.16	132.47	124.68
30	d	406	CLA	CMB-C2B-C3B	4.16	132.47	124.68
30	34	306	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
41	17	314	A86	C41-C32-C31	-4.15	106.76	110.47
41	39	309	A86	C4-C5-C6	-4.15	121.39	127.31
41	37	314	A86	C41-C32-C31	-4.15	106.76	110.47
30	C	502	CLA	CMB-C2B-C3B	4.14	132.43	124.68
41	18	313	A86	C25-C26-C27	-4.14	121.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	31	305	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
41	20	210	A86	C3-C2-C1	-4.13	121.42	127.31
41	38	313	A86	C25-C26-C27	-4.12	121.43	127.31
41	11	313	A86	C41-C32-C31	-4.12	106.79	110.47
41	19	309	A86	C4-C5-C6	-4.11	121.44	127.31
30	b	604	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
41	40	210	A86	C3-C2-C1	-4.11	121.45	127.31
41	33	315	A86	C41-C32-C31	-4.10	106.80	110.47
30	c	523	CLA	O2D-CGD-O1D	-4.10	115.82	123.84
30	34	302	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
30	c	509	CLA	CMB-C2B-C3B	4.10	132.34	124.68
41	32	317	A86	C41-C32-C31	-4.09	106.81	110.47
30	32	306	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
41	15	310	A86	C25-C26-C27	-4.09	121.48	127.31
41	33	312	A86	C25-C26-C27	-4.09	121.48	127.31
35	l	102	LHG	O4-P-O5	4.09	132.44	112.24
30	C	509	CLA	CMB-C2B-C3B	4.08	132.31	124.68
30	38	309	CLA	CMB-C2B-C3B	4.08	132.31	124.68
41	35	310	A86	C25-C26-C27	-4.08	121.49	127.31
41	14	311	A86	C25-C26-C27	-4.08	121.49	127.31
41	34	311	A86	C25-C26-C27	-4.08	121.49	127.31
41	13	314	A86	C41-C32-C31	-4.08	106.82	110.47
41	13	311	A86	C25-C26-C27	-4.08	121.49	127.31
30	C	521	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
30	39	307	CLA	CMB-C2B-C3B	4.07	132.29	124.68
35	L	102	LHG	O4-P-O5	4.07	132.34	112.24
33	l	101	SQD	O9-S-C6	4.07	111.77	106.94
30	18	309	CLA	CMB-C2B-C3B	4.06	132.28	124.68
41	15	313	A86	C41-C32-C31	-4.06	106.84	110.47
41	31	313	A86	C41-C32-C31	-4.05	106.85	110.47
30	B	604	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
30	31	302	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
41	12	315	A86	C25-C26-C27	-4.04	121.55	127.31
30	33	304	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
41	35	313	A86	C41-C32-C31	-4.04	106.86	110.47
41	31	310	A86	C25-C26-C27	-4.03	121.56	127.31
41	32	314	A86	C25-C26-C27	-4.03	121.56	127.31
41	12	318	A86	C41-C32-C31	-4.03	106.86	110.47
41	14	314	A86	C41-C32-C31	-4.03	106.86	110.47
41	11	310	A86	C25-C26-C27	-4.03	121.56	127.31
30	19	307	CLA	CMB-C2B-C3B	4.03	132.21	124.68
41	34	314	A86	C41-C32-C31	-4.02	106.87	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	L	103	SQD	O9-S-C6	4.02	111.72	106.94
41	13	317	A86	C25-C24-C1	-4.02	115.11	126.42
30	34	309	CLA	C2A-C1A-CHA	4.02	130.89	123.86
41	15	314	A86	C25-C24-C1	-4.02	115.12	126.42
41	18	315	A86	C41-C32-C31	-4.02	106.88	110.47
41	35	314	A86	C25-C24-C1	-4.02	115.14	126.42
41	17	316	A86	C25-C24-C1	-4.01	115.14	126.42
41	37	316	A86	C25-C24-C1	-4.01	115.15	126.42
41	33	317	A86	C25-C24-C1	-4.01	115.15	126.42
41	11	314	A86	C25-C24-C1	-4.01	115.16	126.42
30	35	303	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
41	32	319	A86	C25-C24-C1	-4.01	115.16	126.42
32	c	521	BCR	C24-C23-C22	-4.01	120.18	126.23
41	38	315	A86	C41-C32-C31	-4.01	106.89	110.47
30	C	510	CLA	CMB-C2B-C3B	4.01	132.17	124.68
41	13	315	A86	C25-C24-C1	-4.01	115.16	126.42
41	31	314	A86	C25-C24-C1	-4.00	115.17	126.42
30	33	310	CLA	C2A-C1A-CHA	4.00	130.86	123.86
33	B	621	SQD	O7-S-C6	4.00	111.69	106.94
30	32	312	CLA	C2A-C1A-CHA	4.00	130.85	123.86
32	C	518	BCR	C24-C23-C22	-4.00	120.20	126.23
30	14	303	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
30	c	512	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
41	32	318	A86	C25-C24-C1	-3.99	115.20	126.42
30	37	305	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
30	17	305	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
30	31	308	CLA	C2A-C1A-CHA	3.99	130.84	123.86
41	16	313	A86	C25-C24-C1	-3.99	115.21	126.42
33	b	620	SQD	O7-S-C6	3.99	111.68	106.94
30	b	602	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
30	15	303	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
42	32	302	LMU	O1'-C1'-C2'	3.98	114.52	108.30
41	12	319	A86	C25-C24-C1	-3.98	115.23	126.42
41	36	313	A86	C25-C24-C1	-3.98	115.24	126.42
41	33	312	A86	C41-C32-C31	-3.98	106.91	110.47
30	13	303	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
30	34	303	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
30	c	510	CLA	CMB-C2B-C3B	3.97	132.11	124.68
32	B	618	BCR	C2-C1-C6	3.97	116.59	110.48
30	b	622	CLA	CBA-CAA-C2A	3.97	125.58	113.86
41	13	311	A86	C41-C32-C31	-3.97	106.92	110.47
30	13	302	CLA	CMB-C2B-C1B	-3.96	122.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	41	305	CLA	CMB-C2B-C3B	3.96	132.08	124.68
42	32	302	LMU	C1B-O1B-C4'	-3.96	108.17	117.96
30	11	301	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
30	w	102	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
30	12	306	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
30	11	308	CLA	C2A-C1A-CHA	3.95	130.76	123.86
30	21	305	CLA	CMB-C2B-C3B	3.94	132.06	124.68
30	17	308	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
30	37	308	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
30	C	512	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
30	13	309	CLA	C2A-C1A-CHA	3.93	130.74	123.86
41	21	313	A86	C3-C4-C5	-3.93	115.42	123.47
30	B	602	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
30	12	305	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
30	12	313	CLA	C2A-C1A-CHA	3.93	130.72	123.86
30	11	302	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
30	17	303	CLA	CHB-C4A-NA	3.92	129.94	124.51
32	b	617	BCR	C2-C1-C6	3.92	116.52	110.48
41	41	313	A86	C3-C4-C5	-3.92	115.44	123.47
30	14	304	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
30	12	307	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
30	36	303	CLA	C2A-C1A-CHA	3.91	130.70	123.86
30	a	402	CLA	CMB-C2B-C3B	3.91	132.00	124.68
30	16	303	CLA	C2A-C1A-CHA	3.91	130.70	123.86
30	13	304	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
41	17	315	A86	C25-C26-C27	-3.91	121.73	127.31
41	31	310	A86	C41-C32-C31	-3.91	106.97	110.47
30	34	304	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
30	14	309	CLA	C2A-C1A-CHA	3.90	130.68	123.86
30	B	623	CLA	CBA-CAA-C2A	3.90	125.37	113.86
30	11	303	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
41	11	310	A86	C41-C32-C31	-3.90	106.99	110.47
41	37	315	A86	C25-C26-C27	-3.89	121.76	127.31
32	B	616	BCR	C15-C16-C17	-3.89	115.50	123.47
41	21	312	A86	O1-C15-C14	-3.89	105.40	113.21
41	41	312	A86	O1-C15-C14	-3.89	105.41	113.21
30	37	303	CLA	CHB-C4A-NA	3.89	129.89	124.51
30	A	402	CLA	CMB-C2B-C3B	3.88	131.94	124.68
30	14	302	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
30	33	305	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
30	21	302	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
30	31	303	CLA	CMB-C2B-C1B	-3.87	122.51	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	35	307	CLA	CMB-C2B-C3B	3.87	131.92	124.68
32	m	103	BCR	C15-C16-C17	-3.87	115.55	123.47
30	41	302	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
30	W	102	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
30	B	614	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
31	D	403	PHO	CMB-C2B-C3B	3.86	131.90	124.68
30	12	310	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
42	12	302	LMU	O1'-C1'-C2'	3.86	114.33	108.30
30	40	202	CLA	CMB-C2B-C3B	3.85	131.89	124.68
30	15	307	CLA	CMB-C2B-C3B	3.85	131.89	124.68
38	h	102	DGD	C1D-C2D-C3D	-3.85	101.97	110.00
30	c	508	CLA	CMB-C2B-C3B	3.85	131.88	124.68
33	l	101	SQD	C4-C3-C2	3.85	117.55	110.82
41	14	311	A86	C41-C32-C31	-3.85	107.03	110.47
33	A	406	SQD	O47-C7-C8	3.85	119.79	111.50
41	32	314	A86	C41-C32-C31	-3.84	107.03	110.47
30	37	304	CLA	CMB-C2B-C3B	3.84	131.87	124.68
33	a	405	SQD	O47-C7-C8	3.84	119.78	111.50
30	20	202	CLA	CMB-C2B-C3B	3.84	131.86	124.68
30	b	614	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
38	C	517	DGD	O6D-C1D-O3G	-3.84	100.89	109.97
30	32	307	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
30	C	508	CLA	CMB-C2B-C3B	3.83	131.85	124.68
38	c	518	DGD	O6D-C1D-O3G	-3.83	100.90	109.97
41	12	315	A86	C41-C32-C31	-3.83	107.05	110.47
41	21	312	A86	C12-C11-C13	3.83	122.45	116.02
30	14	307	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
41	15	310	A86	C41-C32-C31	-3.82	107.05	110.47
41	35	310	A86	C41-C32-C31	-3.82	107.05	110.47
41	41	312	A86	C12-C11-C13	3.82	122.44	116.02
30	35	308	CLA	C2A-C1A-CHA	3.82	130.53	123.86
30	C	521	CLA	CHB-C4A-NA	3.81	129.78	124.51
30	16	304	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
30	17	304	CLA	CMB-C2B-C3B	3.81	131.81	124.68
31	d	404	PHO	CMB-C2B-C3B	3.81	131.81	124.68
41	20	210	A86	C9-C8-C6	-3.81	115.72	126.42
30	35	305	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
30	36	304	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
41	34	311	A86	C41-C32-C31	-3.80	107.07	110.47
30	17	308	CLA	C1B-CHB-C4A	-3.80	122.59	130.12
30	11	306	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
42	12	302	LMU	C1B-O1B-C4'	-3.80	108.56	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	307	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
30	16	302	CLA	C1B-CHB-C4A	-3.80	122.59	130.12
38	H	102	DGD	C1D-C2D-C3D	-3.80	102.09	110.00
30	15	305	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
30	36	302	CLA	C1B-CHB-C4A	-3.79	122.60	130.12
41	40	210	A86	C9-C8-C6	-3.79	115.76	126.42
41	12	315	A86	C12-C11-C13	3.79	122.39	116.02
41	18	313	A86	C41-C32-C31	-3.79	107.08	110.47
30	17	303	CLA	C1B-CHB-C4A	-3.79	122.61	130.12
41	33	312	A86	C12-C11-C13	3.79	122.39	116.02
41	15	310	A86	C12-C11-C13	3.79	122.39	116.02
33	L	103	SQD	C4-C3-C2	3.79	117.44	110.82
30	37	308	CLA	C1B-CHB-C4A	-3.78	122.62	130.12
30	c	522	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
41	37	313	A86	C25-C26-C27	-3.78	121.91	127.31
41	40	210	A86	C33-C32-C31	3.78	112.89	109.21
30	15	308	CLA	C2A-C1A-CHA	3.78	130.47	123.86
41	13	311	A86	C12-C11-C13	3.78	122.37	116.02
41	32	314	A86	C12-C11-C13	3.78	122.37	116.02
41	38	313	A86	C41-C32-C31	-3.78	107.09	110.47
41	21	314	A86	C33-C32-C31	3.78	112.88	109.21
30	36	302	CLA	CHB-C4A-NA	3.78	129.74	124.51
30	c	523	CLA	CHB-C4A-NA	3.77	129.73	124.51
41	20	213	A86	C33-C32-C31	3.77	112.88	109.21
41	20	201	A86	C25-C26-C27	-3.77	121.93	127.31
33	b	620	SQD	O9-S-O7	-3.77	100.90	113.95
41	40	213	A86	C33-C32-C31	3.76	112.87	109.21
33	B	621	SQD	O9-S-O7	-3.76	100.93	113.95
30	31	306	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
41	12	319	A86	C4-C5-C6	-3.76	121.95	127.31
41	11	310	A86	C12-C11-C13	3.76	122.33	116.02
41	12	317	A86	C25-C26-C27	-3.76	121.95	127.31
30	B	615	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
41	31	310	A86	C12-C11-C13	3.75	122.33	116.02
41	20	210	A86	C33-C32-C31	3.75	112.86	109.21
30	34	307	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
30	40	207	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
41	40	201	A86	C25-C26-C27	-3.75	121.96	127.31
41	41	314	A86	C33-C32-C31	3.75	112.85	109.21
30	37	303	CLA	C1B-CHB-C4A	-3.75	122.70	130.12
30	D	406	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
30	C	520	CLA	CMB-C2B-C1B	-3.75	122.71	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	19	305	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
30	39	305	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
30	16	302	CLA	CHB-C4A-NA	3.74	129.69	124.51
30	33	308	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
41	35	310	A86	C12-C11-C13	3.74	122.31	116.02
30	32	310	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
41	18	313	A86	C12-C11-C13	3.74	122.30	116.02
30	15	302	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
30	14	308	CLA	CMB-C2B-C3B	3.74	131.67	124.68
30	16	307	CLA	C1B-CHB-C4A	-3.74	122.72	130.12
41	14	311	A86	C12-C11-C13	3.74	122.30	116.02
30	21	304	CLA	CMB-C2B-C3B	3.73	131.66	124.68
30	20	207	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
30	34	308	CLA	CMB-C2B-C3B	3.73	131.66	124.68
41	14	312	A86	C41-C32-C31	-3.73	107.14	110.47
41	17	313	A86	C25-C26-C27	-3.73	121.99	127.31
33	b	620	SQD	O47-C7-C8	3.72	119.53	111.50
30	36	309	CLA	CAA-C2A-C3A	-3.72	102.58	112.78
41	15	312	A86	C25-C26-C27	-3.72	122.00	127.31
41	13	317	A86	C4-C5-C6	-3.72	122.00	127.31
41	32	318	A86	C4-C5-C6	-3.72	122.00	127.31
41	36	311	A86	C41-C32-C31	-3.72	107.14	110.47
41	35	312	A86	C25-C26-C27	-3.72	122.00	127.31
41	34	312	A86	C41-C32-C31	-3.72	107.14	110.47
30	11	307	CLA	CMB-C2B-C3B	3.72	131.64	124.68
30	z	101	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
30	b	622	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
41	35	314	A86	C4-C5-C6	-3.72	122.01	127.31
30	16	309	CLA	CAA-C2A-C3A	-3.72	102.60	112.78
41	15	314	A86	C4-C5-C6	-3.72	122.01	127.31
41	35	311	A86	C41-C32-C31	-3.72	107.15	110.47
33	B	621	SQD	O47-C7-C8	3.71	119.51	111.50
30	41	304	CLA	CMB-C2B-C3B	3.71	131.62	124.68
30	d	407	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
41	11	314	A86	C4-C5-C6	-3.71	122.01	127.31
41	20	213	A86	C25-C24-C1	-3.71	115.99	126.42
30	36	302	CLA	CAA-C2A-C1A	3.71	124.13	111.97
41	38	313	A86	C12-C11-C13	3.71	122.25	116.02
30	C	519	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
41	14	313	A86	C25-C26-C27	-3.71	122.02	127.31
41	37	316	A86	C4-C5-C6	-3.71	122.02	127.31
41	40	213	A86	C25-C24-C1	-3.71	116.00	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	34	313	A86	C25-C26-C27	-3.71	122.02	127.31
41	16	313	A86	C4-C5-C6	-3.71	122.02	127.31
41	34	311	A86	C12-C11-C13	3.70	122.25	116.02
30	36	307	CLA	C1B-CHB-C4A	-3.70	122.78	130.12
41	16	311	A86	C41-C32-C31	-3.70	107.16	110.47
41	21	314	A86	C25-C24-C1	-3.70	116.01	126.42
30	C	513	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
30	39	301	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
41	13	313	A86	C25-C26-C27	-3.70	122.03	127.31
41	32	316	A86	C25-C26-C27	-3.70	122.03	127.31
41	37	312	A86	C41-C32-C31	-3.70	107.16	110.47
30	16	302	CLA	CAA-C2A-C1A	3.70	124.10	111.97
41	12	316	A86	C41-C32-C31	-3.70	107.16	110.47
33	L	103	SQD	O5-C5-C4	3.70	116.41	109.69
41	33	314	A86	C25-C26-C27	-3.70	122.03	127.31
30	A	404	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
30	b	622	CLA	CAA-C2A-C3A	-3.69	102.66	112.78
30	C	521	CLA	CMB-C2B-C3B	3.69	131.59	124.68
30	c	523	CLA	CMB-C2B-C3B	3.69	131.59	124.68
41	36	313	A86	C4-C5-C6	-3.69	122.04	127.31
30	19	308	CLA	CMB-C2B-C3B	3.69	131.59	124.68
30	c	513	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
30	13	308	CLA	CMB-C2B-C3B	3.69	131.58	124.68
30	a	403	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
30	20	209	CLA	CMB-C2B-C3B	3.69	131.58	124.68
30	39	308	CLA	CMB-C2B-C3B	3.69	131.58	124.68
41	33	317	A86	C4-C5-C6	-3.69	122.04	127.31
33	l	101	SQD	O47-C7-C8	3.69	119.45	111.50
41	15	311	A86	C41-C32-C31	-3.69	107.17	110.47
33	L	103	SQD	O47-C7-C8	3.69	119.45	111.50
41	31	312	A86	C25-C26-C27	-3.69	122.05	127.31
41	31	314	A86	C4-C5-C6	-3.69	122.05	127.31
41	32	319	A86	C4-C5-C6	-3.69	122.05	127.31
41	32	315	A86	C41-C32-C31	-3.69	107.17	110.47
30	15	301	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
41	11	311	A86	C41-C32-C31	-3.69	107.17	110.47
30	19	301	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
30	40	209	CLA	CMB-C2B-C3B	3.68	131.56	124.68
41	11	312	A86	C25-C26-C27	-3.68	122.06	127.31
41	17	312	A86	C41-C32-C31	-3.68	107.18	110.47
30	31	315	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
41	41	314	A86	C25-C24-C1	-3.67	116.10	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	35	302	CLA	CHB-C4A-NA	3.67	129.59	124.51
41	17	316	A86	C4-C5-C6	-3.67	122.07	127.31
30	33	311	CLA	CAA-C2A-C3A	-3.67	102.73	112.78
30	35	302	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
30	d	401	CLA	CMB-C2B-C3B	3.66	131.53	124.68
30	35	301	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
41	31	311	A86	C41-C32-C31	-3.66	107.19	110.47
30	12	311	CLA	CMB-C2B-C3B	3.66	131.53	124.68
41	13	312	A86	C41-C32-C31	-3.66	107.20	110.47
41	13	315	A86	C4-C5-C6	-3.66	122.09	127.31
38	J	101	DGD	O3G-C3G-C2G	-3.65	102.08	110.90
30	31	307	CLA	CMB-C2B-C3B	3.65	131.51	124.68
30	33	309	CLA	CMB-C2B-C3B	3.65	131.51	124.68
30	B	623	CLA	CAA-C2A-C3A	-3.65	102.78	112.78
30	17	310	CLA	CAA-C2A-C3A	-3.65	102.80	112.78
33	A	406	SQD	O9-S-C6	3.64	111.27	106.94
30	39	303	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
30	b	615	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
30	15	302	CLA	CHB-C4A-NA	3.64	129.55	124.51
30	37	310	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
30	31	309	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
30	32	313	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
30	32	306	CLA	CMB-C2B-C3B	3.64	131.49	124.68
33	a	405	SQD	O9-S-O7	-3.64	101.36	113.95
30	33	301	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
41	38	314	A86	C41-C32-C31	-3.64	107.22	110.47
30	33	304	CLA	CMB-C2B-C3B	3.63	131.48	124.68
30	b	610	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
33	A	406	SQD	O5-C5-C4	3.63	116.29	109.69
30	34	310	CLA	CAA-C2A-C3A	-3.63	102.83	112.78
30	B	623	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
41	33	313	A86	C41-C32-C31	-3.63	107.22	110.47
33	a	405	SQD	O6-C1-C2	3.63	113.97	108.30
30	D	401	CLA	CMB-C2B-C3B	3.63	131.47	124.68
33	l	101	SQD	O5-C5-C4	3.63	116.28	109.69
30	32	303	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
33	A	406	SQD	O6-C1-C2	3.63	113.97	108.30
41	32	318	A86	C12-C11-C13	3.63	122.11	116.02
41	36	312	A86	C25-C26-C27	-3.62	122.14	127.31
41	18	314	A86	C41-C32-C31	-3.62	107.23	110.47
30	32	311	CLA	CMB-C2B-C3B	3.62	131.45	124.68
41	15	314	A86	C12-C11-C13	3.62	122.10	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	16	312	A86	C25-C26-C27	-3.62	122.14	127.31
38	j	101	DGD	O3G-C3G-C2G	-3.62	102.17	110.90
30	20	204	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
30	21	307	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
41	37	311	A86	C41-C32-C31	-3.61	107.24	110.47
41	36	313	A86	C12-C11-C13	3.61	122.09	116.02
33	A	406	SQD	O9-S-O7	-3.61	101.44	113.95
33	a	405	SQD	O9-S-C6	3.61	111.23	106.94
30	31	302	CLA	CMB-C2B-C3B	3.61	131.44	124.68
30	19	303	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
30	41	307	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
41	16	313	A86	C12-C11-C13	3.61	122.09	116.02
30	34	303	CLA	CMB-C2B-C3B	3.61	131.43	124.68
30	33	311	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
38	J	101	DGD	O6D-C1D-O3G	-3.61	101.43	109.97
30	38	312	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
41	12	319	A86	C12-C11-C13	3.61	122.08	116.02
30	16	308	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
41	39	309	A86	C25-C26-C27	-3.61	122.17	127.31
30	36	308	CLA	C1B-CHB-C4A	-3.60	122.98	130.12
30	c	505	CLA	CHB-C4A-NA	3.60	129.50	124.51
30	34	310	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
30	33	307	CLA	CMB-C2B-C3B	3.60	131.42	124.68
41	11	314	A86	C12-C11-C13	3.60	122.07	116.02
30	35	309	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
30	15	309	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
41	13	313	A86	C36-C31-C32	-3.59	116.13	119.70
30	11	305	CLA	CMB-C2B-C3B	3.59	131.40	124.68
38	j	101	DGD	O6D-C1D-O3G	-3.59	101.47	109.97
30	34	302	CLA	CHB-C4A-NA	3.59	129.47	124.51
41	19	309	A86	C25-C24-C1	-3.59	116.33	126.42
30	B	610	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
41	33	317	A86	C12-C11-C13	3.59	122.05	116.02
30	14	306	CLA	CMB-C2B-C3B	3.58	131.38	124.68
41	31	314	A86	C12-C11-C13	3.58	122.04	116.02
30	18	312	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
41	21	310	A86	C25-C26-C27	-3.58	122.20	127.31
41	37	316	A86	C12-C11-C13	3.58	122.04	116.02
30	12	305	CLA	CHB-C4A-NA	3.58	129.46	124.51
30	12	314	CLA	CAA-C2A-C3A	-3.58	102.97	112.78
41	17	311	A86	C25-C26-C27	-3.58	122.20	127.31
30	39	304	CLA	CMB-C2B-C3B	3.58	131.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	19	309	A86	C25-C26-C27	-3.58	122.20	127.31
30	19	304	CLA	CMB-C2B-C3B	3.58	131.37	124.68
30	32	313	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
30	40	204	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
41	35	314	A86	C12-C11-C13	3.58	122.03	116.02
41	39	309	A86	C25-C24-C1	-3.58	116.37	126.42
30	12	309	CLA	CMB-C2B-C3B	3.58	131.37	124.68
33	a	405	SQD	O5-C5-C4	3.57	116.19	109.69
41	32	319	A86	C36-C31-C32	-3.57	116.15	119.70
41	11	314	A86	C36-C31-C32	-3.57	116.15	119.70
41	13	317	A86	C36-C31-C32	-3.57	116.15	119.70
41	19	311	A86	C17-C16-C15	3.57	112.80	109.16
41	37	302	A86	C17-C16-C15	3.57	112.80	109.16
30	13	310	CLA	CAA-C2A-C3A	-3.57	103.01	112.78
41	13	317	A86	C12-C11-C13	3.57	122.02	116.02
41	15	314	A86	C36-C31-C32	-3.57	116.16	119.70
30	14	303	CLA	CMB-C2B-C3B	3.57	131.35	124.68
30	13	303	CLA	CMB-C2B-C3B	3.57	131.35	124.68
30	17	309	CLA	CBA-CAA-C2A	3.56	124.39	113.86
30	33	303	CLA	CHB-C4A-NA	3.56	129.44	124.51
30	11	309	CLA	CAA-C2A-C3A	-3.56	103.02	112.78
30	31	309	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
41	17	316	A86	C12-C11-C13	3.56	122.01	116.02
41	35	314	A86	C36-C31-C32	-3.56	116.16	119.70
41	17	311	A86	C41-C32-C31	-3.56	107.28	110.47
30	14	310	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
41	13	315	A86	C12-C11-C13	3.56	122.00	116.02
30	32	305	CLA	CHB-C4A-NA	3.56	129.43	124.51
30	13	306	CLA	CMB-C2B-C3B	3.56	131.33	124.68
30	37	309	CLA	CBA-CAA-C2A	3.56	124.36	113.86
30	Z	102	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
41	32	319	A86	C12-C11-C13	3.55	121.99	116.02
30	13	302	CLA	CHB-C4A-NA	3.55	129.43	124.51
41	37	311	A86	C25-C26-C27	-3.55	122.24	127.31
30	20	203	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
30	c	505	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
41	41	310	A86	C25-C26-C27	-3.54	122.25	127.31
30	14	302	CLA	CHB-C4A-NA	3.54	129.41	124.51
41	17	316	A86	C36-C31-C32	-3.54	116.18	119.70
41	34	313	A86	C36-C31-C32	-3.54	116.18	119.70
30	37	310	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
41	21	312	A86	C4-C3-C2	-3.54	116.22	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	17	302	A86	C17-C16-C15	3.54	112.78	109.16
30	d	402	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
30	c	524	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
41	13	315	A86	C36-C31-C32	-3.54	116.18	119.70
30	40	203	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
32	Z	101	BCR	C15-C16-C17	-3.54	116.23	123.47
41	33	317	A86	C36-C31-C32	-3.54	116.19	119.70
41	16	313	A86	C36-C31-C32	-3.54	116.19	119.70
36	D	408	LMG	C1-C2-C3	-3.54	102.63	110.00
41	12	319	A86	C36-C31-C32	-3.54	116.19	119.70
30	12	306	CLA	CMB-C2B-C3B	3.53	131.29	124.68
30	38	307	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
30	11	302	CLA	CMB-C2B-C3B	3.53	131.29	124.68
32	Z	101	BCR	C11-C10-C9	-3.53	122.27	127.31
30	31	301	CLA	CHB-C4A-NA	3.53	129.39	124.51
41	17	302	A86	C25-C26-C27	-3.53	122.27	127.31
41	37	313	A86	C36-C31-C32	-3.53	116.19	119.70
41	37	316	A86	C36-C31-C32	-3.53	116.19	119.70
33	b	620	SQD	O8-S-C6	3.53	111.36	105.74
36	d	410	LMG	C1-C2-C3	-3.53	102.65	110.00
30	40	205	CLA	C1B-CHB-C4A	-3.53	123.13	130.12
41	14	313	A86	C36-C31-C32	-3.53	116.19	119.70
30	C	505	CLA	CHB-C4A-NA	3.53	129.39	124.51
41	36	313	A86	C36-C31-C32	-3.53	116.20	119.70
30	33	303	CLA	C1-C2-C3	-3.53	119.94	126.04
41	39	311	A86	C17-C16-C15	3.53	112.76	109.16
30	W	103	CLA	CMB-C2B-C3B	3.53	131.28	124.68
41	36	312	A86	C36-C31-C32	-3.53	116.20	119.70
41	41	312	A86	C4-C3-C2	-3.53	116.25	123.47
30	11	309	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
33	L	103	SQD	O9-S-O7	-3.52	101.75	113.95
41	15	316	A86	C4-C3-C2	-3.52	116.25	123.47
30	13	310	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
30	C	505	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
41	21	313	A86	C12-C11-C13	3.52	121.93	116.02
41	12	317	A86	C3-C2-C1	-3.52	122.29	127.31
30	34	306	CLA	CMB-C2B-C3B	3.52	131.26	124.68
30	21	301	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
41	19	311	A86	C3-C2-C1	-3.52	122.29	127.31
30	17	309	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
30	32	309	CLA	CMB-C2B-C3B	3.51	131.25	124.68
30	41	301	CLA	CMB-C2B-C1B	-3.51	123.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	33	303	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
41	39	311	A86	C3-C2-C1	-3.51	122.30	127.31
30	34	301	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
30	34	302	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
30	20	205	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
30	d	407	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
41	31	316	A86	C4-C3-C2	-3.51	116.29	123.47
30	17	310	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
30	18	307	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
41	32	316	A86	C3-C2-C1	-3.51	122.31	127.31
41	37	302	A86	C25-C26-C27	-3.51	122.31	127.31
30	D	402	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
30	32	305	CLA	C1-C2-C3	-3.50	119.98	126.04
41	33	314	A86	C36-C31-C32	-3.50	116.22	119.70
32	C	518	BCR	C15-C16-C17	-3.50	116.30	123.47
30	31	305	CLA	CMB-C2B-C3B	3.50	131.23	124.68
32	c	515	BCR	C15-C16-C17	-3.50	116.30	123.47
41	35	315	A86	C4-C3-C2	-3.50	116.30	123.47
41	35	312	A86	C3-C2-C1	-3.50	122.31	127.31
41	15	310	A86	C34-O4-C38	-3.50	111.37	117.90
33	l	101	SQD	O9-S-O7	-3.50	101.83	113.95
41	35	316	A86	C4-C3-C2	-3.50	116.30	123.47
30	D	406	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
41	14	313	A86	C3-C2-C1	-3.50	122.31	127.31
38	c	518	DGD	O3G-C3G-C2G	-3.50	102.45	110.90
30	34	302	CLA	C1-C2-C3	-3.50	119.99	126.04
41	17	313	A86	C36-C31-C32	-3.50	116.22	119.70
30	C	507	CLA	CMB-C2B-C3B	3.50	131.22	124.68
41	11	316	A86	C4-C3-C2	-3.50	116.31	123.47
32	a	404	BCR	C15-C16-C17	-3.50	116.31	123.47
30	11	301	CLA	CHB-C4A-NA	3.50	129.35	124.51
30	b	602	CLA	CMB-C2B-C3B	3.50	131.22	124.68
41	31	314	A86	C36-C31-C32	-3.50	116.23	119.70
30	14	301	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
41	33	316	A86	C4-C3-C2	-3.50	116.31	123.47
41	31	312	A86	C3-C2-C1	-3.50	122.32	127.31
30	14	310	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
30	17	304	CLA	C2A-C1A-CHA	3.49	129.97	123.86
41	17	313	A86	C3-C2-C1	-3.49	122.33	127.31
41	11	310	A86	C34-O4-C38	-3.49	111.39	117.90
30	32	305	CLA	C1B-CHB-C4A	-3.49	123.21	130.12
30	m	101	CLA	CMB-C2B-C3B	3.49	131.21	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	13	316	A86	C4-C3-C2	-3.49	116.33	123.47
41	15	312	A86	C3-C2-C1	-3.49	122.33	127.31
30	20	206	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
30	M	101	CLA	CMB-C2B-C3B	3.49	131.20	124.68
41	16	312	A86	C36-C31-C32	-3.48	116.24	119.70
33	B	621	SQD	O8-S-C6	3.48	111.29	105.74
41	36	312	A86	C3-C2-C1	-3.48	122.34	127.31
41	40	211	A86	C12-C11-C13	3.48	121.88	116.02
30	B	602	CLA	CMB-C2B-C3B	3.48	131.20	124.68
30	15	306	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
41	31	310	A86	C34-O4-C38	-3.48	111.41	117.90
41	21	310	A86	C20-C19-C18	-3.48	105.86	112.75
41	12	304	A86	C4-C3-C2	-3.48	116.34	123.47
41	21	311	A86	C12-C11-C13	3.48	121.87	116.02
41	15	312	A86	C36-C31-C32	-3.48	116.24	119.70
41	41	311	A86	C12-C11-C13	3.48	121.86	116.02
41	14	312	A86	C36-C31-C32	-3.48	116.25	119.70
41	11	312	A86	C3-C2-C1	-3.48	122.35	127.31
41	35	310	A86	C34-O4-C38	-3.48	111.42	117.90
41	11	316	A86	C3-C2-C1	-3.48	122.35	127.31
41	13	313	A86	C3-C2-C1	-3.48	122.35	127.31
30	37	304	CLA	C2A-C1A-CHA	3.48	129.94	123.86
30	38	303	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
41	37	313	A86	C3-C2-C1	-3.47	122.35	127.31
41	16	312	A86	C3-C2-C1	-3.47	122.35	127.31
41	41	313	A86	C12-C11-C13	3.47	121.85	116.02
41	15	315	A86	C4-C3-C2	-3.47	116.36	123.47
41	34	312	A86	C36-C31-C32	-3.47	116.25	119.70
30	40	206	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
41	31	312	A86	C36-C31-C32	-3.47	116.25	119.70
30	31	301	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
41	19	310	A86	C12-C11-C13	3.47	121.85	116.02
41	31	316	A86	C3-C2-C1	-3.47	122.36	127.31
41	32	304	A86	C4-C3-C2	-3.47	116.37	123.47
41	38	302	A86	C4-C3-C2	-3.47	116.37	123.47
30	21	308	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
41	36	311	A86	C36-C31-C32	-3.47	116.26	119.70
41	38	313	A86	C34-O4-C38	-3.46	111.44	117.90
30	c	512	CLA	CMB-C2B-C3B	3.46	131.16	124.68
41	20	211	A86	C12-C11-C13	3.46	121.84	116.02
30	b	604	CLA	CMB-C2B-C3B	3.46	131.15	124.68
41	33	314	A86	C3-C2-C1	-3.46	122.37	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	34	313	A86	C3-C2-C1	-3.46	122.37	127.31
30	21	309	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
30	41	308	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
32	A	405	BCR	C15-C16-C17	-3.46	116.39	123.47
30	c	507	CLA	CMB-C2B-C3B	3.46	131.15	124.68
41	18	302	A86	C4-C3-C2	-3.46	116.39	123.47
41	32	314	A86	C34-O4-C38	-3.46	111.45	117.90
30	37	309	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
32	c	515	BCR	C11-C10-C9	-3.45	122.38	127.31
41	13	301	A86	C4-C3-C2	-3.45	116.40	123.47
41	12	317	A86	C36-C31-C32	-3.45	116.27	119.70
41	16	311	A86	C36-C31-C32	-3.45	116.27	119.70
30	31	301	CLA	C1-C2-C3	-3.45	120.08	126.04
38	C	517	DGD	O3G-C3G-C2G	-3.45	102.57	110.90
41	39	310	A86	C12-C11-C13	3.45	121.82	116.02
41	34	311	A86	C34-O4-C38	-3.45	111.47	117.90
41	12	315	A86	C34-O4-C38	-3.45	111.47	117.90
30	18	303	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
30	18	311	CLA	C2A-C1A-CHA	3.45	129.88	123.86
41	11	312	A86	C36-C31-C32	-3.45	116.28	119.70
30	34	304	CLA	CMB-C2B-C3B	3.44	131.12	124.68
41	33	312	A86	C34-O4-C38	-3.44	111.48	117.90
41	32	316	A86	C36-C31-C32	-3.44	116.28	119.70
30	38	311	CLA	C2A-C1A-CHA	3.44	129.88	123.86
41	13	311	A86	C34-O4-C38	-3.44	111.48	117.90
41	14	311	A86	C34-O4-C38	-3.44	111.48	117.90
41	35	315	A86	C3-C2-C1	-3.44	122.40	127.31
41	18	313	A86	C34-O4-C38	-3.44	111.48	117.90
41	41	310	A86	C20-C19-C18	-3.44	105.94	112.75
30	41	309	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
41	37	316	A86	C20-C19-C18	-3.44	105.95	112.75
30	w	103	CLA	CMB-C2B-C3B	3.44	131.11	124.68
41	17	316	A86	C20-C19-C18	-3.44	105.95	112.75
30	17	307	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
41	18	302	A86	C3-C2-C1	-3.44	122.41	127.31
30	12	314	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
41	33	302	A86	C4-C3-C2	-3.44	116.44	123.47
41	15	316	A86	C40-C32-C31	-3.43	107.40	110.47
41	41	312	A86	C41-C32-C31	-3.43	107.40	110.47
41	12	316	A86	C36-C31-C32	-3.43	116.29	119.70
41	13	312	A86	C36-C31-C32	-3.43	116.29	119.70
41	12	304	A86	C3-C2-C1	-3.43	122.41	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	35	312	A86	C36-C31-C32	-3.43	116.29	119.70
41	12	319	A86	C20-C19-C18	-3.43	105.96	112.75
32	c	521	BCR	C15-C16-C17	-3.43	116.45	123.47
31	D	403	PHO	O1D-CGD-CBD	3.43	130.45	124.74
30	36	306	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
41	32	318	A86	C36-C31-C32	-3.43	116.29	119.70
41	37	312	A86	C36-C31-C32	-3.43	116.29	119.70
30	35	306	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
30	39	308	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
41	37	302	A86	C9-C8-C6	-3.43	116.79	126.42
30	12	312	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
41	38	302	A86	C40-C32-C31	-3.43	107.41	110.47
41	15	314	A86	C20-C19-C18	-3.43	105.97	112.75
38	c	517	DGD	O5D-C6D-C5D	-3.43	102.71	109.05
41	11	316	A86	C40-C32-C31	-3.42	107.41	110.47
41	33	316	A86	C3-C2-C1	-3.42	122.42	127.31
41	32	315	A86	C36-C31-C32	-3.42	116.30	119.70
30	c	514	CLA	CHB-C4A-NA	3.42	129.25	124.51
41	15	316	A86	C3-C2-C1	-3.42	122.42	127.31
41	38	302	A86	C3-C2-C1	-3.42	122.42	127.31
41	32	318	A86	C20-C19-C18	-3.42	105.98	112.75
30	11	315	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
30	c	506	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
30	38	304	CLA	CMB-C2B-C3B	3.42	131.08	124.68
30	35	303	CLA	CMB-C2B-C3B	3.42	131.08	124.68
30	38	308	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
41	32	304	A86	C40-C32-C31	-3.42	107.41	110.47
30	37	307	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
41	32	319	A86	C20-C19-C18	-3.42	105.99	112.75
30	12	305	CLA	C1-C2-C3	-3.42	120.13	126.04
41	31	316	A86	C40-C32-C31	-3.42	107.41	110.47
30	C	512	CLA	CMB-C2B-C3B	3.42	131.07	124.68
41	16	312	A86	C26-C25-C24	-3.42	112.56	123.22
41	13	317	A86	C20-C19-C18	-3.42	105.99	112.75
30	11	303	CLA	CMB-C2B-C3B	3.42	131.07	124.68
30	18	304	CLA	CMB-C2B-C3B	3.42	131.07	124.68
41	14	313	A86	C26-C25-C24	-3.41	112.56	123.22
41	36	313	A86	C20-C19-C18	-3.41	105.99	112.75
41	21	310	A86	C4-C5-C6	-3.41	122.44	127.31
41	36	312	A86	C26-C25-C24	-3.41	112.56	123.22
41	17	302	A86	C9-C8-C6	-3.41	116.83	126.42
41	19	311	A86	C9-C10-C11	-3.41	116.57	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	18	302	A86	C40-C32-C31	-3.41	107.42	110.47
30	19	308	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
41	16	313	A86	C20-C19-C18	-3.41	106.00	112.75
30	b	601	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
41	13	301	A86	C3-C2-C1	-3.41	122.44	127.31
41	33	317	A86	C20-C19-C18	-3.41	106.00	112.75
41	35	311	A86	C36-C31-C32	-3.41	116.31	119.70
41	11	312	A86	C26-C25-C24	-3.41	112.58	123.22
30	B	604	CLA	CMB-C2B-C3B	3.41	131.06	124.68
30	B	601	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
41	13	315	A86	C20-C19-C18	-3.41	106.01	112.75
41	35	314	A86	C20-C19-C18	-3.41	106.01	112.75
30	33	305	CLA	CMB-C2B-C3B	3.41	131.05	124.68
41	32	304	A86	C3-C2-C1	-3.40	122.45	127.31
41	33	314	A86	C26-C25-C24	-3.40	112.60	123.22
30	12	307	CLA	CMB-C2B-C3B	3.40	131.04	124.68
30	C	514	CLA	CHB-C4A-NA	3.40	129.22	124.51
41	17	312	A86	C36-C31-C32	-3.40	116.32	119.70
41	15	311	A86	C36-C31-C32	-3.40	116.32	119.70
41	31	312	A86	C26-C25-C24	-3.40	112.60	123.22
30	13	304	CLA	CMB-C2B-C3B	3.40	131.04	124.68
30	41	303	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
41	13	316	A86	C3-C2-C1	-3.40	122.46	127.31
41	17	313	A86	C26-C25-C24	-3.40	112.61	123.22
30	35	306	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
30	16	306	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
30	b	610	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
30	14	304	CLA	CMB-C2B-C3B	3.40	131.03	124.68
41	15	315	A86	C3-C2-C1	-3.40	122.46	127.31
30	21	303	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
30	37	305	CLA	CMB-C2B-C3B	3.40	131.03	124.68
41	34	313	A86	C26-C25-C24	-3.40	112.62	123.22
41	39	311	A86	C9-C10-C11	-3.40	116.62	126.61
30	15	307	CLA	CHB-C4A-NA	3.40	129.21	124.51
41	33	302	A86	C3-C2-C1	-3.39	122.47	127.31
41	11	314	A86	C20-C19-C18	-3.39	106.03	112.75
41	35	316	A86	C3-C2-C1	-3.39	122.47	127.31
30	15	303	CLA	CMB-C2B-C3B	3.39	131.03	124.68
41	31	314	A86	C20-C19-C18	-3.39	106.04	112.75
31	d	404	PHO	O1D-CGD-CBD	3.39	130.39	124.74
30	18	308	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
30	31	303	CLA	CMB-C2B-C3B	3.39	131.02	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	306	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
41	37	313	A86	C26-C25-C24	-3.39	112.64	123.22
30	13	302	CLA	C1-C2-C3	-3.39	120.18	126.04
41	12	317	A86	C26-C25-C24	-3.39	112.65	123.22
30	C	506	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
41	13	313	A86	C26-C25-C24	-3.38	112.66	123.22
41	32	316	A86	C26-C25-C24	-3.38	112.66	123.22
41	31	311	A86	C36-C31-C32	-3.38	116.34	119.70
30	12	303	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
41	21	312	A86	C41-C32-C31	-3.38	107.45	110.47
30	17	305	CLA	CMB-C2B-C3B	3.38	131.00	124.68
30	B	612	CLA	CHB-C4A-NA	3.38	129.18	124.51
32	B	618	BCR	C24-C23-C22	-3.38	121.13	126.23
30	14	303	CLA	CHB-C4A-NA	3.37	129.18	124.51
41	41	310	A86	C4-C5-C6	-3.37	122.49	127.31
30	16	307	CLA	CHB-C4A-NA	3.37	129.18	124.51
41	35	316	A86	C40-C32-C31	-3.37	107.45	110.47
30	b	614	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
30	18	301	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
39	d	405	PL9	C7-C3-C2	-3.37	118.87	123.30
41	33	316	A86	C40-C32-C31	-3.37	107.46	110.47
30	15	301	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
30	b	612	CLA	CHB-C4A-NA	3.37	129.17	124.51
30	14	302	CLA	C1-C2-C3	-3.37	120.22	126.04
41	41	310	A86	C34-O4-C38	-3.37	111.62	117.90
41	35	312	A86	C26-C25-C24	-3.36	112.72	123.22
30	36	302	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
38	C	516	DGD	O5D-C6D-C5D	-3.36	102.82	109.05
41	33	313	A86	C36-C31-C32	-3.36	116.36	119.70
30	41	306	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
41	15	312	A86	C26-C25-C24	-3.36	112.72	123.22
30	34	303	CLA	CHB-C4A-NA	3.36	129.16	124.51
41	33	315	A86	C3-C4-C5	-3.36	116.59	123.47
30	38	301	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
30	16	302	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
30	33	304	CLA	CHB-C4A-NA	3.36	129.16	124.51
30	35	307	CLA	CHB-C4A-NA	3.36	129.16	124.51
41	21	310	A86	C34-O4-C38	-3.36	111.64	117.90
30	B	610	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
32	b	617	BCR	C24-C23-C22	-3.36	121.17	126.23
30	B	614	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
30	21	306	CLA	CMB-C2B-C1B	-3.35	123.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	11	311	A86	C36-C31-C32	-3.35	116.37	119.70
30	15	308	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
41	13	316	A86	C40-C32-C31	-3.35	107.47	110.47
30	32	307	CLA	CMB-C2B-C3B	3.35	130.95	124.68
30	11	301	CLA	C1-C2-C3	-3.35	120.25	126.04
30	14	308	CLA	CHB-C4A-NA	3.35	129.15	124.51
41	18	314	A86	C36-C31-C32	-3.35	116.37	119.70
30	32	306	CLA	CHB-C4A-NA	3.35	129.14	124.51
30	16	308	CLA	C2A-C1A-CHA	3.35	129.71	123.86
30	B	605	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
38	h	102	DGD	O3G-C3G-C2G	-3.35	102.83	110.90
41	37	314	A86	C3-C4-C5	-3.34	116.62	123.47
41	12	304	A86	C40-C32-C31	-3.34	107.48	110.47
30	12	306	CLA	CHB-C4A-NA	3.34	129.13	124.51
30	36	307	CLA	CHB-C4A-NA	3.34	129.13	124.51
30	c	522	CLA	CMB-C2B-C3B	3.34	130.93	124.68
30	12	305	CLA	CMB-C2B-C3B	3.34	130.93	124.68
41	13	314	A86	C3-C4-C5	-3.34	116.63	123.47
32	a	404	BCR	C15-C14-C13	-3.34	122.54	127.31
41	38	315	A86	C3-C4-C5	-3.34	116.63	123.47
30	35	308	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
38	H	102	DGD	O3G-C3G-C2G	-3.34	102.85	110.90
30	13	308	CLA	CHB-C4A-NA	3.34	129.13	124.51
30	B	603	CLA	CMB-C2B-C3B	3.34	130.92	124.68
30	b	601	CLA	CHB-C4A-NA	3.34	129.12	124.51
30	31	302	CLA	CHB-C4A-NA	3.33	129.12	124.51
30	41	304	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
41	33	302	A86	C40-C32-C31	-3.33	107.49	110.47
41	17	314	A86	C3-C4-C5	-3.33	116.65	123.47
41	18	315	A86	C3-C4-C5	-3.33	116.65	123.47
30	B	601	CLA	CHB-C4A-NA	3.33	129.12	124.51
30	13	303	CLA	CHB-C4A-NA	3.33	129.12	124.51
30	35	301	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
41	32	317	A86	C3-C4-C5	-3.33	116.66	123.47
41	19	310	A86	C28-C27-C26	-3.33	118.26	122.92
30	C	512	CLA	CHB-C4A-NA	3.33	129.11	124.51
30	12	305	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
30	31	301	CLA	CMB-C2B-C3B	3.33	130.90	124.68
41	38	314	A86	C36-C31-C32	-3.33	116.40	119.70
30	11	301	CLA	C1B-CHB-C4A	-3.32	123.53	130.12
41	31	313	A86	C3-C4-C5	-3.32	116.67	123.47
30	39	306	CLA	CMB-C2B-C1B	-3.32	123.36	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	12	318	A86	C3-C4-C5	-3.32	116.67	123.47
30	36	308	CLA	C2A-C1A-CHA	3.32	129.67	123.86
30	15	301	CLA	CHB-C4A-NA	3.32	129.10	124.51
30	18	303	CLA	CHB-C4A-NA	3.32	129.10	124.51
30	b	605	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
30	16	309	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
30	19	306	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
30	21	304	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
30	C	520	CLA	CMB-C2B-C3B	3.32	130.89	124.68
30	32	305	CLA	CMB-C2B-C3B	3.32	130.89	124.68
41	13	301	A86	C40-C32-C31	-3.32	107.50	110.47
41	14	314	A86	C3-C4-C5	-3.32	116.68	123.47
30	11	301	CLA	CMB-C2B-C3B	3.31	130.88	124.68
32	A	405	BCR	C15-C14-C13	-3.31	122.58	127.31
30	11	302	CLA	CHB-C4A-NA	3.31	129.09	124.51
41	37	314	A86	C12-C11-C13	3.31	121.58	116.02
41	11	313	A86	C3-C4-C5	-3.31	116.69	123.47
41	35	313	A86	C3-C4-C5	-3.31	116.69	123.47
41	39	310	A86	C28-C27-C26	-3.31	118.29	122.92
41	15	315	A86	C40-C32-C31	-3.31	107.51	110.47
30	21	302	CLA	CMB-C2B-C3B	3.31	130.87	124.68
41	15	313	A86	C3-C4-C5	-3.31	116.70	123.47
41	34	314	A86	C3-C4-C5	-3.31	116.70	123.47
30	13	302	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
30	12	313	CLA	CHB-C4A-NA	3.31	129.08	124.51
30	36	309	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
30	38	303	CLA	CHB-C4A-NA	3.30	129.08	124.51
41	32	317	A86	C12-C11-C13	3.30	121.57	116.02
30	33	303	CLA	CMB-C2B-C3B	3.30	130.85	124.68
30	13	302	CLA	CMB-C2B-C3B	3.30	130.85	124.68
30	34	308	CLA	CHB-C4A-NA	3.30	129.07	124.51
30	18	305	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
41	15	313	A86	C12-C11-C13	3.30	121.56	116.02
39	D	407	PL9	C7-C8-C9	-3.29	121.31	126.79
30	38	305	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
30	11	307	CLA	CHB-C4A-NA	3.29	129.07	124.51
30	b	603	CLA	CMB-C2B-C3B	3.29	130.84	124.68
30	15	302	CLA	CMB-C2B-C3B	3.29	130.84	124.68
30	14	302	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
30	41	302	CLA	CMB-C2B-C3B	3.28	130.82	124.68
30	17	303	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
41	35	313	A86	C12-C11-C13	3.28	121.53	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	18	303	CLA	C1B-CHB-C4A	-3.28	123.63	130.12
39	D	404	PL9	C7-C3-C2	-3.28	118.99	123.30
30	B	614	CLA	CMB-C2B-C3B	3.27	130.80	124.68
41	32	304	A86	C36-C31-C32	-3.27	116.45	119.70
41	11	313	A86	C12-C11-C13	3.27	121.52	116.02
41	18	315	A86	C12-C11-C13	3.27	121.52	116.02
41	34	314	A86	C12-C11-C13	3.27	121.52	116.02
30	34	309	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
30	a	403	CLA	CHB-C4A-NA	3.27	129.04	124.51
30	16	301	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
30	A	404	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
30	c	512	CLA	CHB-C4A-NA	3.27	129.03	124.51
41	35	315	A86	C40-C32-C31	-3.27	107.55	110.47
30	32	311	CLA	CHB-C4A-NA	3.27	129.03	124.51
30	35	301	CLA	CHB-C4A-NA	3.27	129.03	124.51
33	l	101	SQD	C1-O5-C5	3.27	120.10	113.69
30	35	305	CLA	CMB-C2B-C3B	3.27	130.79	124.68
30	37	303	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
30	32	312	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
30	34	309	CLA	CHB-C4A-NA	3.27	129.03	124.51
41	12	304	A86	C36-C31-C32	-3.27	116.46	119.70
41	31	313	A86	C12-C11-C13	3.26	121.51	116.02
33	a	405	SQD	O8-S-C6	3.26	110.94	105.74
41	12	318	A86	C12-C11-C13	3.26	121.50	116.02
41	14	314	A86	C12-C11-C13	3.26	121.50	116.02
30	31	308	CLA	CHB-C4A-NA	3.26	129.02	124.51
41	17	314	A86	C12-C11-C13	3.26	121.50	116.02
33	L	103	SQD	C1-O5-C5	3.26	120.09	113.69
41	34	314	A86	C10-C9-C8	-3.26	113.04	123.22
30	A	404	CLA	CHB-C4A-NA	3.26	129.02	124.51
30	35	302	CLA	CMB-C2B-C3B	3.26	130.78	124.68
41	20	201	A86	C10-C9-C8	-3.26	113.04	123.22
30	36	308	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
30	31	303	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
41	40	201	A86	C10-C9-C8	-3.26	113.06	123.22
30	16	306	CLA	CHB-C4A-NA	3.26	129.01	124.51
30	b	614	CLA	CMB-C2B-C3B	3.26	130.77	124.68
30	a	403	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
30	34	302	CLA	CMB-C2B-C3B	3.25	130.77	124.68
30	14	302	CLA	CMB-C2B-C3B	3.25	130.76	124.68
30	36	301	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
30	35	306	CLA	C1B-CHB-C4A	-3.25	123.68	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	604	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
30	33	310	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
41	13	314	A86	C12-C11-C13	3.25	121.48	116.02
41	33	315	A86	C12-C11-C13	3.25	121.48	116.02
30	C	506	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
30	16	308	CLA	CMB-C2B-C1B	-3.25	123.48	128.46
30	35	306	CLA	CHB-C4A-NA	3.24	129.00	124.51
41	38	315	A86	C12-C11-C13	3.24	121.47	116.02
42	32	302	LMU	O5B-C5B-C4B	3.24	115.58	109.69
41	40	211	A86	C4-C3-C2	-3.24	116.83	123.47
41	14	314	A86	C10-C9-C8	-3.24	113.10	123.22
39	d	408	PL9	C7-C8-C9	-3.24	121.40	126.79
30	15	306	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
30	14	309	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
30	38	303	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
30	15	305	CLA	CMB-C2B-C3B	3.24	130.74	124.68
41	13	316	A86	C36-C31-C32	-3.24	116.48	119.70
30	36	306	CLA	CHB-C4A-NA	3.24	128.99	124.51
30	C	506	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
30	M	101	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
30	c	506	CLA	O2D-CGD-O1D	-3.23	117.51	123.84
30	31	308	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
30	14	309	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	15	306	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	17	308	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	B	605	CLA	CHB-C4A-NA	3.23	128.98	124.51
41	15	316	A86	C36-C31-C32	-3.23	116.49	119.70
30	31	307	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	33	306	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
30	C	505	CLA	C3C-C4C-NC	-3.23	106.95	110.57
30	12	311	CLA	CHB-C4A-NA	3.23	128.98	124.51
30	11	308	CLA	CHB-C4A-NA	3.23	128.98	124.51
41	20	211	A86	C4-C3-C2	-3.23	116.86	123.47
41	35	316	A86	C36-C31-C32	-3.23	116.49	119.70
30	B	608	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
30	b	608	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
30	31	304	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
30	37	308	CLA	CHB-C4A-NA	3.23	128.97	124.51
41	38	315	A86	C10-C9-C8	-3.22	113.15	123.22
30	33	306	CLA	CHB-C4A-NA	3.22	128.97	124.51
41	37	312	A86	C12-C11-C13	3.22	121.44	116.02
41	35	311	A86	C12-C11-C13	3.22	121.43	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	608	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
30	c	506	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
41	17	312	A86	C12-C11-C13	3.22	121.43	116.02
41	15	313	A86	C10-C9-C8	-3.22	113.17	123.22
41	18	315	A86	C10-C9-C8	-3.22	113.17	123.22
41	32	317	A86	C10-C9-C8	-3.22	113.18	123.22
30	d	401	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
41	11	313	A86	C10-C9-C8	-3.22	113.18	123.22
30	12	308	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
41	20	212	A86	C17-C16-C15	3.22	112.44	109.16
33	A	406	SQD	O8-S-C6	3.22	110.86	105.74
30	19	304	CLA	CHB-C4A-NA	3.21	128.96	124.51
41	31	313	A86	C10-C9-C8	-3.21	113.19	123.22
41	15	311	A86	C12-C11-C13	3.21	121.42	116.02
30	D	401	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
30	34	305	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
30	C	508	CLA	CHB-C4A-NA	3.21	128.95	124.51
30	b	608	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
32	a	404	BCR	C24-C23-C22	-3.21	121.39	126.23
30	13	304	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
30	11	308	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
41	31	316	A86	C36-C31-C32	-3.21	116.51	119.70
41	12	318	A86	C10-C9-C8	-3.21	113.21	123.22
30	13	309	CLA	CHB-C4A-NA	3.21	128.95	124.51
30	33	305	CLA	CAA-C2A-C3A	-3.21	104.00	112.78
30	32	312	CLA	CHB-C4A-NA	3.21	128.94	124.51
41	35	313	A86	C10-C9-C8	-3.21	113.21	123.22
41	17	314	A86	C10-C9-C8	-3.20	113.22	123.22
41	20	210	A86	C12-C11-C13	3.20	121.40	116.02
30	B	604	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
30	37	310	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
30	13	309	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
40	E	101	HEM	CMC-C2C-C3C	3.20	130.67	124.68
41	41	311	A86	C4-C3-C2	-3.20	116.92	123.47
41	20	210	A86	C41-C32-C31	-3.20	107.61	110.47
30	b	602	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
41	13	314	A86	C10-C9-C8	-3.20	113.23	123.22
41	13	312	A86	C12-C11-C13	3.20	121.40	116.02
41	21	311	A86	C4-C3-C2	-3.20	116.92	123.47
41	33	315	A86	C10-C9-C8	-3.20	113.23	123.22
41	33	313	A86	C12-C11-C13	3.20	121.40	116.02
32	A	405	BCR	C24-C23-C22	-3.20	121.40	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	m	101	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
30	32	308	CLA	C2A-C1A-CHA	3.20	129.45	123.86
41	37	314	A86	C10-C9-C8	-3.20	113.24	123.22
30	34	304	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
30	B	602	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
30	15	302	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
41	40	210	A86	C41-C32-C31	-3.19	107.62	110.47
41	41	311	A86	C4-C5-C6	-3.19	122.76	127.31
41	11	316	A86	C36-C31-C32	-3.19	116.53	119.70
41	15	315	A86	C36-C31-C32	-3.19	116.53	119.70
30	20	206	CLA	CHB-C4A-NA	3.19	128.92	124.51
41	31	311	A86	C12-C11-C13	3.19	121.38	116.02
41	11	311	A86	C12-C11-C13	3.19	121.37	116.02
30	32	307	CLA	CAA-C2A-C3A	-3.19	104.06	112.78
30	33	310	CLA	CHB-C4A-NA	3.18	128.92	124.51
40	e	101	HEM	CMC-C2C-C3C	3.18	130.64	124.68
30	b	605	CLA	CHB-C4A-NA	3.18	128.91	124.51
41	21	313	A86	C7-C6-C8	3.18	123.09	118.08
30	12	313	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
30	11	304	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
30	12	307	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
30	39	304	CLA	CHB-C4A-NA	3.18	128.91	124.51
41	35	315	A86	C36-C31-C32	-3.18	116.54	119.70
30	40	207	CLA	CMB-C2B-C3B	3.18	130.63	124.68
30	14	305	CLA	CHB-C4A-NA	3.18	128.91	124.51
38	C	516	DGD	O6D-C1D-O3G	-3.18	102.44	109.97
41	33	316	A86	C36-C31-C32	-3.18	116.54	119.70
30	35	302	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
30	33	309	CLA	CHB-C4A-NA	3.18	128.91	124.51
41	13	301	A86	C36-C31-C32	-3.18	116.54	119.70
30	32	308	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
30	14	304	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
41	33	302	A86	C36-C31-C32	-3.18	116.54	119.70
30	12	308	CLA	CHB-C4A-NA	3.18	128.91	124.51
30	20	207	CLA	CMB-C2B-C3B	3.18	130.62	124.68
30	13	305	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
30	17	310	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
41	18	314	A86	C12-C11-C13	3.17	121.35	116.02
30	17	309	CLA	CHB-C4A-NA	3.17	128.90	124.51
30	31	307	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
30	14	305	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
30	11	303	CLA	CAA-C2A-C3A	-3.17	104.09	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	40	210	A86	C12-C11-C13	3.17	121.35	116.02
30	B	608	CLA	CHB-C4A-NA	3.17	128.90	124.51
30	b	609	CLA	CHB-C4A-NA	3.17	128.90	124.51
41	21	311	A86	C4-C5-C6	-3.17	122.78	127.31
41	34	312	A86	C12-C11-C13	3.17	121.35	116.02
41	20	211	A86	C4-C5-C6	-3.17	122.78	127.31
30	b	608	CLA	CHB-C4A-NA	3.17	128.90	124.51
41	41	313	A86	C7-C6-C8	3.17	123.07	118.08
30	32	311	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
30	c	513	CLA	CMB-C2B-C3B	3.17	130.61	124.68
42	12	302	LMU	C3'-C4'-C5'	3.17	118.19	110.93
41	12	316	A86	C12-C11-C13	3.17	121.34	116.02
30	40	206	CLA	CHB-C4A-NA	3.17	128.89	124.51
30	B	609	CLA	CHB-C4A-NA	3.17	128.89	124.51
41	14	312	A86	C12-C11-C13	3.16	121.34	116.02
30	32	308	CLA	CHB-C4A-NA	3.16	128.89	124.51
30	31	304	CLA	C2A-C1A-CHA	3.16	129.39	123.86
30	18	311	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
30	W	102	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
38	c	517	DGD	O6D-C1D-O3G	-3.16	102.50	109.97
30	20	204	CLA	CMB-C2B-C3B	3.16	130.58	124.68
30	36	303	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
30	38	304	CLA	CHB-C4A-NA	3.15	128.87	124.51
41	37	302	A86	C40-C32-C31	-3.15	107.65	110.47
30	33	309	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
30	34	308	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
42	12	302	LMU	O5B-C5B-C4B	3.15	115.41	109.69
41	31	314	A86	C10-C9-C8	-3.15	113.39	123.22
41	16	310	A86	C41-C32-C31	-3.15	107.65	110.47
41	41	314	A86	C3-C4-C5	-3.15	117.02	123.47
41	13	317	A86	C10-C9-C8	-3.15	113.39	123.22
41	32	315	A86	C12-C11-C13	3.15	121.31	116.02
42	32	302	LMU	C3'-C4'-C5'	3.15	118.14	110.93
30	16	303	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
41	36	313	A86	C10-C9-C8	-3.15	113.40	123.22
30	c	505	CLA	C3C-C4C-NC	-3.15	107.04	110.57
30	37	309	CLA	CHB-C4A-NA	3.15	128.86	124.51
41	13	315	A86	C10-C9-C8	-3.15	113.40	123.22
30	w	103	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
30	c	508	CLA	CHB-C4A-NA	3.14	128.86	124.51
41	40	212	A86	C17-C16-C15	3.14	112.37	109.16
30	34	305	CLA	CHB-C4A-NA	3.14	128.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	11	314	A86	C10-C9-C8	-3.14	113.41	123.22
30	31	304	CLA	CHB-C4A-NA	3.14	128.86	124.51
41	40	211	A86	C4-C5-C6	-3.14	122.83	127.31
30	34	305	CLA	C2A-C1A-CHA	3.14	129.35	123.86
41	16	313	A86	C10-C9-C8	-3.14	113.42	123.22
41	17	302	A86	C40-C32-C31	-3.14	107.66	110.47
30	d	406	CLA	CAA-C2A-C3A	-3.14	104.18	112.78
41	33	317	A86	C10-C9-C8	-3.14	113.43	123.22
41	38	314	A86	C12-C11-C13	3.14	121.29	116.02
30	20	204	CLA	CHB-C4A-NA	3.14	128.85	124.51
41	15	314	A86	C10-C9-C8	-3.14	113.43	123.22
41	41	310	A86	C25-C24-C1	-3.14	117.61	126.42
30	16	303	CLA	CHB-C4A-NA	3.13	128.85	124.51
41	35	314	A86	C10-C9-C8	-3.13	113.44	123.22
41	32	318	A86	C10-C9-C8	-3.13	113.44	123.22
30	40	204	CLA	CMB-C2B-C3B	3.13	130.54	124.68
30	38	311	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
30	D	405	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
41	32	319	A86	C10-C9-C8	-3.13	113.44	123.22
30	18	304	CLA	CHB-C4A-NA	3.13	128.84	124.51
41	37	316	A86	C10-C9-C8	-3.13	113.46	123.22
41	18	302	A86	C36-C31-C32	-3.13	116.59	119.70
30	W	103	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
41	21	310	A86	C25-C24-C1	-3.13	117.63	126.42
30	C	521	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
30	w	102	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
30	36	303	CLA	CHB-C4A-NA	3.12	128.83	124.51
30	19	301	CLA	CMB-C2B-C3B	3.12	130.52	124.68
41	21	314	A86	C3-C4-C5	-3.12	117.08	123.47
41	39	310	A86	C40-C32-C31	-3.12	107.68	110.47
30	39	301	CLA	CMB-C2B-C3B	3.12	130.51	124.68
30	33	306	CLA	C2A-C1A-CHA	3.12	129.31	123.86
41	36	311	A86	C12-C11-C13	3.12	121.26	116.02
41	16	311	A86	C12-C11-C13	3.12	121.26	116.02
41	40	213	A86	C3-C4-C5	-3.11	117.09	123.47
41	12	319	A86	C10-C9-C8	-3.11	113.50	123.22
41	38	302	A86	C36-C31-C32	-3.11	116.61	119.70
41	19	310	A86	C40-C32-C31	-3.11	107.69	110.47
41	41	314	A86	C4-C5-C6	-3.11	122.87	127.31
30	C	513	CLA	CMB-C2B-C3B	3.11	130.50	124.68
30	14	309	CLA	CAA-C2A-C1A	3.11	122.17	111.97
30	13	309	CLA	CAA-C2A-C1A	3.11	122.17	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	624	BCR	C7-C8-C9	-3.11	121.54	126.23
41	36	310	A86	C41-C32-C31	-3.11	107.69	110.47
30	37	301	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
30	c	523	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
41	17	316	A86	C10-C9-C8	-3.10	113.53	123.22
41	40	213	A86	C4-C5-C6	-3.10	122.88	127.31
30	17	308	CLA	C4-C3-C5	3.10	120.49	115.27
30	34	308	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
30	C	505	CLA	CMB-C2B-C3B	3.10	130.47	124.68
30	31	307	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
41	41	310	A86	C36-C31-C32	-3.09	116.63	119.70
30	11	308	CLA	CAA-C2A-C1A	3.09	122.11	111.97
41	21	314	A86	C4-C5-C6	-3.09	122.90	127.31
30	b	622	CLA	CAA-C2A-C1A	3.09	122.10	111.97
41	20	213	A86	C3-C4-C5	-3.09	117.14	123.47
32	c	515	BCR	C24-C23-C22	-3.09	121.56	126.23
30	D	402	CLA	CMB-C2B-C3B	3.09	130.46	124.68
30	15	307	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
30	14	309	CLA	CMB-C2B-C3B	3.09	130.46	124.68
30	32	312	CLA	CAA-C2A-C1A	3.09	122.09	111.97
41	20	213	A86	C4-C5-C6	-3.09	122.90	127.31
30	12	313	CLA	CAA-C2A-C1A	3.09	122.09	111.97
30	35	307	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
41	40	212	A86	C25-C24-C1	-3.08	117.75	126.42
30	33	309	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
30	33	310	CLA	CMB-C2B-C3B	3.08	130.45	124.68
30	39	304	CLA	C2A-C1A-CHA	3.08	129.25	123.86
30	40	204	CLA	CHB-C4A-NA	3.08	128.77	124.51
30	c	508	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
30	37	310	CLA	CMB-C2B-C3B	3.08	130.44	124.68
30	31	307	CLA	C1-C2-C3	-3.08	120.72	126.04
30	17	301	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
30	w	102	CLA	CMB-C2B-C3B	3.08	130.44	124.68
30	12	313	CLA	CMB-C2B-C3B	3.08	130.44	124.68
30	32	311	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
30	d	402	CLA	CMB-C2B-C3B	3.07	130.43	124.68
30	11	304	CLA	C2A-C1A-CHA	3.07	129.24	123.86
33	l	101	SQD	C3-C4-C5	3.07	115.72	110.24
30	35	304	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
41	20	212	A86	C25-C24-C1	-3.07	117.78	126.42
30	c	505	CLA	CMB-C2B-C3B	3.07	130.43	124.68
30	18	311	CLA	CHB-C4A-NA	3.07	128.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	304	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
38	C	516	DGD	C1D-C2D-C3D	-3.07	103.60	110.00
30	c	505	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	31	308	CLA	CAA-C2A-C1A	3.07	122.03	111.97
30	37	308	CLA	C4-C3-C5	3.07	120.43	115.27
30	12	307	CLA	CBA-CAA-C2A	3.07	122.92	113.86
30	34	304	CLA	CBA-CAA-C2A	3.07	122.92	113.86
30	32	311	CLA	C1-C2-C3	-3.07	120.74	126.04
30	B	615	CLA	CMB-C2B-C3B	3.07	130.41	124.68
30	34	309	CLA	CMB-C2B-C3B	3.07	130.41	124.68
32	A	409	BCR	C11-C10-C9	-3.06	122.94	127.31
30	33	310	CLA	CAA-C2A-C1A	3.06	122.01	111.97
41	36	310	A86	C26-C25-C24	-3.06	113.66	123.22
30	17	310	CLA	CMB-C2B-C3B	3.06	130.41	124.68
30	41	301	CLA	CMB-C2B-C3B	3.06	130.41	124.68
30	11	304	CLA	CHB-C4A-NA	3.06	128.75	124.51
30	33	309	CLA	C1-C2-C3	-3.06	120.75	126.04
30	32	312	CLA	CMB-C2B-C3B	3.06	130.40	124.68
30	34	309	CLA	CAA-C2A-C1A	3.06	122.00	111.97
30	16	304	CLA	CMB-C2B-C3B	3.06	130.40	124.68
30	11	303	CLA	CBA-CAA-C2A	3.06	122.89	113.86
30	C	504	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
30	d	407	CLA	CMB-C2B-C3B	3.06	130.40	124.68
41	11	313	A86	C36-C31-C32	-3.06	116.66	119.70
30	B	623	CLA	CAA-C2A-C1A	3.06	121.99	111.97
30	13	305	CLA	CHB-C4A-NA	3.06	128.74	124.51
30	33	307	CLA	CHB-C4A-NA	3.06	128.74	124.51
30	14	304	CLA	CBA-CAA-C2A	3.06	122.88	113.86
35	a	407	LHG	O8-C23-C24	3.06	121.50	111.91
30	C	508	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
41	16	310	A86	C26-C25-C24	-3.05	113.69	123.22
30	13	309	CLA	CMB-C2B-C3B	3.05	130.38	124.68
41	17	302	A86	C12-C11-C13	3.05	121.14	116.02
41	21	310	A86	C36-C31-C32	-3.05	116.67	119.70
30	18	311	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
30	21	301	CLA	CMB-C2B-C3B	3.05	130.38	124.68
30	c	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
30	38	311	CLA	CHB-C4A-NA	3.05	128.72	124.51
30	13	304	CLA	CBA-CAA-C2A	3.04	122.85	113.86
32	a	408	BCR	C11-C10-C9	-3.04	122.97	127.31
30	19	304	CLA	C2A-C1A-CHA	3.04	129.18	123.86
35	A	408	LHG	O8-C23-C24	3.04	121.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	19	303	CLA	CHB-C4A-NA	3.04	128.72	124.51
30	38	311	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
30	34	310	CLA	CMB-C2B-C3B	3.04	130.37	124.68
30	39	302	CLA	CHB-C4A-NA	3.04	128.71	124.51
30	B	601	CLA	CMB-C2B-C3B	3.04	130.36	124.68
33	L	103	SQD	C3-C4-C5	3.04	115.66	110.24
41	37	302	A86	C12-C11-C13	3.04	121.12	116.02
30	13	308	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
41	21	313	A86	C10-C9-C8	-3.03	113.75	123.22
30	19	302	CLA	CHB-C4A-NA	3.03	128.71	124.51
30	D	406	CLA	CMB-C2B-C3B	3.03	130.35	124.68
32	b	616	BCR	C15-C14-C13	-3.03	122.98	127.31
30	33	305	CLA	CBA-CAA-C2A	3.03	122.81	113.86
30	31	303	CLA	CBA-CAA-C2A	3.03	122.81	113.86
41	33	315	A86	C36-C31-C32	-3.03	116.69	119.70
30	c	507	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
41	41	313	A86	C10-C9-C8	-3.03	113.77	123.22
42	32	302	LMU	O5'-C5'-C4'	3.03	116.14	109.75
33	B	621	SQD	O9-S-C6	3.03	110.54	106.94
30	34	308	CLA	C1-C2-C3	-3.03	120.81	126.04
30	b	601	CLA	CMB-C2B-C3B	3.03	130.34	124.68
30	d	402	CLA	CHB-C4A-NA	3.03	128.70	124.51
30	14	308	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
41	18	314	A86	C3-C4-C5	-3.03	117.28	123.47
30	16	309	CLA	CMB-C2B-C3B	3.03	130.34	124.68
39	d	405	PL9	C41-C39-C38	-3.02	115.00	121.12
41	18	315	A86	C36-C31-C32	-3.02	116.69	119.70
30	13	305	CLA	C2A-C1A-CHA	3.02	129.15	123.86
30	32	307	CLA	CBA-CAA-C2A	3.02	122.79	113.86
41	13	314	A86	C36-C31-C32	-3.02	116.70	119.70
32	B	617	BCR	C15-C14-C13	-3.02	123.00	127.31
30	36	304	CLA	CMB-C2B-C3B	3.02	130.33	124.68
30	40	207	CLA	CHB-C4A-NA	3.02	128.69	124.51
30	W	102	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
30	35	302	CLA	C2A-C1A-CHA	3.02	129.14	123.86
30	11	308	CLA	CMB-C2B-C3B	3.02	130.33	124.68
38	C	517	DGD	CDB-CCB-CBB	-3.02	99.10	114.42
30	31	308	CLA	CMB-C2B-C3B	3.02	130.32	124.68
30	39	303	CLA	CHB-C4A-NA	3.02	128.69	124.51
32	C	515	BCR	C11-C10-C9	-3.02	123.00	127.31
41	37	311	A86	C9-C10-C11	-3.02	117.74	126.61
30	17	304	CLA	CHB-C4A-NA	3.02	128.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	512	CLA	CAA-CBA-CGA	-3.02	104.44	113.25
30	B	609	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
41	17	302	A86	C41-C32-C31	-3.01	107.77	110.47
41	39	311	A86	C9-C8-C6	-3.01	117.95	126.42
30	12	311	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
30	D	406	CLA	CHB-C4A-NA	3.01	128.68	124.51
41	32	316	A86	C35-C34-C33	3.01	115.13	109.88
30	C	502	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
41	20	213	A86	C10-C9-C8	-3.01	113.82	123.22
33	b	620	SQD	O9-S-C6	3.01	110.52	106.94
30	w	102	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
30	15	308	CLA	CMB-C2B-C3B	3.01	130.31	124.68
41	31	313	A86	C36-C31-C32	-3.01	116.71	119.70
30	d	407	CLA	CHB-C4A-NA	3.01	128.68	124.51
30	32	307	CLA	CHB-C4A-NA	3.01	128.68	124.51
41	13	313	A86	C35-C34-C33	3.01	115.13	109.88
34	A	407	BCT	O3-C-O1	-3.01	111.74	119.55
41	17	315	A86	C7-C6-C5	-3.01	118.71	122.92
30	C	507	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
34	a	406	BCT	O3-C-O1	-3.01	111.74	119.55
41	33	314	A86	C35-C34-C33	3.01	115.13	109.88
38	c	517	DGD	C1D-C2D-C3D	-3.01	103.73	110.00
41	19	311	A86	C9-C8-C6	-3.01	117.97	126.42
41	38	314	A86	C3-C4-C5	-3.01	117.31	123.47
30	31	309	CLA	CMB-C2B-C3B	3.01	130.30	124.68
30	B	605	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
30	b	614	CLA	O2D-CGD-CBD	3.01	116.61	111.27
30	11	307	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
30	b	615	CLA	CMB-C2B-C3B	3.01	130.30	124.68
41	37	313	A86	C35-C34-C33	3.01	115.12	109.88
41	41	310	A86	C12-C11-C13	3.01	121.07	116.02
41	17	311	A86	C9-C10-C11	-3.01	117.77	126.61
30	b	605	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
41	41	310	A86	C3-C4-C5	-3.00	117.32	123.47
41	35	313	A86	C36-C31-C32	-3.00	116.72	119.70
30	c	508	CLA	C2A-C1A-CHA	3.00	129.11	123.86
30	36	309	CLA	CMB-C2B-C3B	3.00	130.30	124.68
30	37	304	CLA	CHB-C4A-NA	3.00	128.66	124.51
41	31	313	A86	C25-C24-C1	-3.00	117.98	126.42
38	c	518	DGD	CDB-CCB-CBB	-3.00	99.19	114.42
41	40	213	A86	C10-C9-C8	-3.00	113.85	123.22
41	31	316	A86	C7-C6-C5	-3.00	118.72	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	12	302	LMU	O5'-C5'-C4'	3.00	116.08	109.75
30	W	102	CLA	CMB-C2B-C3B	3.00	130.29	124.68
30	19	305	CLA	CHB-C4A-NA	3.00	128.66	124.51
30	34	306	CLA	CHB-C4A-NA	3.00	128.66	124.51
33	a	405	SQD	O48-C23-C24	3.00	121.32	111.91
30	15	309	CLA	CMB-C2B-C3B	3.00	130.29	124.68
41	21	310	A86	C12-C11-C13	3.00	121.06	116.02
30	b	614	CLA	CHB-C4A-NA	3.00	128.66	124.51
41	34	313	A86	C35-C34-C33	3.00	115.11	109.88
41	21	314	A86	C10-C9-C8	-3.00	113.87	123.22
41	21	310	A86	C3-C4-C5	-3.00	117.34	123.47
30	B	611	CLA	CMB-C2B-C3B	3.00	130.28	124.68
41	14	314	A86	C25-C24-C1	-2.99	118.00	126.42
41	17	313	A86	C35-C34-C33	2.99	115.10	109.88
30	35	308	CLA	CMB-C2B-C3B	2.99	130.28	124.68
30	b	609	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
41	34	314	A86	C36-C31-C32	-2.99	116.72	119.70
41	12	317	A86	C35-C34-C33	2.99	115.10	109.88
30	35	309	CLA	CMB-C2B-C3B	2.99	130.28	124.68
30	c	512	CLA	CAA-CBA-CGA	-2.99	104.50	113.25
41	34	314	A86	C25-C24-C1	-2.99	118.01	126.42
30	38	312	CLA	CMB-C2B-C3B	2.99	130.28	124.68
41	37	312	A86	C3-C4-C5	-2.99	117.34	123.47
30	c	505	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
41	41	314	A86	C10-C9-C8	-2.99	113.88	123.22
41	15	314	A86	C41-C32-C31	-2.99	107.80	110.47
30	15	302	CLA	C2A-C1A-CHA	2.99	129.09	123.86
41	12	304	A86	C7-C6-C5	-2.99	118.73	122.92
30	C	505	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
41	12	318	A86	C25-C24-C1	-2.99	118.02	126.42
30	39	305	CLA	CMB-C2B-C3B	2.99	130.27	124.68
41	32	317	A86	C36-C31-C32	-2.99	116.73	119.70
30	B	614	CLA	CHB-C4A-NA	2.99	128.65	124.51
41	15	313	A86	C25-C24-C1	-2.99	118.02	126.42
30	17	306	CLA	CHB-C4A-NA	2.99	128.64	124.51
41	38	315	A86	C25-C24-C1	-2.99	118.02	126.42
32	Z	101	BCR	C24-C23-C22	-2.99	121.72	126.23
30	32	313	CLA	CMB-C2B-C3B	2.99	130.27	124.68
30	33	311	CLA	CMB-C2B-C3B	2.99	130.26	124.68
30	19	308	CLA	CHB-C4A-NA	2.98	128.64	124.51
30	20	207	CLA	CHB-C4A-NA	2.98	128.64	124.51
33	A	406	SQD	O48-C23-C24	2.98	121.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	15	313	A86	C36-C31-C32	-2.98	116.73	119.70
30	C	519	CLA	CMB-C2B-C3B	2.98	130.26	124.68
41	11	313	A86	C25-C24-C1	-2.98	118.03	126.42
39	D	404	PL9	C41-C39-C38	-2.98	115.08	121.12
30	39	308	CLA	CHB-C4A-NA	2.98	128.64	124.51
30	12	308	CLA	C2A-C1A-CHA	2.98	129.07	123.86
41	14	313	A86	C35-C34-C33	2.98	115.08	109.88
41	17	312	A86	C3-C4-C5	-2.98	117.36	123.47
30	12	310	CLA	CMB-C2B-C3B	2.98	130.26	124.68
41	35	313	A86	C25-C24-C1	-2.98	118.04	126.42
30	19	305	CLA	CMB-C2B-C3B	2.98	130.26	124.68
30	18	312	CLA	CMB-C2B-C3B	2.98	130.26	124.68
41	33	302	A86	C7-C6-C5	-2.98	118.75	122.92
41	36	312	A86	C35-C34-C33	2.98	115.08	109.88
32	c	516	BCR	C11-C10-C9	-2.98	123.06	127.31
30	18	311	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
30	15	308	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
41	15	311	A86	C3-C4-C5	-2.98	117.37	123.47
41	32	317	A86	C25-C24-C1	-2.98	118.05	126.42
41	37	315	A86	C7-C6-C5	-2.98	118.75	122.92
30	35	304	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
30	31	315	CLA	CHB-C4A-NA	2.98	128.63	124.51
30	38	311	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
30	18	305	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
41	18	315	A86	C25-C24-C1	-2.98	118.06	126.42
30	38	307	CLA	CMB-C2B-C3B	2.98	130.25	124.68
36	b	619	LMG	O6-C1-O1	-2.98	102.93	109.97
30	15	304	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
35	B	622	LHG	O8-C23-C24	2.97	121.24	111.91
41	34	312	A86	C3-C4-C5	-2.97	117.38	123.47
30	b	604	CLA	CHB-C4A-NA	2.97	128.62	124.51
30	z	101	CLA	CMB-C2B-C3B	2.97	130.24	124.68
30	18	307	CLA	CMB-C2B-C3B	2.97	130.24	124.68
32	A	405	BCR	C11-C10-C9	-2.97	123.07	127.31
30	37	306	CLA	CHB-C4A-NA	2.97	128.62	124.51
30	C	508	CLA	C2A-C1A-CHA	2.97	129.06	123.86
30	13	307	CLA	CMB-C2B-C3B	2.97	130.24	124.68
30	14	305	CLA	C2A-C1A-CHA	2.97	129.06	123.86
41	36	311	A86	C3-C4-C5	-2.97	117.39	123.47
30	41	309	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
30	C	506	CLA	C2D-C1D-ND	-2.97	107.92	110.10
41	15	316	A86	C7-C6-C5	-2.97	118.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	621	LHG	O8-C23-C24	2.97	121.23	111.91
30	35	305	CLA	CHB-C4A-NA	2.97	128.62	124.51
41	33	315	A86	C25-C24-C1	-2.97	118.08	126.42
41	38	315	A86	C36-C31-C32	-2.97	116.75	119.70
30	15	305	CLA	CHB-C4A-NA	2.97	128.62	124.51
30	14	308	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
30	38	305	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
41	11	316	A86	C7-C6-C5	-2.97	118.77	122.92
41	35	315	A86	C7-C6-C5	-2.97	118.77	122.92
30	17	306	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
41	13	301	A86	C7-C6-C5	-2.97	118.77	122.92
41	13	314	A86	C25-C24-C1	-2.97	118.08	126.42
41	15	312	A86	C35-C34-C33	2.97	115.05	109.88
41	14	314	A86	C36-C31-C32	-2.97	116.75	119.70
41	32	304	A86	C7-C6-C5	-2.97	118.77	122.92
30	35	308	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
30	b	610	CLA	CMB-C2B-C3B	2.97	130.23	124.68
41	33	313	A86	C3-C4-C5	-2.97	117.40	123.47
41	35	316	A86	C7-C6-C5	-2.96	118.77	122.92
41	12	318	A86	C36-C31-C32	-2.96	116.75	119.70
32	B	624	BCR	C11-C10-C9	-2.96	123.08	127.31
30	33	301	CLA	CHB-C4A-NA	2.96	128.61	124.51
30	20	208	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	12	303	CLA	CHB-C4A-NA	2.96	128.61	124.51
30	32	310	CLA	CHB-C4A-NA	2.96	128.61	124.51
30	41	302	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
30	16	305	CLA	CHB-C4A-NA	2.96	128.61	124.51
30	b	611	CLA	CMB-C2B-C3B	2.96	130.22	124.68
30	39	305	CLA	CHB-C4A-NA	2.96	128.60	124.51
41	35	311	A86	C3-C4-C5	-2.96	117.41	123.47
30	37	306	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
30	C	505	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
41	12	316	A86	C3-C4-C5	-2.96	117.42	123.47
41	16	311	A86	C3-C4-C5	-2.96	117.42	123.47
41	37	314	A86	C25-C24-C1	-2.96	118.11	126.42
41	16	312	A86	C35-C34-C33	2.96	115.04	109.88
30	12	311	CLA	C1-C2-C3	-2.96	120.93	126.04
30	21	307	CLA	CMB-C2B-C3B	2.96	130.21	124.68
32	c	516	BCR	C15-C16-C17	-2.96	117.42	123.47
32	C	515	BCR	C15-C16-C17	-2.96	117.42	123.47
41	37	302	A86	C41-C32-C31	-2.96	107.83	110.47
41	17	314	A86	C25-C24-C1	-2.96	118.11	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	13	312	A86	C3-C4-C5	-2.95	117.42	123.47
41	35	312	A86	C35-C34-C33	2.95	115.03	109.88
41	37	313	A86	C12-C11-C13	2.95	120.98	116.02
41	35	314	A86	C41-C32-C31	-2.95	107.83	110.47
30	B	605	CLA	CMB-C2B-C3B	2.95	130.20	124.68
41	15	312	A86	C12-C11-C13	2.95	120.98	116.02
41	35	312	A86	C12-C11-C13	2.95	120.98	116.02
30	36	305	CLA	CHB-C4A-NA	2.95	128.59	124.51
30	16	306	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
30	21	302	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
30	32	309	CLA	CHB-C4A-NA	2.95	128.59	124.51
30	38	303	CLA	CMB-C2B-C3B	2.95	130.20	124.68
41	16	313	A86	C41-C32-C31	-2.95	107.83	110.47
30	21	308	CLA	CMB-C2B-C3B	2.95	130.19	124.68
41	19	311	A86	C7-C6-C5	-2.95	118.79	122.92
41	31	311	A86	C3-C4-C5	-2.95	117.44	123.47
30	B	610	CLA	CMB-C2B-C3B	2.95	130.19	124.68
41	12	317	A86	C12-C11-C13	2.95	120.97	116.02
41	37	314	A86	C36-C31-C32	-2.95	116.77	119.70
30	17	308	CLA	CMB-C2B-C3B	2.95	130.19	124.68
41	15	315	A86	C7-C6-C5	-2.95	118.80	122.92
30	B	614	CLA	O2D-CGD-CBD	2.94	116.50	111.27
30	11	305	CLA	CHB-C4A-NA	2.94	128.58	124.51
30	41	308	CLA	CMB-C2B-C3B	2.94	130.19	124.68
41	14	314	A86	C7-C6-C8	2.94	122.72	118.08
30	13	308	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
30	40	208	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
41	14	313	A86	C12-C11-C13	2.94	120.96	116.02
41	13	316	A86	C7-C6-C5	-2.94	118.80	122.92
41	11	312	A86	C35-C34-C33	2.94	115.01	109.88
41	31	312	A86	C35-C34-C33	2.94	115.01	109.88
41	32	316	A86	C12-C11-C13	2.94	120.96	116.02
30	14	307	CLA	CHB-C4A-NA	2.94	128.58	124.51
36	B	620	LMG	O6-C1-O1	-2.94	103.01	109.97
30	15	301	CLA	CMB-C2B-C3B	2.94	130.18	124.68
41	18	302	A86	C7-C6-C5	-2.94	118.81	122.92
41	33	316	A86	C7-C6-C5	-2.94	118.81	122.92
41	39	311	A86	C7-C6-C5	-2.94	118.81	122.92
30	35	301	CLA	CMB-C2B-C3B	2.94	130.18	124.68
31	d	403	PHO	O1D-CGD-CBD	2.94	129.63	124.74
30	33	308	CLA	CHB-C4A-NA	2.94	128.57	124.51
30	d	402	CLA	C1B-CHB-C4A	-2.94	124.30	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	40	201	A86	C4-C5-C6	-2.94	123.12	127.31
30	41	307	CLA	CMB-C2B-C3B	2.94	130.17	124.68
30	D	402	CLA	CHB-C4A-NA	2.94	128.57	124.51
41	11	311	A86	C3-C4-C5	-2.94	117.46	123.47
30	33	305	CLA	CHB-C4A-NA	2.94	128.57	124.51
41	17	313	A86	C12-C11-C13	2.94	120.95	116.02
30	12	309	CLA	CHB-C4A-NA	2.94	128.57	124.51
41	38	302	A86	C7-C6-C5	-2.93	118.81	122.92
30	18	306	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
30	11	306	CLA	CMB-C2B-C3B	2.93	130.17	124.68
41	34	313	A86	C12-C11-C13	2.93	120.95	116.02
41	20	201	A86	C4-C5-C6	-2.93	123.12	127.31
41	37	315	A86	C17-C16-C15	2.93	112.16	109.16
30	c	502	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	13	306	CLA	CHB-C4A-NA	2.93	128.57	124.51
41	14	312	A86	C3-C4-C5	-2.93	117.47	123.47
30	b	613	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	33	308	CLA	CMB-C2B-C3B	2.93	130.16	124.68
30	37	309	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	32	303	CLA	CHB-C4A-NA	2.93	128.56	124.51
30	18	303	CLA	CMB-C2B-C3B	2.93	130.16	124.68
30	37	308	CLA	CMB-C2B-C3B	2.93	130.16	124.68
30	21	309	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
30	38	306	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
31	A	403	PHO	O1D-CGD-CBD	2.93	129.61	124.74
30	C	509	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
41	16	312	A86	C12-C11-C13	2.93	120.94	116.02
41	36	312	A86	C12-C11-C13	2.93	120.94	116.02
30	c	509	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
41	34	314	A86	C7-C6-C8	2.93	122.69	118.08
30	13	310	CLA	CMB-C2B-C3B	2.93	130.15	124.68
30	41	303	CLA	CMB-C2B-C3B	2.93	130.15	124.68
30	11	307	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
41	32	319	A86	C41-C32-C31	-2.92	107.86	110.47
30	36	306	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
30	11	303	CLA	CHB-C4A-NA	2.92	128.56	124.51
41	17	314	A86	C36-C31-C32	-2.92	116.80	119.70
30	31	305	CLA	CHB-C4A-NA	2.92	128.55	124.51
30	14	310	CLA	CMB-C2B-C3B	2.92	130.14	124.68
41	17	312	A86	C34-O4-C38	-2.92	112.45	117.90
30	41	305	CLA	CHB-C4A-NA	2.92	128.55	124.51
41	17	315	A86	C17-C16-C15	2.92	112.14	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	33	315	A86	C4-C5-C6	-2.92	123.14	127.31
30	11	309	CLA	CMB-C2B-C3B	2.92	130.14	124.68
30	19	304	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
41	32	315	A86	C3-C4-C5	-2.92	117.50	123.47
30	11	315	CLA	CHB-C4A-NA	2.92	128.54	124.51
30	12	312	CLA	CHB-C4A-NA	2.92	128.54	124.51
41	31	313	A86	C7-C6-C8	2.92	122.67	118.08
30	11	306	CLA	CHB-C4A-NA	2.92	128.54	124.51
30	21	305	CLA	CHB-C4A-NA	2.92	128.54	124.51
30	34	301	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	12	310	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
30	15	303	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	37	310	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
41	36	313	A86	C41-C32-C31	-2.91	107.86	110.47
30	16	301	CLA	CHB-C4A-NA	2.91	128.54	124.51
32	b	623	BCR	C7-C8-C9	-2.91	121.83	126.23
30	C	513	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	B	607	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	13	304	CLA	CHB-C4A-NA	2.91	128.54	124.51
41	12	318	A86	C7-C6-C8	2.91	122.66	118.08
30	31	306	CLA	CHB-C4A-NA	2.91	128.54	124.51
30	b	608	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
41	37	316	A86	C41-C32-C31	-2.91	107.87	110.47
30	21	303	CLA	CMB-C2B-C3B	2.91	130.12	124.68
30	c	510	CLA	CHB-C4A-NA	2.91	128.53	124.51
30	B	608	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
41	11	313	A86	C7-C6-C8	2.91	122.66	118.08
41	12	319	A86	C41-C32-C31	-2.91	107.87	110.47
30	17	308	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
30	16	305	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
30	17	308	CLA	C2D-C1D-ND	-2.91	107.96	110.10
41	31	312	A86	C12-C11-C13	2.91	120.90	116.02
41	38	315	A86	C7-C6-C8	2.91	122.66	118.08
30	35	303	CLA	CHB-C4A-NA	2.91	128.53	124.51
30	36	305	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
30	17	310	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
30	12	307	CLA	CHB-C4A-NA	2.90	128.53	124.51
41	13	317	A86	C41-C32-C31	-2.90	107.87	110.47
30	34	307	CLA	CMB-C2B-C3B	2.90	130.11	124.68
30	C	510	CLA	O2D-CGD-CBD	2.90	116.43	111.27
41	39	309	A86	C33-C32-C31	2.90	112.03	109.21
30	37	308	CLA	CAA-C2A-C3A	-2.90	104.83	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	39	307	CLA	CHB-C4A-NA	2.90	128.53	124.51
30	B	607	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
32	a	404	BCR	C11-C10-C9	-2.90	123.17	127.31
30	14	307	CLA	CMB-C2B-C3B	2.90	130.10	124.68
41	36	311	A86	C34-O4-C38	-2.90	112.49	117.90
41	33	314	A86	C12-C11-C13	2.90	120.89	116.02
30	12	311	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
30	b	605	CLA	CMB-C2B-C3B	2.90	130.10	124.68
30	17	309	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
30	36	302	CLA	CMA-C3A-C2A	-2.90	102.13	113.83
41	13	312	A86	C34-O4-C38	-2.90	112.49	117.90
30	41	309	CLA	CMB-C2B-C3B	2.90	130.10	124.68
30	35	308	CLA	CHB-C4A-NA	2.90	128.52	124.51
30	c	512	CLA	C2A-C1A-CHA	2.90	128.93	123.86
30	31	302	CLA	C2A-C1A-CHA	2.90	128.93	123.86
41	14	312	A86	C34-O4-C38	-2.90	112.50	117.90
41	33	315	A86	C7-C6-C8	2.90	122.64	118.08
41	18	315	A86	C7-C6-C8	2.90	122.64	118.08
30	14	303	CLA	C2A-C1A-CHA	2.90	128.93	123.86
38	J	101	DGD	O2D-C2D-C1D	-2.90	103.01	110.05
41	11	312	A86	C12-C11-C13	2.90	120.89	116.02
41	35	311	A86	C34-O4-C38	-2.89	112.50	117.90
41	13	314	A86	C7-C6-C8	2.89	122.64	118.08
41	17	316	A86	C41-C32-C31	-2.89	107.88	110.47
30	16	302	CLA	CMA-C3A-C2A	-2.89	102.16	113.83
41	17	314	A86	C7-C6-C8	2.89	122.64	118.08
30	14	304	CLA	CHB-C4A-NA	2.89	128.51	124.51
30	11	302	CLA	C2A-C1A-CHA	2.89	128.92	123.86
30	D	402	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
30	34	303	CLA	C2A-C1A-CHA	2.89	128.92	123.86
30	16	305	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
30	b	607	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
41	37	314	A86	C7-C6-C8	2.89	122.63	118.08
30	36	305	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
41	32	317	A86	C7-C6-C8	2.89	122.63	118.08
41	37	312	A86	C34-O4-C38	-2.89	112.51	117.90
30	39	304	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
41	16	311	A86	C34-O4-C38	-2.89	112.51	117.90
30	21	309	CLA	CMB-C2B-C3B	2.89	130.08	124.68
30	13	307	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
30	A	402	CLA	C7-C6-C5	-2.89	105.52	113.36
41	12	316	A86	C34-O4-C38	-2.89	112.51	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	620	LMG	O3-C3-C2	-2.89	103.67	110.35
30	c	513	CLA	CHB-C4A-NA	2.89	128.50	124.51
41	40	201	A86	C-C1-C2	-2.89	118.88	122.92
30	34	307	CLA	CHB-C4A-NA	2.89	128.50	124.51
30	c	524	CLA	CMB-C2B-C3B	2.89	130.08	124.68
30	c	506	CLA	C2D-C1D-ND	-2.89	107.98	110.10
41	19	309	A86	C33-C32-C31	2.89	112.02	109.21
41	18	314	A86	C34-O4-C38	-2.89	112.52	117.90
41	32	315	A86	C34-O4-C38	-2.89	112.52	117.90
30	c	510	CLA	O2D-CGD-CBD	2.89	116.40	111.27
30	32	310	CLA	CMB-C2B-C3B	2.89	130.08	124.68
30	b	604	CLA	C1B-CHB-C4A	-2.88	124.40	130.12
41	17	315	A86	C3-C4-C5	-2.88	117.56	123.47
30	31	306	CLA	CMB-C2B-C3B	2.88	130.07	124.68
30	11	307	CLA	C1-C2-C3	-2.88	121.06	126.04
32	Y	101	BCR	C24-C23-C22	-2.88	121.88	126.23
30	C	512	CLA	C2A-C1A-CHA	2.88	128.90	123.86
41	11	314	A86	C41-C32-C31	-2.88	107.89	110.47
41	15	313	A86	C7-C6-C8	2.88	122.62	118.08
32	Y	101	BCR	C11-C10-C9	-2.88	123.20	127.31
41	15	313	A86	C4-C5-C6	-2.88	123.20	127.31
30	B	604	CLA	CHB-C4A-NA	2.88	128.50	124.51
41	37	315	A86	C3-C4-C5	-2.88	117.57	123.47
41	13	313	A86	C12-C11-C13	2.88	120.86	116.02
30	B	604	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
41	37	314	A86	C4-C5-C6	-2.88	123.20	127.31
30	B	602	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
30	B	606	CLA	CMB-C2B-C3B	2.88	130.06	124.68
32	c	520	BCR	C16-C15-C14	-2.88	117.58	123.47
41	35	313	A86	C4-C5-C6	-2.88	123.20	127.31
41	11	311	A86	C34-O4-C38	-2.88	112.53	117.90
41	15	311	A86	C34-O4-C38	-2.88	112.53	117.90
41	38	314	A86	C34-O4-C38	-2.88	112.53	117.90
30	36	301	CLA	CHB-C4A-NA	2.88	128.49	124.51
41	20	201	A86	C-C1-C2	-2.88	118.89	122.92
38	j	101	DGD	O2D-C2D-C1D	-2.88	103.06	110.05
41	31	311	A86	C34-O4-C38	-2.88	112.53	117.90
30	c	506	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	18	305	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	19	307	CLA	CHB-C4A-NA	2.88	128.49	124.51
41	35	313	A86	C7-C6-C8	2.88	122.61	118.08
30	B	613	CLA	CHB-C4A-NA	2.87	128.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	34	312	A86	C34-O4-C38	-2.87	112.54	117.90
30	17	307	CLA	CMB-C2B-C3B	2.87	130.06	124.68
30	21	306	CLA	CMB-C2B-C3B	2.87	130.06	124.68
30	41	306	CLA	CMB-C2B-C3B	2.87	130.06	124.68
30	c	523	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
41	13	314	A86	C4-C5-C6	-2.87	123.21	127.31
41	33	313	A86	C34-O4-C38	-2.87	112.54	117.90
32	c	520	BCR	C24-C23-C22	-2.87	121.89	126.23
36	b	619	LMG	O3-C3-C2	-2.87	103.71	110.35
30	19	301	CLA	C1-C2-C3	-2.87	121.08	126.04
30	37	307	CLA	CMB-C2B-C3B	2.87	130.05	124.68
30	38	305	CLA	CMB-C2B-C3B	2.87	130.05	124.68
30	C	521	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
32	b	623	BCR	C11-C10-C9	-2.87	123.22	127.31
30	14	308	CLA	C1-C2-C3	-2.87	121.08	126.04
30	Z	102	CLA	CMB-C2B-C3B	2.87	130.04	124.68
41	17	314	A86	C4-C5-C6	-2.87	123.22	127.31
41	31	313	A86	C4-C5-C6	-2.87	123.22	127.31
30	39	301	CLA	C1-C2-C3	-2.86	121.09	126.04
41	32	318	A86	C41-C32-C31	-2.86	107.91	110.47
30	C	506	CLA	CMB-C2B-C3B	2.86	130.04	124.68
30	13	308	CLA	C1-C2-C3	-2.86	121.09	126.04
30	18	306	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
30	33	304	CLA	C2A-C1A-CHA	2.86	128.86	123.86
30	12	314	CLA	CMB-C2B-C3B	2.86	130.03	124.68
41	11	313	A86	C4-C5-C6	-2.86	123.23	127.31
30	a	402	CLA	C7-C6-C5	-2.86	105.59	113.36
32	Y	101	BCR	C16-C15-C14	-2.86	117.62	123.47
30	13	307	CLA	CHB-C4A-NA	2.86	128.47	124.51
30	b	612	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
30	b	606	CLA	CMB-C2B-C3B	2.86	130.03	124.68
30	39	301	CLA	C4D-C3D-CAD	-2.86	104.73	108.10
41	40	201	A86	C33-C32-C31	2.86	111.99	109.21
38	J	101	DGD	O5D-C6D-C5D	-2.86	103.76	109.05
41	33	317	A86	C41-C32-C31	-2.86	107.92	110.47
30	19	301	CLA	C4D-C3D-CAD	-2.86	104.73	108.10
30	31	303	CLA	CHB-C4A-NA	2.86	128.46	124.51
30	34	304	CLA	CHB-C4A-NA	2.86	128.46	124.51
30	B	612	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
41	11	310	A86	C3-C4-C5	-2.85	117.63	123.47
41	34	314	A86	C4-C5-C6	-2.85	123.24	127.31
30	31	309	CLA	O2D-CGD-O1D	-2.85	118.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	303	CLA	C2A-C1A-CHA	2.85	128.84	123.86
30	38	308	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	32	312	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
30	c	511	CLA	C2D-C1D-ND	-2.85	108.00	110.10
30	12	310	CLA	CHB-C4A-NA	2.85	128.45	124.51
41	18	313	A86	C3-C4-C5	-2.85	117.64	123.47
41	14	314	A86	C4-C5-C6	-2.85	123.25	127.31
41	31	314	A86	C41-C32-C31	-2.85	107.92	110.47
30	32	306	CLA	C2A-C1A-CHA	2.85	128.84	123.86
30	38	306	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
41	18	315	A86	C4-C5-C6	-2.85	123.25	127.31
30	B	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
30	B	610	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	15	308	CLA	CHB-C4A-NA	2.85	128.45	124.51
41	38	315	A86	C4-C5-C6	-2.85	123.25	127.31
30	40	202	CLA	CHB-C4A-NA	2.85	128.45	124.51
30	b	602	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
30	b	607	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
30	14	310	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
30	18	311	CLA	CMB-C2B-C3B	2.84	130.00	124.68
30	35	307	CLA	C2A-C1A-CHA	2.84	128.83	123.86
30	34	309	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
30	18	308	CLA	CHB-C4A-NA	2.84	128.44	124.51
30	31	315	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
30	40	203	CLA	CMB-C2B-C3B	2.84	129.99	124.68
41	12	315	A86	C3-C4-C5	-2.84	117.66	123.47
30	41	301	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
41	39	310	A86	C33-C32-C31	2.84	111.97	109.21
30	c	507	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
30	31	308	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
30	12	314	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
41	19	311	A86	C40-C32-C31	-2.84	107.93	110.47
30	38	305	CLA	CHB-C4A-NA	2.84	128.43	124.51
30	14	301	CLA	CHB-C4A-NA	2.83	128.43	124.51
30	b	611	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
30	11	306	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	32	313	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
31	A	403	PHO	CMB-C2B-C3B	2.83	129.98	124.68
41	15	310	A86	C3-C4-C5	-2.83	117.67	123.47
41	31	310	A86	C3-C4-C5	-2.83	117.67	123.47
30	20	203	CLA	CMB-C2B-C3B	2.83	129.98	124.68
30	b	601	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	h	102	DGD	CDB-CCB-CBB	-2.83	100.05	114.42
41	34	311	A86	C3-C4-C5	-2.83	117.67	123.47
30	12	306	CLA	C2A-C1A-CHA	2.83	128.81	123.86
41	14	311	A86	C3-C4-C5	-2.83	117.68	123.47
41	13	315	A86	C41-C32-C31	-2.83	107.94	110.47
41	21	314	A86	C25-C26-C27	-2.83	123.27	127.31
30	38	311	CLA	CMB-C2B-C3B	2.83	129.97	124.68
30	33	311	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
38	j	101	DGD	O5D-C6D-C5D	-2.83	103.81	109.05
30	33	301	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
30	21	301	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
30	14	306	CLA	CHB-C4A-NA	2.83	128.42	124.51
30	41	301	CLA	CHB-C4A-NA	2.83	128.42	124.51
30	15	307	CLA	C2A-C1A-CHA	2.83	128.80	123.86
30	B	610	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
32	c	516	BCR	C15-C14-C13	-2.82	123.28	127.31
41	20	201	A86	C33-C32-C31	2.82	111.95	109.21
30	b	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
41	36	310	A86	C40-C32-C31	-2.82	107.95	110.47
30	31	315	CLA	CMB-C2B-C3B	2.82	129.96	124.68
30	C	509	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	21	301	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	C	503	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	c	509	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	20	203	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
41	38	313	A86	C3-C4-C5	-2.82	117.70	123.47
41	13	311	A86	C3-C4-C5	-2.82	117.70	123.47
39	D	404	PL9	C40-C39-C41	2.82	120.01	115.27
30	36	301	CLA	CMB-C2B-C3B	2.82	129.95	124.68
41	35	310	A86	C3-C4-C5	-2.82	117.71	123.47
41	41	312	A86	C26-C25-C24	-2.82	114.43	123.22
41	20	212	A86	C3-C4-C5	-2.82	117.71	123.47
30	34	301	CLA	CAA-C2A-C3A	-2.81	105.07	112.78
30	14	307	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
30	36	309	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
32	C	515	BCR	C15-C14-C13	-2.81	123.30	127.31
41	41	314	A86	C25-C26-C27	-2.81	123.30	127.31
41	21	313	A86	C8-C6-C5	-2.81	114.63	118.94
39	D	407	PL9	C40-C39-C41	2.81	120.00	115.27
30	18	301	CLA	CMB-C2B-C3B	2.81	129.94	124.68
41	21	312	A86	C26-C25-C24	-2.81	114.45	123.22
41	39	311	A86	C40-C32-C31	-2.81	107.96	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	H	102	DGD	CDB-CCB-CBB	-2.81	100.16	114.42
30	18	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
30	16	306	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
30	18	301	CLA	CHB-C4A-NA	2.81	128.40	124.51
30	37	307	CLA	CHB-C4A-NA	2.81	128.40	124.51
30	B	603	CLA	O2D-CGD-CBD	2.81	116.26	111.27
38	J	101	DGD	C3G-C2G-C1G	-2.81	105.15	111.79
30	b	607	CLA	CHB-C4A-NA	2.81	128.39	124.51
30	38	301	CLA	CMB-C2B-C3B	2.81	129.93	124.68
30	41	301	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	16	301	CLA	CMB-C2B-C3B	2.81	129.93	124.68
30	b	622	CLA	CMD-C2D-C1D	-2.81	119.77	124.71
41	33	312	A86	C3-C4-C5	-2.81	117.73	123.47
41	32	314	A86	C3-C4-C5	-2.81	117.73	123.47
41	12	318	A86	C4-C5-C6	-2.80	123.31	127.31
41	41	313	A86	C8-C6-C5	-2.80	114.64	118.94
30	c	509	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	37	305	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	19	306	CLA	CMB-C2B-C3B	2.80	129.92	124.68
30	12	313	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
30	39	303	CLA	CMB-C2B-C3B	2.80	129.92	124.68
41	19	310	A86	C19-C18-C17	2.80	116.18	110.77
30	11	309	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	21	308	CLA	CHB-C4A-NA	2.80	128.38	124.51
30	40	204	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	20	206	CLA	CMB-C2B-C3B	2.80	129.91	124.68
30	12	303	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
30	21	301	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	d	405	PL9	C40-C39-C41	2.80	119.98	115.27
30	41	308	CLA	CHB-C4A-NA	2.80	128.38	124.51
30	C	511	CLA	C2D-C1D-ND	-2.80	108.04	110.10
32	c	520	BCR	C11-C10-C9	-2.80	123.32	127.31
41	40	213	A86	C25-C26-C27	-2.80	123.32	127.31
30	14	301	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
30	14	301	CLA	CMB-C2B-C3B	2.80	129.91	124.68
30	b	606	CLA	C1-C2-C3	-2.79	121.21	126.04
30	B	602	CLA	CHB-C4A-NA	2.79	128.38	124.51
30	16	307	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
30	20	202	CLA	CHB-C4A-NA	2.79	128.38	124.51
30	36	306	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
30	34	310	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
41	41	314	A86	C12-C11-C13	2.79	120.71	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	408	BCR	C15-C16-C17	-2.79	117.75	123.47
41	32	317	A86	C4-C5-C6	-2.79	123.33	127.31
30	11	315	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
30	35	303	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
41	20	213	A86	C25-C26-C27	-2.79	123.33	127.31
41	17	315	A86	C41-C32-C31	-2.79	107.97	110.47
31	d	403	PHO	CMB-C2B-C3B	2.79	129.90	124.68
30	C	510	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	40	206	CLA	CMB-C2B-C3B	2.79	129.90	124.68
30	38	311	CLA	CAA-C2A-C1A	2.79	121.12	111.97
30	16	309	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
41	41	311	A86	C20-C19-C18	-2.79	107.23	112.75
33	a	405	SQD	C1-O5-C5	2.79	119.16	113.69
30	12	312	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
30	17	305	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	21	303	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	38	301	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	21	309	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	41	303	CLA	CHB-C4A-NA	2.79	128.37	124.51
30	13	310	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	41	309	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	33	301	CLA	CMB-C2B-C3B	2.79	129.89	124.68
41	19	310	A86	C33-C32-C31	2.79	111.92	109.21
30	17	309	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
30	20	204	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	40	203	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
30	32	303	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
30	31	304	CLA	C3A-C2A-C1A	2.79	105.51	101.34
39	d	408	PL9	C40-C39-C41	2.79	119.96	115.27
41	20	211	A86	C10-C9-C8	-2.78	114.53	123.22
36	Q	301	LMG	O6-C1-O1	-2.78	103.38	109.97
36	c	519	LMG	O6-C1-O1	-2.78	103.38	109.97
30	39	301	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
30	W	102	CLA	CHB-C4A-NA	2.78	128.36	124.51
38	J	101	DGD	CDB-CCB-CBB	-2.78	100.30	114.42
41	40	211	A86	C10-C9-C8	-2.78	114.53	123.22
30	39	306	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	b	602	CLA	CHB-C4A-NA	2.78	128.36	124.51
30	b	601	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
30	17	307	CLA	CHB-C4A-NA	2.78	128.36	124.51
30	19	303	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	B	607	CLA	O2D-CGD-O1D	-2.78	118.40	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	603	CLA	O2D-CGD-CBD	2.78	116.21	111.27
30	B	609	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
32	B	616	BCR	C7-C8-C9	-2.78	122.03	126.23
30	36	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
30	b	605	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	B	601	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
41	20	211	A86	C20-C19-C18	-2.78	107.26	112.75
30	B	611	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
30	C	520	CLA	CHB-C4A-NA	2.77	128.35	124.51
33	A	406	SQD	C1-O5-C5	2.77	119.13	113.69
41	21	311	A86	C20-C19-C18	-2.77	107.26	112.75
41	40	213	A86	C12-C11-C13	2.77	120.68	116.02
30	32	303	CLA	CMB-C2B-C3B	2.77	129.87	124.68
30	13	309	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
38	j	101	DGD	C3G-C2G-C1G	-2.77	105.23	111.79
30	d	402	CLA	O2D-CGD-CBD	2.77	116.19	111.27
41	40	211	A86	C20-C19-C18	-2.77	107.26	112.75
41	40	212	A86	C3-C4-C5	-2.77	117.80	123.47
30	C	507	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
41	39	310	A86	C19-C18-C17	2.77	116.12	110.77
30	18	311	CLA	CAA-C2A-C1A	2.77	121.06	111.97
30	33	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	37	309	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
32	A	409	BCR	C15-C16-C17	-2.77	117.80	123.47
41	21	314	A86	C12-C11-C13	2.77	120.67	116.02
30	17	309	CLA	CMB-C2B-C3B	2.77	129.86	124.68
30	34	301	CLA	CMB-C2B-C3B	2.77	129.86	124.68
41	19	310	A86	C-C1-C2	-2.77	119.05	122.92
30	c	503	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
41	21	311	A86	C10-C9-C8	-2.77	114.58	123.22
30	19	301	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
30	21	307	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	37	306	CLA	C2D-C1D-ND	-2.77	108.06	110.10
38	j	101	DGD	CDB-CCB-CBB	-2.77	100.38	114.42
30	11	304	CLA	C3A-C2A-C1A	2.77	105.48	101.34
30	15	308	CLA	CAA-C2A-C1A	2.77	121.04	111.97
30	35	308	CLA	CAA-C2A-C1A	2.77	121.04	111.97
41	40	201	A86	C4-C3-C2	-2.76	117.81	123.47
30	16	304	CLA	CHB-C4A-NA	2.76	128.33	124.51
30	M	101	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
30	41	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	11	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	601	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
41	20	213	A86	C12-C11-C13	2.76	120.66	116.02
30	C	509	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
41	37	302	A86	C7-C6-C5	-2.76	119.06	122.92
30	B	609	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
30	D	402	CLA	O2D-CGD-CBD	2.76	116.17	111.27
30	m	101	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
30	A	402	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
30	35	309	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
30	33	305	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
30	34	307	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
41	16	310	A86	C40-C32-C31	-2.75	108.01	110.47
30	18	312	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
30	16	308	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	32	310	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
41	37	315	A86	C41-C32-C31	-2.75	108.01	110.47
32	b	616	BCR	C11-C10-C9	-2.75	123.38	127.31
30	c	502	CLA	CHB-C4A-NA	2.75	128.32	124.51
38	C	516	DGD	C3G-C2G-C1G	-2.75	105.28	111.79
30	b	610	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
30	33	310	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
30	B	615	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
41	20	201	A86	C4-C3-C2	-2.75	117.84	123.47
41	41	311	A86	C10-C9-C8	-2.75	114.64	123.22
30	15	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	32	307	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
41	17	302	A86	C7-C6-C5	-2.75	119.07	122.92
30	37	304	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	37	309	CLA	CMB-C2B-C3B	2.75	129.82	124.68
30	17	306	CLA	C2D-C1D-ND	-2.75	108.08	110.10
30	15	309	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
30	12	307	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	17	301	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	b	609	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
30	14	309	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
41	16	310	A86	C12-C11-C13	2.74	120.63	116.02
30	19	303	CLA	CAA-CBA-CGA	2.74	121.27	113.25
30	C	503	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
30	b	610	CLA	CHB-C4A-NA	2.74	128.30	124.51
32	m	103	BCR	C7-C8-C9	-2.74	122.09	126.23
30	b	606	CLA	CHB-C4A-NA	2.74	128.30	124.51
30	B	605	CLA	O2D-CGD-O1D	-2.74	118.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	32	308	CLA	C3A-C2A-C1A	2.74	105.44	101.34
30	36	307	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
30	B	603	CLA	CHB-C4A-NA	2.74	128.30	124.51
30	14	304	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
30	34	304	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
30	38	309	CLA	C2A-C1A-CHA	2.74	128.64	123.86
30	21	302	CLA	CHB-C4A-NA	2.74	128.30	124.51
30	B	606	CLA	CHB-C4A-NA	2.74	128.29	124.51
30	b	603	CLA	CHB-C4A-NA	2.74	128.29	124.51
30	38	306	CLA	CHB-C4A-NA	2.74	128.29	124.51
30	37	308	CLA	C2D-C1D-ND	-2.74	108.09	110.10
38	c	517	DGD	C3G-C2G-C1G	-2.74	105.32	111.79
30	36	304	CLA	CHB-C4A-NA	2.73	128.29	124.51
41	21	313	A86	C26-C25-C24	-2.73	114.68	123.22
30	39	303	CLA	CAA-CBA-CGA	2.73	121.24	113.25
30	12	303	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
30	c	522	CLA	CHB-C4A-NA	2.73	128.29	124.51
30	15	306	CLA	CMB-C2B-C3B	2.73	129.79	124.68
30	41	302	CLA	CHB-C4A-NA	2.73	128.29	124.51
30	b	615	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	37	301	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
41	36	310	A86	C12-C11-C13	2.73	120.61	116.02
30	B	606	CLA	C1-C2-C3	-2.73	121.32	126.04
30	18	309	CLA	C2A-C1A-CHA	2.73	128.63	123.86
36	b	618	LMG	C1-C2-C3	-2.73	104.31	110.00
30	21	303	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	11	308	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
30	C	502	CLA	CHB-C4A-NA	2.73	128.29	124.51
30	13	304	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	41	303	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	18	306	CLA	CHB-C4A-NA	2.73	128.28	124.51
30	21	307	CLA	CHB-C4A-NA	2.73	128.28	124.51
30	31	303	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
30	34	305	CLA	C3A-C2A-C1A	2.73	105.42	101.34
41	39	310	A86	C-C1-C2	-2.73	119.10	122.92
30	38	312	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
38	j	101	DGD	O3G-C1D-C2D	-2.73	104.05	108.30
32	C	515	BCR	C28-C27-C26	-2.72	109.21	114.08
30	w	103	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
36	B	619	LMG	C1-C2-C3	-2.72	104.32	110.00
30	38	307	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
30	18	307	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	20	206	CLA	C2A-C1A-CHA	2.72	128.62	123.86
41	21	310	A86	C41-C32-C31	-2.72	108.04	110.47
30	41	306	CLA	CHB-C4A-NA	2.72	128.27	124.51
41	41	310	A86	C41-C32-C31	-2.72	108.04	110.47
30	40	209	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
30	40	206	CLA	C2A-C1A-CHA	2.72	128.61	123.86
30	w	102	CLA	CHB-C4A-NA	2.72	128.27	124.51
41	41	313	A86	C26-C25-C24	-2.72	114.74	123.22
30	b	603	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
40	e	101	HEM	CMB-C2B-C1B	-2.72	120.90	125.04
30	20	209	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	21	306	CLA	CHB-C4A-NA	2.71	128.27	124.51
30	D	406	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
30	C	519	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	b	609	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	c	507	CLA	C2A-C1A-CHA	2.71	128.60	123.86
30	17	304	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	c	503	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	c	508	CLA	O1D-CGD-CBD	2.71	130.03	124.48
30	35	306	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	c	522	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	18	307	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	34	301	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	33	306	CLA	C3A-C2A-C1A	2.71	105.39	101.34
41	14	313	A86	C3-C4-C5	-2.71	117.93	123.47
32	B	617	BCR	C11-C10-C9	-2.71	123.45	127.31
30	31	306	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
30	B	603	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
30	39	306	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
36	32	301	LMG	O3-C3-C2	-2.70	104.10	110.35
30	z	101	CLA	CHB-C4A-NA	2.70	128.25	124.51
30	41	307	CLA	CHB-C4A-NA	2.70	128.25	124.51
30	C	507	CLA	C2A-C1A-CHA	2.70	128.59	123.86
30	16	303	CLA	CAA-C2A-C1A	2.70	120.83	111.97
30	40	209	CLA	CHB-C4A-NA	2.70	128.25	124.51
30	31	315	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
30	34	305	CLA	C2D-C1D-ND	-2.70	108.11	110.10
30	41	309	CLA	CHB-C4A-NA	2.70	128.25	124.51
30	35	309	CLA	CHB-C4A-NA	2.70	128.25	124.51
30	d	407	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
30	C	520	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
30	19	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	37	307	CLA	C2D-C1D-ND	-2.70	108.12	110.10
30	19	302	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
30	c	504	CLA	CAA-CBA-CGA	-2.70	105.37	113.25
30	c	510	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
30	38	304	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
30	38	309	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	39	302	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
30	37	306	CLA	CAA-C2A-C3A	-2.69	105.40	112.78
30	20	205	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	C	510	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
41	39	309	A86	C3-C4-C5	-2.69	117.96	123.47
41	19	309	A86	C3-C4-C5	-2.69	117.96	123.47
41	32	316	A86	C3-C4-C5	-2.69	117.96	123.47
30	11	315	CLA	CMB-C2B-C3B	2.69	129.71	124.68
30	b	606	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
32	c	521	BCR	C27-C26-C25	2.69	126.64	122.73
41	16	312	A86	C3-C4-C5	-2.69	117.97	123.47
36	d	410	LMG	O1-C7-C8	-2.69	104.41	110.90
41	36	312	A86	C3-C4-C5	-2.69	117.97	123.47
36	12	301	LMG	O3-C3-C2	-2.69	104.14	110.35
30	D	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	40	205	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	C	504	CLA	CAA-CBA-CGA	-2.69	105.40	113.25
30	d	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	12	308	CLA	C3A-C2A-C1A	2.69	105.36	101.34
36	D	408	LMG	O1-C7-C8	-2.69	104.42	110.90
30	36	303	CLA	CAA-C2A-C1A	2.69	120.78	111.97
39	D	407	PL9	C22-C23-C24	-2.69	121.19	127.66
30	14	305	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
32	m	103	BCR	C11-C10-C9	-2.69	123.48	127.31
41	17	313	A86	C3-C4-C5	-2.68	117.98	123.47
41	34	313	A86	C3-C4-C5	-2.68	117.98	123.47
30	17	306	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
30	B	606	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
30	b	622	CLA	CMB-C2B-C3B	2.68	129.70	124.68
30	18	312	CLA	CHB-C4A-NA	2.68	128.22	124.51
38	J	101	DGD	O3G-C1D-C2D	-2.68	104.12	108.30
32	c	516	BCR	C28-C27-C26	-2.68	109.29	114.08
30	38	312	CLA	CHB-C4A-NA	2.68	128.22	124.51
30	W	103	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
41	21	310	A86	C10-C9-C8	-2.68	114.86	123.22
30	13	305	CLA	C3A-C2A-C1A	2.68	105.35	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	604	CLA	C1-C2-C3	-2.68	121.41	126.04
41	15	312	A86	C3-C4-C5	-2.68	117.99	123.47
30	C	502	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
30	36	302	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
41	31	312	A86	C20-C19-C18	-2.68	107.45	112.75
30	b	622	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
30	b	604	CLA	C1-C2-C3	-2.68	121.42	126.04
30	20	203	CLA	CHB-C4A-NA	2.68	128.21	124.51
30	18	308	CLA	CMB-C2B-C3B	2.68	129.68	124.68
30	b	604	CLA	C2D-C1D-ND	-2.67	108.13	110.10
30	18	309	CLA	CHB-C4A-NA	2.67	128.21	124.51
30	38	307	CLA	CHB-C4A-NA	2.67	128.21	124.51
30	c	510	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
30	C	504	CLA	CHB-C4A-NA	2.67	128.21	124.51
30	c	502	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
30	38	308	CLA	CMB-C2B-C3B	2.67	129.68	124.68
30	33	306	CLA	C2D-C1D-ND	-2.67	108.14	110.10
41	37	313	A86	C20-C19-C18	-2.67	107.46	112.75
30	18	304	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
41	17	313	A86	C20-C19-C18	-2.67	107.47	112.75
39	d	408	PL9	C22-C23-C24	-2.67	121.23	127.66
30	C	506	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	34	308	CLA	C2A-C1A-CHA	2.67	128.53	123.86
30	C	504	CLA	CMB-C2B-C3B	2.67	129.67	124.68
41	16	312	A86	C20-C19-C18	-2.67	107.47	112.75
41	33	314	A86	C3-C4-C5	-2.67	118.01	123.47
30	33	301	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
41	35	312	A86	C3-C4-C5	-2.67	118.01	123.47
41	15	312	A86	C20-C19-C18	-2.67	107.47	112.75
41	41	310	A86	C10-C9-C8	-2.67	114.89	123.22
30	c	506	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	37	310	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	12	303	CLA	CMB-C2B-C3B	2.66	129.66	124.68
30	20	209	CLA	CHB-C4A-NA	2.66	128.20	124.51
41	31	312	A86	C3-C4-C5	-2.66	118.02	123.47
30	a	402	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
41	11	312	A86	C20-C19-C18	-2.66	107.48	112.75
30	C	508	CLA	O1D-CGD-CBD	2.66	129.93	124.48
30	D	401	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	21	309	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
30	C	503	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
41	14	314	A86	C8-C6-C5	-2.66	114.86	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	622	CLA	CHB-C4A-NA	2.66	128.19	124.51
41	12	317	A86	C3-C4-C5	-2.66	118.02	123.47
30	B	604	CLA	C2D-C1D-ND	-2.66	108.14	110.10
30	17	307	CLA	C2D-C1D-ND	-2.66	108.14	110.10
41	36	312	A86	C20-C19-C18	-2.66	107.49	112.75
30	C	514	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	37	309	CLA	O2A-CGA-O1A	-2.66	116.67	123.30
30	b	604	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
41	13	313	A86	C3-C4-C5	-2.66	118.03	123.47
30	40	209	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
41	37	313	A86	C3-C4-C5	-2.66	118.03	123.47
30	12	312	CLA	CMB-C2B-C3B	2.66	129.65	124.68
30	11	315	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	c	503	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
41	35	312	A86	C20-C19-C18	-2.66	107.49	112.75
41	11	312	A86	C3-C4-C5	-2.66	118.03	123.47
41	39	310	A86	O-C13-C14	-2.66	116.26	121.66
41	33	315	A86	C8-C6-C5	-2.65	114.87	118.94
40	E	101	HEM	CMB-C2B-C1B	-2.65	121.00	125.04
41	34	314	A86	C8-C6-C5	-2.65	114.87	118.94
30	C	510	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
30	21	309	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	c	504	CLA	CMB-C2B-C3B	2.65	129.64	124.68
30	35	307	CLA	C1-C2-C3	-2.65	121.46	126.04
30	c	524	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
41	38	315	A86	C8-C6-C5	-2.65	114.87	118.94
41	37	311	A86	C40-C32-C31	-2.65	108.10	110.47
30	15	309	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	36	309	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	41	309	CLA	CAA-C2A-C1A	-2.65	103.29	111.97
30	16	308	CLA	CMB-C2B-C3B	2.65	129.64	124.68
30	z	101	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	11	304	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	17	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	C	519	CLA	CHB-C4A-NA	2.65	128.18	124.51
30	37	307	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
38	c	517	DGD	C1E-O6E-C5E	2.65	118.89	113.69
30	17	307	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
30	20	209	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
38	h	102	DGD	O6D-C1D-O3G	-2.65	103.70	109.97
30	c	514	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	16	302	CLA	O2D-CGD-O1D	-2.65	118.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	21	308	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	39	303	CLA	C1-O2A-CGA	2.65	123.39	116.44
30	12	312	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
41	14	313	A86	C20-C19-C18	-2.65	107.52	112.75
30	12	308	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
30	18	301	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
38	H	102	DGD	O6D-C1D-O3G	-2.64	103.71	109.97
41	32	316	A86	C20-C19-C18	-2.64	107.52	112.75
30	36	308	CLA	O2A-CGA-O1A	-2.64	116.71	123.30
30	C	519	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
41	13	313	A86	C20-C19-C18	-2.64	107.52	112.75
30	34	310	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
30	17	309	CLA	O2A-CGA-O1A	-2.64	116.71	123.30
38	C	517	DGD	CBB-CAB-C9B	-2.64	101.02	114.42
30	B	623	CLA	CHB-C4A-NA	2.64	128.16	124.51
32	c	521	BCR	C11-C10-C9	-2.64	123.54	127.31
30	Z	102	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
41	40	210	A86	C17-C16-C15	2.64	111.86	109.16
30	16	308	CLA	O2A-CGA-O1A	-2.64	116.72	123.30
30	31	304	CLA	C2D-C1D-ND	-2.64	108.16	110.10
30	15	307	CLA	C1-C2-C3	-2.64	121.48	126.04
30	d	401	CLA	CHB-C4A-NA	2.64	128.16	124.51
30	40	203	CLA	CHB-C4A-NA	2.64	128.16	124.51
30	19	303	CLA	C1-O2A-CGA	2.64	123.36	116.44
32	B	616	BCR	C11-C10-C9	-2.64	123.55	127.31
30	B	604	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
41	37	314	A86	C8-C6-C5	-2.64	114.90	118.94
30	14	305	CLA	C3A-C2A-C1A	2.63	105.28	101.34
35	L	102	LHG	C20-C19-C18	-2.63	101.05	114.42
30	b	606	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
30	B	614	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
30	14	301	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
30	17	306	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
30	32	303	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
41	15	313	A86	C8-C6-C5	-2.63	114.90	118.94
30	c	523	CLA	O2D-CGD-CBD	2.63	115.94	111.27
41	31	313	A86	C8-C6-C5	-2.63	114.90	118.94
30	z	101	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
30	37	306	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
30	c	512	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	A	403	PHO	O2D-CGD-O1D	-2.63	118.70	123.84
41	19	310	A86	O-C13-C14	-2.63	116.32	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c	518	DGD	O2D-C2D-C1D	-2.63	103.66	110.05
30	14	310	CLA	CHB-C4A-NA	2.63	128.15	124.51
41	12	317	A86	C20-C19-C18	-2.63	107.55	112.75
36	Q	301	LMG	O2-C2-C1	-2.63	103.66	110.05
30	21	302	CLA	C2A-C1A-CHA	2.63	128.45	123.86
38	C	516	DGD	C1E-O6E-C5E	2.63	118.84	113.69
30	41	302	CLA	C2A-C1A-CHA	2.62	128.45	123.86
41	16	310	A86	C3-C4-C5	-2.62	118.10	123.47
30	d	406	CLA	CAA-CBA-CGA	-2.62	105.58	113.25
30	D	405	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
30	15	305	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
30	B	606	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
39	D	407	PL9	C31-C32-C33	-2.62	103.26	111.88
30	B	610	CLA	O2D-CGD-CBD	2.62	115.93	111.27
41	17	314	A86	C8-C6-C5	-2.62	114.92	118.94
30	16	309	CLA	CHB-C4A-NA	2.62	128.14	124.51
30	31	307	CLA	C2A-C1A-CHA	2.62	128.44	123.86
30	32	308	CLA	C2D-C1D-ND	-2.62	108.17	110.10
30	b	614	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
32	B	616	BCR	C24-C23-C22	-2.62	122.28	126.23
31	d	403	PHO	O2D-CGD-O1D	-2.62	118.72	123.84
30	b	610	CLA	O2D-CGD-CBD	2.62	115.92	111.27
41	11	313	A86	C8-C6-C5	-2.62	114.92	118.94
41	35	313	A86	C8-C6-C5	-2.62	114.92	118.94
35	l	102	LHG	C20-C19-C18	-2.62	101.14	114.42
30	m	101	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	16	308	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	33	311	CLA	CHB-C4A-NA	2.62	128.13	124.51
41	18	315	A86	C8-C6-C5	-2.62	114.93	118.94
41	34	313	A86	C20-C19-C18	-2.62	107.57	112.75
30	13	310	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	36	308	CLA	CHB-C4A-NA	2.61	128.13	124.51
38	c	518	DGD	CBB-CAB-C9B	-2.61	101.15	114.42
30	38	301	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
41	13	314	A86	C8-C6-C5	-2.61	114.93	118.94
32	Y	101	BCR	C28-C27-C26	-2.61	109.41	114.08
30	B	623	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
36	M	102	LMG	O3-C3-C2	-2.61	104.31	110.35
32	B	618	BCR	C3-C4-C5	-2.61	109.41	114.08
41	33	314	A86	C20-C19-C18	-2.61	107.58	112.75
30	39	301	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
38	h	102	DGD	C3G-C2G-C1G	-2.61	105.61	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	d	408	PL9	C31-C32-C33	-2.61	103.30	111.88
41	17	302	A86	C34-O4-C38	-2.61	113.03	117.90
32	c	520	BCR	C34-C9-C10	-2.61	119.27	122.92
30	33	311	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
41	32	318	A86	C7-C6-C8	2.61	122.19	118.08
30	13	305	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
30	19	301	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
41	37	302	A86	C34-O4-C38	-2.61	113.03	117.90
30	C	521	CLA	O2D-CGD-CBD	2.61	115.90	111.27
38	C	517	DGD	O2D-C2D-C1D	-2.61	103.71	110.05
30	b	609	CLA	CMB-C2B-C3B	2.61	129.56	124.68
30	36	308	CLA	CMB-C2B-C3B	2.61	129.56	124.68
38	H	102	DGD	C3G-C2G-C1G	-2.61	105.62	111.79
30	19	307	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
30	41	308	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
30	c	502	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
39	d	405	PL9	C7-C8-C9	-2.61	122.45	126.79
41	35	314	A86	C7-C6-C8	2.60	122.18	118.08
30	M	101	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	37	309	CLA	C2A-C3A-C4A	-2.60	97.66	101.87
30	B	609	CLA	CMB-C2B-C3B	2.60	129.55	124.68
30	35	305	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
41	20	210	A86	C17-C16-C15	2.60	111.82	109.16
41	17	311	A86	C40-C32-C31	-2.60	108.14	110.47
30	32	313	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
30	39	307	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
30	B	623	CLA	CMB-C2B-C3B	2.60	129.54	124.68
32	m	103	BCR	C24-C23-C22	-2.60	122.31	126.23
30	37	301	CLA	CMA-C3A-C2A	-2.60	103.34	113.83
30	32	313	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	34	305	CLA	O2D-CGD-CBD	2.60	115.89	111.27
39	D	404	PL9	C7-C8-C9	-2.60	122.47	126.79
41	20	201	A86	C34-O4-C38	-2.60	113.05	117.90
30	32	311	CLA	C2A-C1A-CHA	2.60	128.40	123.86
32	C	518	BCR	C11-C10-C9	-2.60	123.60	127.31
36	c	519	LMG	O2-C2-C1	-2.60	103.74	110.05
30	Z	102	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	15	304	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	34	310	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	d	406	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
30	39	303	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
30	18	310	CLA	O2D-CGD-O1D	-2.59	118.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	12	318	A86	C8-C6-C5	-2.59	114.96	118.94
41	12	319	A86	C7-C6-C8	2.59	122.16	118.08
30	20	204	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
41	36	310	A86	C3-C4-C5	-2.59	118.16	123.47
41	13	315	A86	C7-C6-C8	2.59	122.16	118.08
30	18	308	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
30	17	301	CLA	CMA-C3A-C2A	-2.59	103.38	113.83
32	b	616	BCR	C27-C26-C25	2.59	126.49	122.73
30	38	303	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
36	W	101	LMG	O3-C3-C2	-2.59	104.36	110.35
30	19	303	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
36	w	101	LMG	O3-C3-C2	-2.59	104.37	110.35
41	32	319	A86	C7-C6-C8	2.59	122.15	118.08
30	38	308	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
36	w	101	LMG	C1-C2-C3	-2.58	104.61	110.00
30	14	310	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
32	c	520	BCR	C28-C27-C26	-2.58	109.46	114.08
32	B	617	BCR	C27-C26-C25	2.58	126.48	122.73
41	32	317	A86	C8-C6-C5	-2.58	114.98	118.94
30	40	204	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
41	13	317	A86	C7-C6-C8	2.58	122.14	118.08
30	c	504	CLA	CHB-C4A-NA	2.58	128.08	124.51
30	17	309	CLA	C2A-C3A-C4A	-2.58	97.70	101.87
30	b	622	CLA	CMD-C2D-C3D	2.58	133.55	127.61
30	33	309	CLA	C2A-C1A-CHA	2.58	128.37	123.86
30	c	524	CLA	CHB-C4A-NA	2.58	128.08	124.51
41	31	314	A86	C7-C6-C8	2.58	122.14	118.08
35	l	102	LHG	O8-C23-C24	2.58	120.00	111.91
32	C	518	BCR	C27-C26-C25	2.58	126.47	122.73
36	m	102	LMG	O3-C3-C2	-2.58	104.39	110.35
30	C	512	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
39	d	408	PL9	C7-C3-C4	2.58	118.97	116.88
30	12	314	CLA	CHB-C4A-NA	2.58	128.07	124.51
32	Y	101	BCR	C34-C9-C10	-2.58	119.31	122.92
41	17	302	A86	C26-C25-C24	-2.58	115.18	123.22
30	41	303	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
30	B	606	CLA	CHD-C1D-ND	-2.58	122.09	124.45
30	B	604	CLA	CAA-CBA-CGA	-2.58	105.73	113.25
36	W	101	LMG	C1-C2-C3	-2.58	104.63	110.00
30	B	610	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
41	11	314	A86	C7-C6-C8	2.57	122.13	118.08
41	33	317	A86	C7-C6-C8	2.57	122.13	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	37	302	A86	C26-C25-C24	-2.57	115.19	123.22
41	15	314	A86	C7-C6-C8	2.57	122.13	118.08
32	b	617	BCR	C3-C4-C5	-2.57	109.48	114.08
41	17	302	A86	C4-C3-C2	-2.57	118.21	123.47
30	33	304	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
30	38	310	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
30	14	305	CLA	O2D-CGD-CBD	2.57	115.83	111.27
30	b	604	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
41	16	310	A86	C34-O4-C38	-2.57	113.11	117.90
30	C	509	CLA	O2D-CGD-CBD	2.57	115.83	111.27
30	d	401	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
41	17	311	A86	O1-C15-C14	2.57	118.36	113.21
32	B	617	BCR	C40-C30-C25	2.57	114.46	110.30
41	16	310	A86	C4-C3-C2	-2.57	118.22	123.47
30	c	504	CLA	C2A-C1A-CHA	2.57	128.35	123.86
41	12	304	A86	C41-C32-C31	-2.57	108.18	110.47
40	e	101	HEM	CBA-CAA-C2A	2.57	117.00	112.62
30	13	310	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
35	L	102	LHG	O8-C23-C24	2.56	119.96	111.91
30	11	304	CLA	O2D-CGD-CBD	2.56	115.83	111.27
30	19	302	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
30	19	305	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
30	D	405	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
36	W	101	LMG	C38-C37-C36	-2.56	101.41	114.42
36	w	101	LMG	C38-C37-C36	-2.56	101.41	114.42
30	35	303	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
41	40	201	A86	C34-O4-C38	-2.56	113.12	117.90
40	E	101	HEM	CBA-CAA-C2A	2.56	116.99	112.62
30	12	305	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
30	18	303	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
41	36	310	A86	C34-O4-C38	-2.56	113.12	117.90
32	a	408	BCR	C15-C14-C13	-2.56	123.65	127.31
30	b	604	CLA	C2A-C1A-CHA	2.56	128.34	123.86
41	19	309	A86	C12-C11-C13	2.56	120.32	116.02
30	12	314	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
41	39	309	A86	C12-C11-C13	2.56	120.32	116.02
30	11	309	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
30	b	610	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
30	11	305	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
30	21	303	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
30	39	302	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
30	32	306	CLA	C1B-CHB-C4A	-2.56	125.06	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	39	305	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
41	37	302	A86	C4-C3-C2	-2.55	118.24	123.47
30	31	309	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
30	13	308	CLA	C2A-C1A-CHA	2.55	128.32	123.86
30	w	103	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	35	304	CLA	CHB-C4A-NA	2.55	128.04	124.51
41	37	311	A86	O1-C15-C14	2.55	118.33	113.21
32	b	623	BCR	C15-C14-C13	-2.55	123.67	127.31
30	16	301	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
41	16	313	A86	C7-C6-C8	2.55	122.09	118.08
41	19	310	A86	O-C13-C11	-2.55	115.52	121.15
32	f	101	BCR	C7-C8-C9	-2.55	122.38	126.23
32	B	616	BCR	C15-C14-C13	-2.55	123.67	127.31
41	36	313	A86	C7-C6-C8	2.55	122.09	118.08
41	39	310	A86	O-C13-C11	-2.55	115.52	121.15
32	B	617	BCR	C15-C16-C17	-2.55	118.26	123.47
30	C	508	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
41	32	304	A86	C41-C32-C31	-2.55	108.19	110.47
30	13	306	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
30	36	301	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
30	C	504	CLA	C2A-C1A-CHA	2.55	128.31	123.86
41	37	316	A86	C7-C6-C8	2.54	122.09	118.08
30	21	309	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
30	B	615	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	11	301	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
30	37	305	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
30	14	306	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
38	c	518	DGD	O6D-C5D-C6D	-2.54	101.53	106.67
30	11	302	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
32	F	101	BCR	C11-C10-C9	-2.54	123.68	127.31
32	b	616	BCR	C15-C16-C17	-2.54	118.27	123.47
30	41	309	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
30	34	307	CLA	C2A-C1A-CHA	2.54	128.30	123.86
30	C	506	CLA	O2D-CGD-CBD	2.54	115.78	111.27
41	17	316	A86	C7-C6-C8	2.54	122.08	118.08
30	B	613	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
30	d	407	CLA	O2D-CGD-CBD	2.54	115.78	111.27
42	32	302	LMU	O5B-C1B-C2B	2.54	115.72	110.35
30	18	304	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
30	D	401	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	14	302	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	38	304	CLA	C1B-CHB-C4A	-2.54	125.09	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	302	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	32	310	CLA	C2A-C1A-CHA	2.54	128.29	123.86
30	11	309	CLA	CHB-C4A-NA	2.53	128.02	124.51
30	12	311	CLA	C2A-C1A-CHA	2.53	128.29	123.86
41	38	315	A86	C40-C32-C31	-2.53	108.20	110.47
30	34	303	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
30	17	303	CLA	CMB-C2B-C3B	2.53	129.42	124.68
30	c	509	CLA	O2D-CGD-CBD	2.53	115.77	111.27
30	20	207	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	32	305	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	15	303	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
41	32	317	A86	C40-C32-C31	-2.53	108.21	110.47
30	32	308	CLA	O2D-CGD-CBD	2.53	115.77	111.27
41	11	314	A86	C3-C4-C5	-2.53	118.29	123.47
30	C	521	CLA	C2A-C1A-CHA	2.53	128.28	123.86
30	31	306	CLA	C2A-C1A-CHA	2.53	128.28	123.86
41	11	310	A86	C25-C24-C1	-2.53	119.31	126.42
30	C	502	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
35	B	622	LHG	C11-C10-C9	-2.53	101.59	114.42
35	L	101	LHG	C20-C19-C18	-2.53	101.59	114.42
41	13	311	A86	C7-C6-C8	2.53	122.06	118.08
30	17	305	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
30	34	305	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
30	39	301	CLA	CHB-C4A-NA	2.53	128.01	124.51
41	31	310	A86	C25-C24-C1	-2.53	119.32	126.42
41	36	310	A86	C4-C3-C2	-2.53	118.30	123.47
30	B	604	CLA	C2A-C1A-CHA	2.53	128.28	123.86
39	D	407	PL9	C7-C3-C4	2.53	118.93	116.88
30	c	508	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
30	16	308	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
41	11	316	A86	C41-C32-C31	-2.53	108.21	110.47
30	C	511	CLA	CHB-C4A-NA	2.53	128.00	124.51
41	35	314	A86	C3-C4-C5	-2.52	118.30	123.47
38	C	517	DGD	O6D-C5D-C6D	-2.52	101.57	106.67
41	33	302	A86	C41-C32-C31	-2.52	108.21	110.47
41	33	312	A86	C25-C24-C1	-2.52	119.33	126.42
32	c	516	BCR	C29-C30-C25	2.52	114.37	110.48
30	c	503	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
35	d	409	LHG	C20-C19-C18	-2.52	101.62	114.42
36	W	101	LMG	O1-C1-C2	-2.52	104.36	108.30
30	11	307	CLA	C2A-C1A-CHA	2.52	128.27	123.86
30	19	306	CLA	C1B-CHB-C4A	-2.52	125.12	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	615	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	C	503	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
32	b	616	BCR	C40-C30-C25	2.52	114.39	110.30
41	14	314	A86	C40-C32-C31	-2.52	108.22	110.47
41	41	313	A86	O1-C15-C14	-2.52	108.15	113.21
32	F	101	BCR	C7-C8-C9	-2.52	122.43	126.23
30	36	306	CLA	CMB-C2B-C3B	2.52	129.39	124.68
32	B	624	BCR	C15-C14-C13	-2.52	123.71	127.31
32	f	101	BCR	C11-C10-C9	-2.52	123.71	127.31
41	34	311	A86	C25-C24-C1	-2.52	119.34	126.42
30	37	305	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
41	37	312	A86	C20-C19-C18	-2.52	107.77	112.75
41	35	310	A86	C25-C24-C1	-2.52	119.34	126.42
30	a	403	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
30	31	309	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	12	309	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
41	14	312	A86	C20-C19-C18	-2.52	107.77	112.75
30	34	305	CLA	CBA-CAA-C2A	-2.52	106.43	113.86
41	38	313	A86	C7-C6-C8	2.52	122.04	118.08
30	39	303	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
41	13	314	A86	C40-C32-C31	-2.52	108.22	110.47
30	21	306	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
33	a	405	SQD	O7-S-C6	2.52	109.93	106.94
41	37	316	A86	C3-C4-C5	-2.52	118.32	123.47
30	b	613	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
41	34	312	A86	C20-C19-C18	-2.51	107.77	112.75
41	15	314	A86	C3-C4-C5	-2.51	118.32	123.47
41	39	310	A86	C9-C10-C11	-2.51	119.22	126.61
41	15	310	A86	C25-C24-C1	-2.51	119.35	126.42
41	32	315	A86	C20-C19-C18	-2.51	107.78	112.75
41	31	316	A86	C41-C32-C31	-2.51	108.22	110.47
30	D	406	CLA	O2D-CGD-CBD	2.51	115.73	111.27
35	A	408	LHG	C20-C19-C18	-2.51	101.67	114.42
30	32	308	CLA	CBA-CAA-C2A	-2.51	106.44	113.86
30	39	306	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
41	12	319	A86	C3-C4-C5	-2.51	118.33	123.47
41	13	317	A86	C3-C4-C5	-2.51	118.33	123.47
41	13	301	A86	C41-C32-C31	-2.51	108.22	110.47
30	c	523	CLA	C2A-C1A-CHA	2.51	128.25	123.86
41	13	311	A86	C25-C24-C1	-2.51	119.36	126.42
41	18	313	A86	C25-C24-C1	-2.51	119.36	126.42
35	b	621	LHG	C11-C10-C9	-2.51	101.68	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	31	314	A86	C3-C4-C5	-2.51	118.33	123.47
30	37	303	CLA	CMB-C2B-C3B	2.51	129.38	124.68
41	33	312	A86	C7-C6-C8	2.51	122.03	118.08
41	17	312	A86	C20-C19-C18	-2.51	107.78	112.75
30	38	309	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
30	19	303	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
36	w	101	LMG	O1-C1-C2	-2.51	104.38	108.30
30	W	103	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	33	308	CLA	C2A-C1A-CHA	2.51	128.25	123.86
30	40	207	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
41	34	311	A86	C7-C6-C8	2.51	122.03	118.08
38	j	101	DGD	O3D-C3D-C4D	-2.51	104.55	110.35
41	19	310	A86	C9-C10-C11	-2.51	119.23	126.61
30	15	301	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
30	41	306	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
30	12	308	CLA	O2D-CGD-CBD	2.51	115.73	111.27
30	c	511	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	36	308	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
30	C	513	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
35	a	407	LHG	C20-C19-C18	-2.51	101.70	114.42
32	m	103	BCR	C15-C14-C13	-2.51	123.73	127.31
36	m	102	LMG	O2-C2-C1	-2.51	103.96	110.05
30	31	302	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
41	33	313	A86	C20-C19-C18	-2.51	107.79	112.75
30	19	301	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	36	302	CLA	C1-C2-C3	-2.50	121.71	126.04
41	18	313	A86	C7-C6-C8	2.50	122.02	118.08
30	17	305	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
30	35	301	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
41	32	318	A86	C3-C4-C5	-2.50	118.35	123.47
41	15	311	A86	C25-C24-C1	-2.50	119.39	126.42
30	34	306	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
41	16	313	A86	C3-C4-C5	-2.50	118.35	123.47
30	17	301	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
30	17	305	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
30	d	406	CLA	CHB-C4A-NA	2.50	127.97	124.51
41	35	311	A86	C20-C19-C18	-2.50	107.80	112.75
41	32	314	A86	C25-C24-C1	-2.50	119.39	126.42
30	15	309	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
36	M	102	LMG	O2-C2-C1	-2.50	103.97	110.05
30	16	302	CLA	C1-C2-C3	-2.50	121.72	126.04
41	12	318	A86	C40-C32-C31	-2.50	108.23	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	33	306	CLA	O2D-CGD-CBD	2.50	115.71	111.27
30	18	308	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
30	37	305	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
30	31	304	CLA	CBA-CAA-C2A	-2.50	106.48	113.86
41	16	310	A86	C10-C9-C8	-2.50	115.42	123.22
30	c	503	CLA	C2A-C1A-CHA	2.50	128.23	123.86
30	37	301	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
30	40	208	CLA	CHB-C4A-NA	2.50	127.97	124.51
41	33	315	A86	C40-C32-C31	-2.50	108.24	110.47
30	18	309	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
41	14	311	A86	C25-C24-C1	-2.50	119.40	126.42
30	13	305	CLA	O2D-CGD-CBD	2.50	115.71	111.27
30	16	304	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
41	15	315	A86	C41-C32-C31	-2.50	108.24	110.47
30	20	208	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	c	506	CLA	O2D-CGD-CBD	2.50	115.70	111.27
41	13	312	A86	C20-C19-C18	-2.50	107.81	112.75
30	31	304	CLA	O2D-CGD-CBD	2.50	115.70	111.27
41	13	316	A86	C41-C32-C31	-2.50	108.24	110.47
30	12	308	CLA	CBA-CAA-C2A	-2.50	106.50	113.86
41	12	315	A86	C25-C24-C1	-2.50	119.40	126.42
30	20	202	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
41	15	316	A86	C12-C11-C13	2.50	120.22	116.02
30	19	308	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
41	11	311	A86	C20-C19-C18	-2.50	107.81	112.75
41	15	311	A86	C20-C19-C18	-2.50	107.81	112.75
38	C	516	DGD	O3D-C3D-C4D	-2.50	104.58	110.35
41	37	311	A86	C4-C3-C2	-2.50	118.36	123.47
30	33	306	CLA	CBA-CAA-C2A	-2.49	106.50	113.86
32	B	616	BCR	C27-C26-C25	2.49	126.35	122.73
41	18	314	A86	C20-C19-C18	-2.49	107.81	112.75
41	21	313	A86	O1-C15-C14	-2.49	108.20	113.21
41	35	315	A86	C41-C32-C31	-2.49	108.24	110.47
30	36	304	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
32	A	409	BCR	C15-C14-C13	-2.49	123.75	127.31
41	32	319	A86	C3-C4-C5	-2.49	118.37	123.47
41	36	311	A86	C20-C19-C18	-2.49	107.82	112.75
30	40	202	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
41	35	316	A86	C12-C11-C13	2.49	120.21	116.02
30	34	308	CLA	CHA-C1A-NA	-2.49	120.69	126.40
41	38	313	A86	C25-C24-C1	-2.49	119.42	126.42
30	b	622	CLA	C1B-CHB-C4A	-2.49	125.18	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	32	307	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
32	C	515	BCR	C29-C30-C25	2.49	114.32	110.48
30	b	606	CLA	CHD-C1D-ND	-2.49	122.17	124.45
30	14	303	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
41	33	316	A86	C41-C32-C31	-2.49	108.24	110.47
38	J	101	DGD	O3D-C3D-C4D	-2.49	104.59	110.35
41	33	317	A86	C3-C4-C5	-2.49	118.37	123.47
30	38	304	CLA	C2A-C1A-CHA	2.49	128.21	123.86
41	35	311	A86	C25-C24-C1	-2.49	119.42	126.42
41	31	311	A86	C25-C24-C1	-2.49	119.42	126.42
31	d	403	PHO	CAA-CBA-CGA	-2.49	105.98	113.25
41	21	312	A86	C40-C32-C31	-2.49	108.24	110.47
41	35	313	A86	C40-C32-C31	-2.49	108.24	110.47
30	13	303	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
30	13	303	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	18	304	CLA	C2A-C1A-CHA	2.49	128.21	123.86
36	b	618	LMG	O6-C1-O1	-2.49	104.08	109.97
30	33	309	CLA	CHA-C1A-NA	-2.49	120.70	126.40
41	12	316	A86	C20-C19-C18	-2.49	107.83	112.75
41	31	311	A86	C20-C19-C18	-2.49	107.83	112.75
30	11	302	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
41	36	313	A86	C3-C4-C5	-2.49	118.38	123.47
30	b	612	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	20	203	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
30	16	304	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	18	312	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
30	39	308	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
41	20	201	A86	O1-C15-C14	2.49	118.20	113.21
36	d	410	LMG	O6-C1-O1	-2.48	104.09	109.97
30	16	306	CLA	CMB-C2B-C3B	2.48	129.33	124.68
30	38	308	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
30	14	305	CLA	CBA-CAA-C2A	-2.48	106.53	113.86
41	15	310	A86	C7-C6-C8	2.48	121.99	118.08
30	12	306	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
36	B	619	LMG	O6-C1-O1	-2.48	104.09	109.97
41	13	312	A86	C25-C24-C1	-2.48	119.44	126.42
32	H	101	BCR	C37-C22-C21	-2.48	119.44	122.92
31	A	403	PHO	CAA-CBA-CGA	-2.48	106.00	113.25
41	12	315	A86	C7-C6-C8	2.48	121.99	118.08
41	38	314	A86	C20-C19-C18	-2.48	107.84	112.75
36	D	408	LMG	O6-C1-O1	-2.48	104.10	109.97
41	36	310	A86	C10-C9-C8	-2.48	115.47	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	17	311	A86	C4-C3-C2	-2.48	118.39	123.47
30	31	307	CLA	CHA-C1A-NA	-2.48	120.72	126.40
30	B	612	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
30	38	310	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
31	D	403	PHO	O2D-CGD-O1D	-2.48	118.99	123.84
41	15	316	A86	C41-C32-C31	-2.48	108.25	110.47
41	33	313	A86	C25-C24-C1	-2.48	119.45	126.42
41	13	315	A86	C3-C4-C5	-2.48	118.39	123.47
41	17	316	A86	C3-C4-C5	-2.48	118.39	123.47
41	14	311	A86	C7-C6-C8	2.48	121.98	118.08
30	14	308	CLA	C2A-C1A-CHA	2.48	128.20	123.86
30	16	302	CLA	CMB-C2B-C3B	2.48	129.32	124.68
30	c	510	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
41	41	313	A86	C4-C5-C6	-2.48	123.77	127.31
41	11	311	A86	C25-C24-C1	-2.48	119.45	126.42
30	C	503	CLA	C2A-C1A-CHA	2.48	128.19	123.86
30	A	404	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
30	31	301	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	33	307	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	36	304	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
41	41	313	A86	C20-C19-C18	-2.48	107.85	112.75
41	40	201	A86	O1-C15-C14	2.48	118.18	113.21
30	C	513	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
41	16	311	A86	C25-C24-C1	-2.48	119.46	126.42
41	32	315	A86	C25-C24-C1	-2.48	119.46	126.42
41	20	213	A86	C7-C6-C8	2.48	121.98	118.08
41	18	314	A86	C25-C24-C1	-2.48	119.46	126.42
30	18	310	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
30	34	303	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
32	Z	101	BCR	C7-C8-C9	-2.48	122.50	126.23
41	34	312	A86	C25-C24-C1	-2.47	119.47	126.42
30	14	303	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
41	35	310	A86	C7-C6-C8	2.47	121.97	118.08
36	Q	301	LMG	C9-C8-C7	-2.47	105.94	111.79
30	c	513	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
30	21	304	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
30	32	311	CLA	CHA-C1A-NA	-2.47	120.73	126.40
41	35	316	A86	C41-C32-C31	-2.47	108.26	110.47
30	16	304	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
41	38	314	A86	C25-C24-C1	-2.47	119.47	126.42
41	34	314	A86	C40-C32-C31	-2.47	108.26	110.47
41	32	314	A86	C7-C6-C8	2.47	121.97	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	40	213	A86	C7-C6-C8	2.47	121.97	118.08
41	18	315	A86	C40-C32-C31	-2.47	108.26	110.47
41	21	313	A86	C4-C5-C6	-2.47	123.78	127.31
38	c	517	DGD	O3D-C3D-C4D	-2.47	104.64	110.35
30	A	404	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
30	C	510	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
30	11	304	CLA	CBA-CAA-C2A	-2.47	106.58	113.86
30	36	304	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
30	38	312	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
30	41	304	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
41	36	311	A86	C25-C24-C1	-2.47	119.48	126.42
30	c	514	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
41	14	312	A86	C25-C24-C1	-2.47	119.49	126.42
30	b	604	CLA	C3C-C4C-NC	-2.47	107.81	110.57
41	17	312	A86	C25-C24-C1	-2.47	119.49	126.42
41	21	313	A86	C20-C19-C18	-2.47	107.87	112.75
30	D	405	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
41	41	314	A86	C7-C6-C8	2.47	121.96	118.08
32	C	518	BCR	C15-C14-C13	-2.47	123.79	127.31
30	17	303	CLA	C1-C2-C3	-2.46	121.78	126.04
30	36	302	CLA	CMB-C2B-C3B	2.46	129.29	124.68
30	b	606	CLA	CHC-C1C-NC	2.46	127.94	124.20
30	35	305	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
30	32	309	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
33	A	406	SQD	O7-S-C6	2.46	109.87	106.94
32	c	515	BCR	C7-C8-C9	-2.46	122.51	126.23
30	B	606	CLA	CHC-C1C-NC	2.46	127.94	124.20
30	40	203	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	13	305	CLA	CBA-CAA-C2A	-2.46	106.60	113.86
30	34	302	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
41	13	316	A86	C12-C11-C13	2.46	120.16	116.02
30	33	303	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	C	514	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
31	D	403	PHO	CMC-C2C-C3C	2.46	129.58	124.94
30	C	520	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
41	16	311	A86	C20-C19-C18	-2.46	107.89	112.75
30	37	303	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	16	303	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
41	11	310	A86	C10-C9-C8	-2.46	115.55	123.22
41	12	315	A86	C10-C9-C8	-2.46	115.55	123.22
30	40	202	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
32	h	101	BCR	C37-C22-C21	-2.46	119.48	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	17	311	A86	C17-C16-C15	2.46	111.67	109.16
30	15	305	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
41	11	310	A86	C7-C6-C8	2.46	121.95	118.08
41	14	311	A86	C10-C9-C8	-2.46	115.55	123.22
30	a	403	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
41	15	313	A86	C40-C32-C31	-2.46	108.27	110.47
30	36	303	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
41	20	210	A86	C26-C25-C24	-2.46	115.55	123.22
41	40	210	A86	C26-C25-C24	-2.46	115.55	123.22
35	l	102	LHG	C11-C10-C9	-2.46	101.96	114.42
41	40	212	A86	C9-C10-C11	-2.45	119.39	126.61
41	13	311	A86	C10-C9-C8	-2.45	115.56	123.22
32	c	521	BCR	C15-C14-C13	-2.45	123.81	127.31
33	b	620	SQD	O48-C23-O10	-2.45	117.40	123.59
41	34	311	A86	C10-C9-C8	-2.45	115.56	123.22
35	L	102	LHG	C11-C10-C9	-2.45	101.97	114.42
41	12	316	A86	C25-C24-C1	-2.45	119.53	126.42
36	B	619	LMG	O3-C3-C2	-2.45	104.68	110.35
41	32	314	A86	C10-C9-C8	-2.45	115.57	123.22
41	35	310	A86	C10-C9-C8	-2.45	115.57	123.22
41	37	312	A86	C25-C24-C1	-2.45	119.53	126.42
30	17	303	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
41	41	312	A86	C40-C32-C31	-2.45	108.28	110.47
41	33	312	A86	C10-C9-C8	-2.45	115.57	123.22
41	38	302	A86	C12-C11-C13	2.45	120.14	116.02
41	17	314	A86	C40-C32-C31	-2.45	108.28	110.47
30	C	504	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
41	31	310	A86	C10-C9-C8	-2.45	115.58	123.22
31	d	404	PHO	CMC-C2C-C3C	2.45	129.56	124.94
41	20	212	A86	C9-C10-C11	-2.45	119.42	126.61
41	12	304	A86	C12-C11-C13	2.45	120.13	116.02
30	19	306	CLA	CHB-C4A-NA	2.44	127.89	124.51
41	11	313	A86	C40-C32-C31	-2.44	108.28	110.47
30	33	307	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
41	31	310	A86	C7-C6-C8	2.44	121.93	118.08
41	31	316	A86	C12-C11-C13	2.44	120.13	116.02
41	18	313	A86	C10-C9-C8	-2.44	115.59	123.22
30	37	303	CLA	C1-C2-C3	-2.44	121.82	126.04
38	j	101	DGD	O3E-C3E-C2E	-2.44	104.70	110.35
41	15	310	A86	C10-C9-C8	-2.44	115.60	123.22
41	39	311	A86	C41-C32-C31	-2.44	108.29	110.47
30	D	405	CLA	CHB-C4A-NA	2.44	127.89	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	J	101	DGD	O3E-C3E-C2E	-2.44	104.70	110.35
41	38	313	A86	C10-C9-C8	-2.44	115.60	123.22
41	33	302	A86	C12-C11-C13	2.44	120.12	116.02
30	14	307	CLA	C2A-C1A-CHA	2.44	128.12	123.86
30	b	609	CLA	C2A-C1A-CHA	2.44	128.12	123.86
36	B	620	LMG	O1-C1-C2	-2.44	104.50	108.30
41	37	313	A86	C9-C10-C11	-2.44	119.44	126.61
36	c	519	LMG	C9-C8-C7	-2.44	106.02	111.79
30	35	309	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
30	B	612	CLA	CMD-C2D-C1D	-2.44	120.42	124.71
30	21	305	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
32	m	103	BCR	C27-C26-C25	2.44	126.27	122.73
30	c	505	CLA	CHD-C1D-ND	-2.44	122.21	124.45
41	35	312	A86	C9-C10-C11	-2.44	119.44	126.61
30	12	307	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
30	c	504	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
30	13	307	CLA	C2A-C1A-CHA	2.44	128.12	123.86
36	b	618	LMG	O3-C3-C2	-2.44	104.72	110.35
41	17	313	A86	C9-C10-C11	-2.44	119.45	126.61
30	13	305	CLA	C2D-C1D-ND	-2.44	108.31	110.10
39	d	405	PL9	C20-C19-C21	2.44	119.37	115.27
30	18	310	CLA	CHB-C4A-NA	2.43	127.88	124.51
41	21	314	A86	C7-C6-C8	2.43	121.91	118.08
30	34	306	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
36	c	519	LMG	C40-C39-C38	-2.43	102.07	114.42
41	19	311	A86	C41-C32-C31	-2.43	108.29	110.47
32	H	101	BCR	C11-C10-C9	-2.43	123.84	127.31
30	13	304	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
30	11	306	CLA	C2A-C1A-CHA	2.43	128.11	123.86
30	c	522	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
30	12	306	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
30	32	308	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
30	19	304	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
32	Y	101	BCR	C7-C8-C9	-2.43	122.56	126.23
41	33	312	A86	C23-C16-C22	-2.43	103.79	107.37
32	F	101	BCR	C35-C13-C14	-2.43	119.52	122.92
33	B	621	SQD	O48-C23-O10	-2.43	117.46	123.59
41	14	313	A86	C9-C10-C11	-2.43	119.47	126.61
42	12	302	LMU	O5B-C1B-C2B	2.43	115.49	110.35
30	C	514	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
32	c	516	BCR	C7-C8-C9	-2.43	122.57	126.23
30	B	623	CLA	C1B-CHB-C4A	-2.43	125.31	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	h	101	BCR	C11-C10-C9	-2.43	123.85	127.31
30	33	305	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
30	d	406	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
41	33	316	A86	C12-C11-C13	2.42	120.09	116.02
30	20	202	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
41	19	309	A86	C34-O4-C38	-2.42	113.38	117.90
30	41	306	CLA	CBA-CAA-C2A	-2.42	106.71	113.86
30	39	304	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
41	12	317	A86	C9-C10-C11	-2.42	119.49	126.61
30	12	310	CLA	C2A-C1A-CHA	2.42	128.09	123.86
30	c	513	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
35	A	408	LHG	C11-C10-C9	-2.42	102.13	114.42
30	31	304	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
30	16	303	CLA	CHA-C1A-NA	-2.42	120.85	126.40
32	f	101	BCR	C35-C13-C14	-2.42	119.53	122.92
41	13	301	A86	C12-C11-C13	2.42	120.09	116.02
41	18	302	A86	C12-C11-C13	2.42	120.09	116.02
41	31	313	A86	C40-C32-C31	-2.42	108.31	110.47
30	33	304	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
30	13	308	CLA	CHA-C1A-NA	-2.42	120.85	126.40
30	A	402	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	21	306	CLA	CBA-CAA-C2A	-2.42	106.72	113.86
30	c	514	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
30	41	305	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
36	D	408	LMG	C6-C5-C4	-2.42	107.34	113.00
41	34	313	A86	C9-C10-C11	-2.42	119.49	126.61
30	B	615	CLA	CHA-C1A-NA	-2.42	120.86	126.40
39	D	407	PL9	C36-C34-C33	-2.42	116.22	121.12
41	21	313	A86	C28-C27-C26	-2.42	119.53	122.92
41	35	315	A86	C12-C11-C13	2.42	120.09	116.02
32	B	624	BCR	C33-C5-C6	-2.42	121.81	124.53
30	C	506	CLA	CMC-C2C-C1C	-2.42	121.36	125.04
30	33	306	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
31	d	404	PHO	O2D-CGD-O1D	-2.42	119.11	123.84
41	41	313	A86	C28-C27-C26	-2.42	119.54	122.92
41	11	316	A86	C12-C11-C13	2.42	120.08	116.02
41	32	304	A86	C12-C11-C13	2.42	120.08	116.02
36	Q	301	LMG	C40-C39-C38	-2.42	102.15	114.42
30	31	305	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
30	38	310	CLA	CHB-C4A-NA	2.42	127.85	124.51
41	17	312	A86	C40-C32-C31	-2.42	108.31	110.47
41	15	312	A86	C9-C10-C11	-2.42	119.51	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	303	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
41	21	313	A86	C34-O4-C38	-2.42	113.39	117.90
30	40	205	CLA	CHB-C4A-NA	2.41	127.85	124.51
41	13	313	A86	C9-C10-C11	-2.41	119.51	126.61
41	33	314	A86	C9-C10-C11	-2.41	119.51	126.61
41	21	312	A86	C7-C6-C8	2.41	121.88	118.08
30	16	302	CLA	C2A-C1A-CHA	2.41	128.08	123.86
30	B	609	CLA	C2A-C1A-CHA	2.41	128.08	123.86
30	B	605	CLA	C3C-C4C-NC	-2.41	107.87	110.57
30	c	508	CLA	CHA-C1A-NA	-2.41	120.88	126.40
41	13	311	A86	C23-C16-C22	-2.41	103.81	107.37
38	c	518	DGD	O3E-C3E-C2E	-2.41	104.77	110.35
35	a	407	LHG	C11-C10-C9	-2.41	102.19	114.42
41	32	316	A86	C9-C10-C11	-2.41	119.52	126.61
35	L	101	LHG	O8-C23-C24	2.41	119.47	111.91
36	d	410	LMG	C6-C5-C4	-2.41	107.36	113.00
41	35	310	A86	C23-C16-C22	-2.41	103.82	107.37
38	c	517	DGD	O6E-C5E-C6E	-2.41	100.45	106.44
30	13	306	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
30	b	615	CLA	CHA-C1A-NA	-2.41	120.88	126.40
41	41	312	A86	C7-C6-C8	2.41	121.87	118.08
30	41	302	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
41	39	309	A86	C34-O4-C38	-2.41	113.41	117.90
41	31	312	A86	C9-C10-C11	-2.41	119.53	126.61
41	15	315	A86	C12-C11-C13	2.41	120.06	116.02
41	16	311	A86	C40-C32-C31	-2.41	108.32	110.47
30	C	512	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
30	14	308	CLA	CHA-C1A-NA	-2.41	120.89	126.40
30	B	604	CLA	C3C-C4C-NC	-2.40	107.87	110.57
30	32	306	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
41	14	311	A86	C23-C16-C22	-2.40	103.83	107.37
41	11	312	A86	C9-C10-C11	-2.40	119.54	126.61
36	c	519	LMG	C38-C37-C36	-2.40	102.23	114.42
30	36	309	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
36	d	410	LMG	O3-C3-C2	-2.40	104.80	110.35
36	Q	301	LMG	C38-C37-C36	-2.40	102.23	114.42
30	18	305	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
30	20	205	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	A	404	CLA	CMB-C2B-C3B	2.40	129.17	124.68
33	B	621	SQD	C4-C3-C2	2.40	115.01	110.82
41	21	312	A86	C35-C34-C33	2.40	114.06	109.88
41	13	312	A86	C40-C32-C31	-2.40	108.32	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	301	CLA	C1-C2-C3	-2.40	121.89	126.04
38	C	516	DGD	CDB-CCB-CBB	-2.40	102.24	114.42
33	a	405	SQD	C1-C2-C3	-2.40	105.00	110.00
39	D	404	PL9	C20-C19-C21	2.40	119.31	115.27
30	38	306	CLA	C2A-C1A-CHA	2.40	128.05	123.86
36	D	408	LMG	O3-C3-C2	-2.40	104.80	110.35
30	21	309	CLA	CHD-C1D-ND	-2.40	122.25	124.45
41	19	309	A86	C10-C9-C8	-2.40	115.73	123.22
30	20	205	CLA	C3A-C2A-C1A	2.40	104.93	101.34
30	37	304	CLA	CHA-C1A-NA	-2.40	120.91	126.40
30	20	207	CLA	C2A-C1A-CHA	2.40	128.05	123.86
41	33	313	A86	C40-C32-C31	-2.40	108.33	110.47
30	37	301	CLA	CMB-C2B-C3B	2.40	129.16	124.68
41	16	312	A86	C9-C10-C11	-2.40	119.56	126.61
30	b	612	CLA	CMD-C2D-C1D	-2.40	120.49	124.71
38	C	517	DGD	O3E-C3E-C2E	-2.40	104.81	110.35
30	32	309	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
36	32	301	LMG	C1-C2-C3	-2.40	105.01	110.00
30	36	303	CLA	CHA-C1A-NA	-2.40	120.91	126.40
30	12	309	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
38	c	518	DGD	C3D-C4D-C5D	-2.40	105.97	110.24
35	d	409	LHG	O8-C23-C24	2.39	119.42	111.91
41	37	311	A86	C17-C16-C15	2.39	111.61	109.16
30	31	315	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
30	21	302	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
30	18	306	CLA	C2A-C1A-CHA	2.39	128.04	123.86
39	d	408	PL9	C36-C34-C33	-2.39	116.27	121.12
41	41	313	A86	C34-O4-C38	-2.39	113.44	117.90
30	12	311	CLA	CHA-C1A-NA	-2.39	120.92	126.40
41	37	312	A86	C40-C32-C31	-2.39	108.33	110.47
41	12	315	A86	C23-C16-C22	-2.39	103.84	107.37
41	38	313	A86	C23-C16-C22	-2.39	103.84	107.37
30	34	304	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
30	14	305	CLA	C2D-C1D-ND	-2.39	108.34	110.10
30	19	306	CLA	O2A-CGA-O1A	-2.39	117.34	123.30
41	31	310	A86	C23-C16-C22	-2.39	103.84	107.37
30	11	307	CLA	CHA-C1A-NA	-2.39	120.92	126.40
30	14	304	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
41	32	314	A86	C23-C16-C22	-2.39	103.84	107.37
39	d	408	PL9	C42-C43-C44	-2.39	121.91	127.66
32	h	101	BCR	C15-C14-C13	-2.39	123.90	127.31
41	41	312	A86	C35-C34-C33	2.39	114.04	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	39	306	CLA	O2A-CGA-O1A	-2.39	117.35	123.30
30	b	612	CLA	CMD-C2D-C3D	2.39	133.11	127.61
41	17	311	A86	C12-C11-C13	2.39	120.03	116.02
30	17	301	CLA	CMB-C2B-C3B	2.39	129.15	124.68
33	A	406	SQD	C1-C2-C3	-2.39	105.02	110.00
30	b	604	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
41	36	312	A86	C9-C10-C11	-2.39	119.59	126.61
30	12	303	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
30	41	309	CLA	CHD-C1D-ND	-2.39	122.26	124.45
30	c	512	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
30	17	304	CLA	CHA-C1A-NA	-2.39	120.93	126.40
30	15	307	CLA	CAA-C2A-C1A	2.39	119.80	111.97
30	c	503	CLA	C1D-ND-C4D	2.39	108.03	106.33
41	34	311	A86	C23-C16-C22	-2.39	103.85	107.37
30	31	305	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
30	B	602	CLA	CHD-C1D-ND	-2.39	122.26	124.45
30	20	206	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
30	35	307	CLA	CAA-C2A-C1A	2.38	119.79	111.97
30	36	301	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
30	C	505	CLA	CHD-C1D-ND	-2.38	122.26	124.45
30	40	205	CLA	C3A-C2A-C1A	2.38	104.91	101.34
30	40	207	CLA	C2A-C1A-CHA	2.38	128.03	123.86
30	c	510	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
30	40	208	CLA	C2A-C1A-CHA	2.38	128.03	123.86
30	16	309	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
41	40	201	A86	C7-C6-C8	2.38	121.83	118.08
30	18	307	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
30	40	206	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
35	A	408	LHG	C18-C17-C16	-2.38	102.34	114.42
33	b	620	SQD	C1-O5-C5	2.38	118.36	113.69
41	12	316	A86	C40-C32-C31	-2.38	108.34	110.47
30	36	302	CLA	C2A-C1A-CHA	2.38	128.02	123.86
30	b	605	CLA	C3C-C4C-NC	-2.38	107.90	110.57
36	D	408	LMG	C40-C39-C38	-2.38	102.34	114.42
41	14	312	A86	C10-C9-C8	-2.38	115.79	123.22
41	18	313	A86	C23-C16-C22	-2.38	103.86	107.37
41	18	314	A86	C10-C9-C8	-2.38	115.79	123.22
41	37	314	A86	C40-C32-C31	-2.38	108.34	110.47
30	15	307	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
30	41	307	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
30	b	611	CLA	CHB-C4A-NA	2.38	127.80	124.51
32	c	520	BCR	C7-C8-C9	-2.38	122.64	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	612	CLA	CMD-C2D-C3D	2.38	133.08	127.61
38	c	517	DGD	CDB-CCB-CBB	-2.38	102.35	114.42
30	21	307	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
41	37	312	A86	C10-C9-C8	-2.38	115.80	123.22
33	B	621	SQD	C1-O5-C5	2.38	118.35	113.69
36	d	410	LMG	C40-C39-C38	-2.38	102.36	114.42
30	35	307	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
41	38	314	A86	C10-C9-C8	-2.38	115.80	123.22
30	31	303	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
30	39	306	CLA	CHB-C4A-NA	2.37	127.80	124.51
30	11	305	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
30	32	303	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	12	308	CLA	C2D-C1D-ND	-2.37	108.36	110.10
30	16	309	CLA	C2D-C1D-ND	-2.37	108.36	110.10
41	20	213	A86	C40-C32-C31	-2.37	108.35	110.47
36	W	101	LMG	C40-C39-C38	-2.37	102.38	114.42
41	37	311	A86	C12-C11-C13	2.37	120.01	116.02
32	C	515	BCR	C7-C8-C9	-2.37	122.65	126.23
41	34	312	A86	C10-C9-C8	-2.37	115.81	123.22
41	15	310	A86	C23-C16-C22	-2.37	103.87	107.37
41	39	309	A86	C10-C9-C8	-2.37	115.81	123.22
30	B	604	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
41	17	312	A86	C10-C9-C8	-2.37	115.82	123.22
32	B	617	BCR	C24-C23-C22	-2.37	122.65	126.23
36	w	101	LMG	C40-C39-C38	-2.37	102.40	114.42
30	33	306	CLA	C1D-ND-C4D	2.37	108.02	106.33
41	33	313	A86	C10-C9-C8	-2.37	115.83	123.22
30	39	308	CLA	CBC-CAC-C3C	2.37	118.96	112.43
33	b	620	SQD	C4-C3-C2	2.37	114.96	110.82
32	b	616	BCR	C24-C23-C22	-2.37	122.66	126.23
30	38	305	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
36	W	101	LMG	O2-C2-C1	-2.37	104.30	110.05
30	c	506	CLA	CMC-C2C-C1C	-2.37	121.43	125.04
35	a	407	LHG	C18-C17-C16	-2.37	102.41	114.42
41	37	302	A86	C9-C10-C11	-2.37	119.65	126.61
30	15	308	CLA	CBA-CAA-C2A	-2.37	106.88	113.86
30	b	608	CLA	CMB-C2B-C3B	2.37	129.10	124.68
38	c	517	DGD	O5E-C6E-C5E	-2.37	103.17	111.29
30	17	309	CLA	CHA-C1A-NA	-2.37	120.98	126.40
30	B	615	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
40	V	201	HEM	CAD-CBD-CGD	-2.36	108.51	113.60
30	20	208	CLA	C2A-C1A-CHA	2.36	127.99	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	F	101	BCR	C16-C15-C14	-2.36	118.63	123.47
30	b	602	CLA	CHD-C1D-ND	-2.36	122.28	124.45
41	13	312	A86	C10-C9-C8	-2.36	115.84	123.22
30	38	307	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
41	31	311	A86	C10-C9-C8	-2.36	115.84	123.22
30	35	308	CLA	CBA-CAA-C2A	-2.36	106.89	113.86
36	m	102	LMG	O6-C1-O1	-2.36	104.38	109.97
30	14	306	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
41	40	213	A86	C40-C32-C31	-2.36	108.36	110.47
32	c	515	BCR	C33-C5-C6	-2.36	121.88	124.53
30	B	611	CLA	C3C-C4C-NC	-2.36	107.92	110.57
41	18	302	A86	C41-C32-C31	-2.36	108.36	110.47
36	w	101	LMG	O2-C2-C1	-2.36	104.31	110.05
36	M	102	LMG	O6-C1-O1	-2.36	104.38	109.97
41	20	201	A86	C7-C6-C8	2.36	121.80	118.08
30	35	301	CLA	C1-C2-C3	-2.36	121.96	126.04
41	11	311	A86	C10-C9-C8	-2.36	115.85	123.22
36	b	619	LMG	O1-C1-C2	-2.36	104.62	108.30
30	39	302	CLA	O2A-CGA-O1A	-2.36	117.42	123.30
30	b	615	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
41	17	302	A86	C9-C10-C11	-2.36	119.67	126.61
36	W	101	LMG	C6-C5-C4	-2.36	107.48	113.00
30	37	309	CLA	CHA-C1A-NA	-2.36	121.00	126.40
30	37	304	CLA	CAA-C2A-C1A	2.36	119.70	111.97
38	C	517	DGD	C3D-C4D-C5D	-2.36	106.03	110.24
41	11	310	A86	C23-C16-C22	-2.36	103.89	107.37
30	16	301	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
30	34	301	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
41	38	302	A86	C41-C32-C31	-2.36	108.36	110.47
30	39	308	CLA	CAA-C2A-C1A	-2.36	104.25	111.97
32	c	515	BCR	C27-C26-C25	2.36	126.15	122.73
41	16	311	A86	C10-C9-C8	-2.36	115.87	123.22
41	15	311	A86	C10-C9-C8	-2.35	115.87	123.22
30	33	301	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
30	C	510	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
36	b	619	LMG	O2-C2-C1	-2.35	104.33	110.05
30	41	305	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
30	40	206	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
30	32	312	CLA	CHA-C1A-NA	-2.35	121.01	126.40
30	a	403	CLA	CMB-C2B-C3B	2.35	129.08	124.68
32	H	101	BCR	C15-C14-C13	-2.35	123.95	127.31
30	19	308	CLA	CAA-C2A-C1A	-2.35	104.27	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	32	315	A86	C10-C9-C8	-2.35	115.88	123.22
41	36	311	A86	C10-C9-C8	-2.35	115.88	123.22
41	31	316	A86	C9-C10-C11	-2.35	119.69	126.61
32	B	618	BCR	C15-C16-C17	-2.35	118.66	123.47
30	34	309	CLA	CHA-C1A-NA	-2.35	121.01	126.40
32	b	616	BCR	C30-C25-C26	-2.35	119.30	122.61
39	D	407	PL9	O1-C4-C3	-2.35	118.13	120.72
30	19	308	CLA	CBC-CAC-C3C	2.35	118.91	112.43
41	12	316	A86	C10-C9-C8	-2.35	115.88	123.22
36	b	619	LMG	O7-C10-O9	-2.35	118.03	123.70
36	w	101	LMG	C6-C5-C4	-2.35	107.50	113.00
30	C	520	CLA	C11-C12-C13	-2.35	108.33	115.92
30	21	306	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
30	20	206	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
30	17	304	CLA	CAA-C2A-C1A	2.35	119.67	111.97
41	20	213	A86	C41-C32-C31	-2.35	108.37	110.47
41	21	314	A86	C40-C32-C31	-2.35	108.37	110.47
41	11	316	A86	C9-C10-C11	-2.35	119.71	126.61
41	14	312	A86	C40-C32-C31	-2.35	108.37	110.47
41	36	311	A86	C40-C32-C31	-2.35	108.37	110.47
41	35	311	A86	C10-C9-C8	-2.35	115.90	123.22
38	C	516	DGD	O6E-C5E-C6E	-2.35	100.60	106.44
40	v	201	HEM	CAD-CBD-CGD	-2.34	108.56	113.60
30	c	522	CLA	C11-C12-C13	-2.34	108.34	115.92
36	B	619	LMG	O1-C7-C8	-2.34	105.24	110.90
30	c	509	CLA	CGD-CBD-CAD	-2.34	103.14	110.73
30	b	606	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
41	13	301	A86	C9-C10-C11	-2.34	119.72	126.61
41	15	316	A86	C9-C10-C11	-2.34	119.72	126.61
30	C	508	CLA	CHA-C1A-NA	-2.34	121.03	126.40
30	11	315	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	34	305	CLA	C1D-ND-C4D	2.34	108.00	106.33
41	12	304	A86	C9-C10-C11	-2.34	119.72	126.61
41	13	316	A86	C9-C10-C11	-2.34	119.72	126.61
41	32	304	A86	C9-C10-C11	-2.34	119.72	126.61
36	B	620	LMG	O7-C10-O9	-2.34	118.04	123.70
30	35	302	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	b	614	CLA	C2A-C1A-CHA	2.34	127.95	123.86
41	40	213	A86	C41-C32-C31	-2.34	108.38	110.47
30	c	503	CLA	C2D-C1D-ND	-2.34	108.38	110.10
30	12	312	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
38	j	101	DGD	CAB-C9B-C8B	-2.34	102.56	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	40	204	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
41	35	311	A86	C40-C32-C31	-2.34	108.38	110.47
30	33	310	CLA	CHA-C1A-NA	-2.34	121.05	126.40
36	B	620	LMG	O2-C2-C1	-2.34	104.37	110.05
36	B	619	LMG	O1-C1-C2	-2.34	104.66	108.30
41	18	314	A86	C40-C32-C31	-2.34	108.38	110.47
36	B	619	LMG	C40-C39-C38	-2.34	102.56	114.42
30	19	302	CLA	O2A-CGA-O1A	-2.33	117.48	123.30
30	B	614	CLA	C2A-C1A-CHA	2.33	127.94	123.86
41	15	311	A86	C40-C32-C31	-2.33	108.38	110.47
41	15	315	A86	C9-C10-C11	-2.33	119.75	126.61
30	c	507	CLA	O1D-CGD-CBD	2.33	129.26	124.48
32	f	101	BCR	C16-C15-C14	-2.33	118.69	123.47
30	B	614	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	15	302	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
36	b	618	LMG	C40-C39-C38	-2.33	102.58	114.42
36	b	618	LMG	O1-C1-C2	-2.33	104.66	108.30
30	12	313	CLA	CHA-C1A-NA	-2.33	121.06	126.40
30	16	305	CLA	C2A-C1A-CHA	2.33	127.94	123.86
30	21	305	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
38	J	101	DGD	CAB-C9B-C8B	-2.33	102.59	114.42
41	41	314	A86	C40-C32-C31	-2.33	108.39	110.47
41	33	316	A86	C9-C10-C11	-2.33	119.76	126.61
41	35	316	A86	C9-C10-C11	-2.33	119.76	126.61
32	b	617	BCR	C15-C16-C17	-2.33	118.70	123.47
30	17	304	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	31	308	CLA	CHA-C1A-NA	-2.33	121.06	126.40
30	B	611	CLA	C7-C6-C5	-2.33	107.03	113.36
30	31	304	CLA	C1D-ND-C4D	2.33	107.99	106.33
30	b	611	CLA	C1-C2-C3	-2.33	122.02	126.04
41	16	310	A86	C7-C6-C8	2.33	121.75	118.08
30	41	306	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
41	35	315	A86	C9-C10-C11	-2.33	119.76	126.61
30	B	613	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
30	B	611	CLA	C1-C2-C3	-2.33	122.02	126.04
30	36	305	CLA	C2A-C1A-CHA	2.33	127.93	123.86
30	c	505	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
36	b	618	LMG	O1-C7-C8	-2.33	105.29	110.90
30	b	613	CLA	C4-C3-C5	2.33	119.18	115.27
30	41	308	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
32	Z	101	BCR	C33-C5-C6	-2.32	121.92	124.53
30	B	608	CLA	CMB-C2B-C3B	2.32	129.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	304	CLA	C2D-C1D-ND	-2.32	108.39	110.10
30	C	509	CLA	CGD-CBD-CAD	-2.32	103.21	110.73
30	37	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
30	21	308	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
30	41	301	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
30	20	204	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
41	32	315	A86	C40-C32-C31	-2.32	108.40	110.47
30	11	308	CLA	CHA-C1A-NA	-2.32	121.09	126.40
32	F	101	BCR	C15-C16-C17	-2.32	118.72	123.47
30	c	511	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
41	34	312	A86	C40-C32-C31	-2.32	108.40	110.47
41	33	302	A86	C9-C10-C11	-2.32	119.79	126.61
30	B	606	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
30	c	504	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
30	b	613	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
30	21	301	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
32	h	101	BCR	C27-C26-C25	2.31	126.09	122.73
30	20	209	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
36	Q	301	LMG	O3-C3-C2	-2.31	105.00	110.35
30	31	302	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
30	C	505	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
41	21	314	A86	C41-C32-C31	-2.31	108.40	110.47
30	c	511	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
30	C	511	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
36	12	301	LMG	C1-C2-C3	-2.31	105.18	110.00
32	Z	101	BCR	C27-C26-C25	2.31	126.09	122.73
30	20	207	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
39	d	408	PL9	C11-C9-C8	-2.31	116.44	121.12
41	12	319	A86	C-C1-C24	2.31	121.72	118.08
36	d	410	LMG	C38-C37-C36	-2.31	102.70	114.42
30	14	301	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
36	D	408	LMG	C38-C37-C36	-2.31	102.70	114.42
38	C	516	DGD	O2D-C2D-C1D	-2.31	104.44	110.05
30	b	611	CLA	C3C-C4C-NC	-2.31	107.98	110.57
30	13	309	CLA	CHA-C1A-NA	-2.31	121.11	126.40
30	37	306	CLA	C2A-C1A-CHA	2.31	127.89	123.86
41	38	302	A86	C9-C10-C11	-2.31	119.82	126.61
41	31	311	A86	C40-C32-C31	-2.31	108.41	110.47
33	L	103	SQD	O8-S-C6	2.31	109.42	105.74
30	b	607	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
30	40	207	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
38	c	517	DGD	O2D-C2D-C1D	-2.31	104.44	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	20	209	CLA	C2A-C1A-CHA	2.31	127.89	123.86
30	15	303	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
30	18	301	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
30	b	611	CLA	C7-C6-C5	-2.30	107.10	113.36
41	15	315	A86	C35-C34-C33	2.30	113.90	109.88
41	41	314	A86	C41-C32-C31	-2.30	108.41	110.47
32	B	617	BCR	C30-C25-C26	-2.30	119.37	122.61
30	C	504	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
30	C	504	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
30	c	504	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
30	B	611	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	40	209	CLA	C2A-C1A-CHA	2.30	127.88	123.86
41	17	316	A86	C-C1-C24	2.30	121.70	118.08
41	32	316	A86	C7-C6-C8	2.30	121.70	118.08
30	b	606	CLA	C3C-C4C-NC	-2.30	107.99	110.57
30	38	301	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
30	40	209	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
30	B	607	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
30	39	307	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
30	14	309	CLA	CHA-C1A-NA	-2.30	121.13	126.40
41	18	302	A86	C9-C10-C11	-2.30	119.85	126.61
36	b	619	LMG	C6-C5-C4	-2.30	107.62	113.00
36	c	519	LMG	O3-C3-C2	-2.30	105.03	110.35
41	21	312	A86	C10-C9-C8	-2.30	116.05	123.22
41	36	310	A86	C7-C6-C8	2.30	121.70	118.08
35	d	409	LHG	C18-C17-C16	-2.30	102.77	114.42
39	d	408	PL9	O1-C4-C3	-2.30	118.19	120.72
39	D	407	PL9	C42-C43-C44	-2.30	122.13	127.66
35	L	101	LHG	C18-C17-C16	-2.30	102.77	114.42
30	b	614	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
31	A	403	PHO	CBA-CAA-C2A	-2.29	107.11	113.81
38	C	516	DGD	O5E-C6E-C5E	-2.29	103.42	111.29
41	21	310	A86	C7-C6-C8	2.29	121.69	118.08
30	B	603	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
30	c	511	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
30	17	306	CLA	C2A-C1A-CHA	2.29	127.87	123.86
41	41	310	A86	C7-C6-C8	2.29	121.69	118.08
30	19	304	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
41	41	312	A86	C10-C9-C8	-2.29	116.06	123.22
32	h	101	BCR	C24-C23-C22	-2.29	122.77	126.23
38	h	102	DGD	CBB-CAB-C9B	-2.29	102.78	114.42
41	11	311	A86	C40-C32-C31	-2.29	108.42	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	622	CLA	C1-C2-C3	-2.29	122.08	126.04
30	35	308	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	C	511	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
41	37	316	A86	C-C1-C24	2.29	121.68	118.08
30	31	307	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
30	34	308	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
30	C	507	CLA	O1D-CGD-CBD	2.29	129.16	124.48
30	19	307	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
35	l	102	LHG	C18-C17-C16	-2.29	102.82	114.42
38	H	102	DGD	CBB-CAB-C9B	-2.29	102.82	114.42
30	C	511	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
41	38	314	A86	C40-C32-C31	-2.29	108.43	110.47
41	36	313	A86	C-C1-C24	2.29	121.68	118.08
30	36	309	CLA	C2D-C1D-ND	-2.29	108.42	110.10
30	39	304	CLA	CAA-C2A-C3A	-2.28	106.52	112.78
30	z	101	CLA	C2A-C1A-CHA	2.28	127.85	123.86
39	D	407	PL9	C11-C9-C8	-2.28	116.49	121.12
39	D	404	PL9	C36-C34-C33	-2.28	116.50	121.12
31	A	403	PHO	CMC-C2C-C3C	2.28	129.25	124.94
41	12	317	A86	C7-C6-C8	2.28	121.67	118.08
41	37	311	A86	C34-O4-C38	-2.28	113.64	117.90
30	a	402	CLA	CHB-C4A-NA	2.28	127.67	124.51
32	b	623	BCR	C33-C5-C6	-2.28	121.97	124.53
41	35	315	A86	C35-C34-C33	2.28	113.86	109.88
41	32	304	A86	C35-C34-C33	2.28	113.86	109.88
30	36	304	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	35	303	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	B	601	CLA	C2A-C1A-CHA	2.28	127.84	123.86
30	B	615	CLA	C2A-C1A-CHA	2.28	127.84	123.86
30	b	603	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	32	311	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	B	613	CLA	C2A-C1A-CHA	2.28	127.84	123.86
30	c	507	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
32	f	101	BCR	C15-C16-C17	-2.28	118.81	123.47
30	B	613	CLA	C4-C3-C5	2.28	119.10	115.27
30	33	304	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
36	B	620	LMG	C6-C5-C4	-2.28	107.67	113.00
30	16	304	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
41	35	316	A86	C35-C34-C33	2.28	113.85	109.88
30	40	205	CLA	C2A-C1A-CHA	2.28	127.84	123.86
31	d	403	PHO	CBA-CAA-C2A	-2.27	107.17	113.81
41	15	316	A86	C35-C34-C33	2.27	113.84	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	613	CLA	C2A-C1A-CHA	2.27	127.84	123.86
30	c	503	CLA	CHA-C1A-NA	-2.27	121.19	126.40
30	B	606	CLA	C3C-C4C-NC	-2.27	108.02	110.57
41	32	318	A86	C-C1-C24	2.27	121.66	118.08
41	12	304	A86	C35-C34-C33	2.27	113.84	109.88
35	L	102	LHG	C18-C17-C16	-2.27	102.89	114.42
41	13	315	A86	C-C1-C24	2.27	121.66	118.08
30	15	308	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
30	20	208	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
30	b	602	CLA	C3C-C4C-NC	-2.27	108.03	110.57
30	C	507	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
30	40	208	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
30	b	622	CLA	CHA-C1A-NA	-2.27	121.20	126.40
30	16	305	CLA	C2D-C1D-ND	-2.27	108.43	110.10
30	b	604	CLA	CHA-C1A-NA	-2.27	121.20	126.40
30	B	602	CLA	C3C-C4C-NC	-2.27	108.03	110.57
32	a	404	BCR	C35-C13-C14	-2.27	119.75	122.92
30	38	301	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
41	13	313	A86	C7-C6-C8	2.27	121.65	118.08
41	21	312	A86	C19-C18-C17	-2.26	106.40	110.77
30	b	601	CLA	C2A-C1A-CHA	2.26	127.82	123.86
30	21	308	CLA	C2A-C1A-CHA	2.26	127.82	123.86
30	c	522	CLA	C2D-C1D-ND	-2.26	108.44	110.10
30	c	504	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
39	d	405	PL9	C36-C34-C33	-2.26	116.54	121.12
32	H	101	BCR	C24-C23-C22	-2.26	122.82	126.23
42	32	302	LMU	C1B-O5B-C5B	2.26	118.13	113.69
30	34	303	CLA	CHA-C1A-NA	-2.26	121.22	126.40
41	18	302	A86	C35-C34-C33	2.26	113.82	109.88
30	20	205	CLA	C2A-C1A-CHA	2.26	127.81	123.86
30	41	308	CLA	C2A-C1A-CHA	2.26	127.81	123.86
41	36	312	A86	C7-C6-C8	2.26	121.64	118.08
30	14	307	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
32	H	101	BCR	C27-C26-C25	2.26	126.01	122.73
32	b	617	BCR	C11-C10-C9	-2.26	124.09	127.31
30	C	504	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
30	W	102	CLA	CAA-CBA-CGA	-2.26	106.65	113.25
41	35	314	A86	C-C1-C24	2.26	121.64	118.08
42	12	302	LMU	C1B-O5B-C5B	2.26	118.12	113.69
32	b	623	BCR	C27-C26-C25	2.26	126.01	122.73
36	12	301	LMG	O2-C2-C3	-2.26	105.13	110.35
36	b	618	LMG	C38-C37-C36	-2.26	102.97	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	D	404	PL9	C37-C38-C39	-2.26	122.23	127.66
30	11	306	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
30	21	306	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
41	15	314	A86	C-C1-C24	2.26	121.63	118.08
30	C	503	CLA	CHA-C1A-NA	-2.25	121.24	126.40
41	16	312	A86	C7-C6-C8	2.25	121.63	118.08
30	15	306	CLA	O2D-CGD-CBD	2.25	115.27	111.27
30	15	306	CLA	CHD-C1D-ND	-2.25	122.39	124.45
41	33	317	A86	C-C1-C24	2.25	121.62	118.08
30	B	602	CLA	O2D-CGD-CBD	2.25	115.27	111.27
41	16	313	A86	C-C1-C24	2.25	121.62	118.08
38	C	517	DGD	O6E-C1E-O5D	-2.25	104.65	109.97
41	13	301	A86	C35-C34-C33	2.25	113.80	109.88
41	20	211	A86	C7-C6-C8	2.25	121.62	118.08
30	B	608	CLA	O2D-CGD-CBD	2.25	115.26	111.27
41	11	316	A86	C35-C34-C33	2.25	113.80	109.88
41	31	316	A86	C35-C34-C33	2.25	113.80	109.88
33	l	101	SQD	O8-S-C6	2.25	109.32	105.74
30	37	308	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
30	18	301	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
30	B	623	CLA	CMD-C2D-C1D	-2.24	120.76	124.71
35	b	621	LHG	C18-C17-C16	-2.24	103.04	114.42
30	B	623	CLA	CMD-C2D-C3D	2.24	132.77	127.61
30	11	307	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
32	c	515	BCR	C15-C14-C13	-2.24	124.11	127.31
30	13	308	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
30	14	308	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
30	31	302	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
30	c	510	CLA	C16-C15-C13	-2.24	108.67	115.92
41	17	313	A86	C7-C6-C8	2.24	121.61	118.08
41	33	302	A86	C35-C34-C33	2.24	113.79	109.88
41	38	302	A86	C35-C34-C33	2.24	113.79	109.88
30	c	508	CLA	C2D-C1D-ND	-2.24	108.45	110.10
30	17	308	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
41	17	311	A86	C34-O4-C38	-2.24	113.72	117.90
41	31	314	A86	C-C1-C24	2.24	121.61	118.08
41	33	314	A86	C7-C6-C8	2.24	121.61	118.08
32	m	103	BCR	C33-C5-C6	-2.24	122.01	124.53
41	35	312	A86	C7-C6-C8	2.24	121.60	118.08
31	d	403	PHO	CMC-C2C-C3C	2.24	129.16	124.94
41	15	312	A86	C7-C6-C8	2.24	121.60	118.08
41	33	316	A86	C35-C34-C33	2.24	113.78	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	505	CLA	CHC-C1C-NC	2.24	127.60	124.20
30	w	102	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
35	B	622	LHG	C18-C17-C16	-2.24	103.07	114.42
41	40	201	A86	C7-C6-C5	-2.24	119.79	122.92
30	39	301	CLA	CHD-C1D-ND	-2.24	122.40	124.45
30	21	309	CLA	O2A-CGA-O1A	-2.24	117.73	123.30
30	32	308	CLA	C1D-ND-C4D	2.24	107.92	106.33
30	C	520	CLA	C2D-C1D-ND	-2.23	108.46	110.10
41	13	317	A86	C-C1-C24	2.23	121.60	118.08
41	41	312	A86	C19-C18-C17	-2.23	106.46	110.77
30	C	510	CLA	C16-C15-C13	-2.23	108.70	115.92
30	C	503	CLA	C1D-ND-C4D	2.23	107.92	106.33
39	d	405	PL9	C37-C38-C39	-2.23	122.28	127.66
32	F	101	BCR	C27-C26-C25	2.23	125.97	122.73
30	40	204	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
36	B	619	LMG	C38-C37-C36	-2.23	103.09	114.42
30	41	306	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
30	C	503	CLA	C2D-C1D-ND	-2.23	108.46	110.10
38	C	517	DGD	O5D-C6D-C5D	-2.23	104.92	109.05
30	35	306	CLA	O2D-CGD-CBD	2.23	115.23	111.27
30	b	615	CLA	C2A-C1A-CHA	2.23	127.76	123.86
41	32	319	A86	C-C1-C24	2.23	121.59	118.08
41	19	310	A86	C26-C25-C24	-2.23	116.26	123.22
30	12	310	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
30	31	302	CLA	CHA-C1A-NA	-2.23	121.30	126.40
41	41	310	A86	C19-C18-C17	-2.23	106.47	110.77
32	A	405	BCR	C35-C13-C14	-2.23	119.80	122.92
41	41	311	A86	O1-C15-C14	-2.23	108.74	113.21
41	21	310	A86	O1-C15-C14	-2.23	108.74	113.21
38	C	517	DGD	CAB-C9B-C8B	-2.23	103.12	114.42
30	B	609	CLA	O1D-CGD-CBD	2.23	129.04	124.48
30	b	609	CLA	O1D-CGD-CBD	2.23	129.04	124.48
30	13	307	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
30	C	519	CLA	C2A-C1A-CHA	2.23	127.75	123.86
41	13	316	A86	C35-C34-C33	2.23	113.76	109.88
32	b	617	BCR	C27-C26-C25	2.23	125.96	122.73
30	b	602	CLA	O2D-CGD-CBD	2.23	115.22	111.27
41	31	312	A86	C7-C6-C8	2.22	121.58	118.08
30	39	304	CLA	C3A-C2A-C1A	2.22	104.67	101.34
30	B	623	CLA	C1-C2-C3	-2.22	122.20	126.04
31	D	403	PHO	C1-C2-C3	-2.22	122.20	126.04
41	21	311	A86	O1-C15-C14	-2.22	108.75	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	39	310	A86	C26-C25-C24	-2.22	116.28	123.22
30	33	309	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
30	C	503	CLA	CHC-C1C-NC	2.22	127.58	124.20
30	18	309	CLA	CAA-C2A-C1A	2.22	119.26	111.97
36	B	620	LMG	C38-C37-C36	-2.22	103.14	114.42
30	35	303	CLA	CHD-C1D-ND	-2.22	122.41	124.45
33	A	406	SQD	O48-C23-O10	-2.22	117.99	123.59
41	11	312	A86	C7-C6-C8	2.22	121.58	118.08
41	40	211	A86	C7-C6-C8	2.22	121.58	118.08
30	33	304	CLA	CHA-C1A-NA	-2.22	121.31	126.40
41	41	311	A86	C7-C6-C8	2.22	121.58	118.08
30	d	401	CLA	O2D-CGD-CBD	2.22	115.21	111.27
41	37	313	A86	C7-C6-C8	2.22	121.57	118.08
38	C	517	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
30	38	305	CLA	CHD-C1D-ND	-2.22	122.42	124.45
30	c	513	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
30	W	102	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
30	38	309	CLA	CAA-C2A-C1A	2.22	119.24	111.97
30	C	505	CLA	CHC-C1C-NC	2.22	127.57	124.20
30	19	301	CLA	CHD-C1D-ND	-2.22	122.42	124.45
41	41	310	A86	O1-C15-C14	-2.22	108.76	113.21
41	21	310	A86	C19-C18-C17	-2.22	106.49	110.77
30	20	204	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
41	11	314	A86	C-C1-C24	2.22	121.57	118.08
30	20	202	CLA	C1-C2-C3	-2.22	122.21	126.04
31	d	404	PHO	C1-C2-C3	-2.21	122.21	126.04
32	B	618	BCR	C11-C10-C9	-2.21	124.15	127.31
32	c	520	BCR	C29-C30-C25	2.21	113.89	110.48
30	19	301	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
30	b	608	CLA	O2D-CGD-CBD	2.21	115.20	111.27
30	32	306	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
30	40	202	CLA	C1-C2-C3	-2.21	122.22	126.04
41	34	313	A86	C7-C6-C8	2.21	121.56	118.08
30	19	308	CLA	O2A-CGA-O1A	-2.21	117.79	123.30
32	B	618	BCR	C15-C14-C13	-2.21	124.16	127.31
30	B	611	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
30	38	306	CLA	C3A-C2A-C1A	2.21	104.65	101.34
30	37	307	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
30	39	308	CLA	O2A-CGA-O1A	-2.21	117.79	123.30
30	12	306	CLA	CHA-C1A-NA	-2.21	121.34	126.40
38	c	518	DGD	O6E-C1E-O5D	-2.21	104.75	109.97
32	b	617	BCR	C15-C14-C13	-2.21	124.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c	518	DGD	C3G-C2G-C1G	-2.21	106.57	111.79
30	B	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
36	b	619	LMG	C38-C37-C36	-2.21	103.22	114.42
30	b	605	CLA	C2D-C1D-ND	-2.21	108.48	110.10
30	14	303	CLA	CHA-C1A-NA	-2.21	121.34	126.40
30	37	307	CLA	CMC-C2C-C3C	2.21	132.10	126.12
30	B	604	CLA	CHA-C1A-NA	-2.21	121.35	126.40
30	17	307	CLA	CMC-C2C-C3C	2.20	132.10	126.12
30	35	306	CLA	CHD-C1D-ND	-2.20	122.43	124.45
32	b	623	BCR	C38-C26-C27	-2.20	109.38	113.62
30	11	308	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	W	102	CLA	C2D-C1D-ND	-2.20	108.48	110.10
30	18	301	CLA	C3C-C4C-NC	-2.20	108.10	110.57
33	L	103	SQD	C44-O6-C1	2.20	118.04	113.74
30	41	305	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	36	305	CLA	C2D-C1D-ND	-2.20	108.48	110.10
30	C	502	CLA	C7-C6-C5	-2.20	107.38	113.36
30	11	302	CLA	CHA-C1A-NA	-2.20	121.36	126.40
30	C	513	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
39	d	408	PL9	C36-C37-C38	-2.20	104.64	111.88
38	j	101	DGD	CBB-CAB-C9B	-2.20	103.25	114.42
32	B	618	BCR	C16-C15-C14	-2.20	118.97	123.47
30	21	305	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
30	39	304	CLA	CHA-C1A-NA	-2.20	121.36	126.40
30	19	304	CLA	C3A-C2A-C1A	2.20	104.63	101.34
30	34	309	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
30	34	303	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
30	39	301	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
30	18	306	CLA	C3A-C2A-C1A	2.20	104.63	101.34
30	41	309	CLA	O2A-CGA-O1A	-2.20	117.83	123.30
41	39	311	A86	C12-C11-C13	2.20	119.71	116.02
30	38	309	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
38	J	101	DGD	C3D-C4D-C5D	-2.20	106.32	110.24
41	12	304	A86	C28-C27-C26	-2.20	119.85	122.92
30	32	306	CLA	CHA-C1A-NA	-2.19	121.37	126.40
38	c	518	DGD	CAB-C9B-C8B	-2.19	103.28	114.42
41	16	310	A86	C9-C10-C11	-2.19	120.16	126.61
38	j	101	DGD	C3D-C4D-C5D	-2.19	106.33	110.24
41	21	311	A86	C7-C6-C8	2.19	121.53	118.08
41	16	310	A86	C8-C6-C5	-2.19	115.58	118.94
33	l	101	SQD	C44-O6-C1	2.19	118.02	113.74
30	13	309	CLA	O2D-CGD-O1D	-2.19	119.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
33	a	405	SQD	O48-C23-O10	-2.19	118.06	123.59
32	f	101	BCR	C27-C26-C25	2.19	125.91	122.73
30	16	308	CLA	CHA-C1A-NA	-2.19	121.38	126.40
32	B	624	BCR	C27-C26-C25	2.19	125.91	122.73
30	35	302	CLA	O2D-CGD-CBD	2.19	115.16	111.27
32	C	518	BCR	C20-C21-C22	-2.19	124.18	127.31
41	14	313	A86	C7-C6-C8	2.19	121.53	118.08
39	D	404	PL9	O2-C1-C6	2.19	124.38	120.59
30	c	502	CLA	C7-C6-C5	-2.19	107.41	113.36
41	20	201	A86	C7-C6-C5	-2.19	119.86	122.92
30	15	303	CLA	CHD-C1D-ND	-2.19	122.44	124.45
41	36	310	A86	C9-C10-C11	-2.19	120.17	126.61
30	17	307	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
41	36	310	A86	C8-C6-C5	-2.19	115.58	118.94
30	39	302	CLA	O1A-CGA-CBA	2.19	130.11	123.08
41	33	302	A86	C28-C27-C26	-2.19	119.86	122.92
30	15	309	CLA	O2A-CGA-O1A	-2.19	117.85	123.30
38	c	518	DGD	O5D-C6D-C5D	-2.19	105.00	109.05
41	20	211	A86	O1-C15-C14	-2.19	108.82	113.21
30	18	301	CLA	CAC-C3C-C4C	2.19	127.65	124.81
30	19	302	CLA	O1A-CGA-CBA	2.19	130.10	123.08
30	16	305	CLA	O2A-CGA-O1A	-2.19	117.85	123.30
30	35	309	CLA	O2A-CGA-O1A	-2.19	117.85	123.30
38	J	101	DGD	CBB-CAB-C9B	-2.19	103.33	114.42
41	40	211	A86	O1-C15-C14	-2.19	108.83	113.21
30	c	503	CLA	CHC-C1C-NC	2.18	127.52	124.20
30	19	304	CLA	CHA-C1A-NA	-2.18	121.40	126.40
32	b	617	BCR	C16-C15-C14	-2.18	119.00	123.47
30	12	313	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
35	b	621	LHG	C20-C19-C18	-2.18	103.34	114.42
30	C	508	CLA	C2D-C1D-ND	-2.18	108.50	110.10
30	d	406	CLA	CAC-C3C-C4C	2.18	127.64	124.81
38	c	518	DGD	O5E-C6E-C5E	-2.18	103.81	111.29
30	13	303	CLA	CHA-C1A-NA	-2.18	121.41	126.40
41	35	315	A86	C28-C27-C26	-2.18	119.87	122.92
30	36	305	CLA	O2A-CGA-O1A	-2.18	117.87	123.30
30	33	308	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
30	B	605	CLA	C2D-C1D-ND	-2.18	108.50	110.10
30	B	606	CLA	C6-C7-C8	-2.18	108.88	115.92
36	M	102	LMG	C1-C2-C3	-2.18	105.46	110.00
30	17	307	CLA	CMC-C2C-C1C	-2.18	121.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	b	619	LMG	C40-C39-C38	-2.18	103.37	114.42
41	38	315	A86	C-C1-C24	2.18	121.51	118.08
30	13	303	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
41	32	304	A86	C28-C27-C26	-2.18	119.87	122.92
41	19	311	A86	C12-C11-C13	2.18	119.68	116.02
30	18	310	CLA	C2A-C1A-CHA	2.18	127.67	123.86
30	w	102	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
35	A	408	LHG	C5-O7-C7	-2.18	112.43	117.79
30	14	309	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
30	15	302	CLA	O2D-CGD-CBD	2.18	115.13	111.27
30	C	508	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
30	38	311	CLA	O2A-CGA-O1A	-2.17	117.88	123.30
30	38	312	CLA	O2A-CGA-O1A	-2.17	117.88	123.30
32	Y	101	BCR	C29-C30-C25	2.17	113.83	110.48
35	B	622	LHG	C20-C19-C18	-2.17	103.39	114.42
30	12	311	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
30	c	512	CLA	CHA-C4D-ND	2.17	137.05	132.50
32	Z	101	BCR	C15-C14-C13	-2.17	124.21	127.31
30	18	309	CLA	CHA-C1A-NA	-2.17	121.42	126.40
30	39	302	CLA	C2A-C1A-CHA	2.17	127.66	123.86
33	b	620	SQD	O48-C23-C24	2.17	118.73	111.91
30	38	301	CLA	C3C-C4C-NC	-2.17	108.13	110.57
30	C	512	CLA	CHA-C4D-ND	2.17	137.04	132.50
30	D	405	CLA	CAC-C3C-C4C	2.17	127.63	124.81
32	h	101	BCR	C40-C30-C25	2.17	113.82	110.30
30	34	301	CLA	C2A-C1A-CHA	2.17	127.66	123.86
30	w	102	CLA	C2D-C1D-ND	-2.17	108.50	110.10
30	37	306	CLA	C3A-C2A-C1A	2.17	104.59	101.34
30	D	401	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
30	11	302	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
32	H	101	BCR	C40-C30-C25	2.17	113.82	110.30
30	c	512	CLA	CHA-C1A-NA	-2.17	121.43	126.40
39	D	407	PL9	C36-C37-C38	-2.17	104.75	111.88
30	38	301	CLA	CAC-C3C-C4C	2.17	127.63	124.81
30	14	303	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
30	21	302	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
32	f	101	BCR	C24-C23-C22	-2.17	122.96	126.23
30	18	307	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
41	33	315	A86	C-C1-C24	2.17	121.49	118.08
38	H	102	DGD	C5B-C4B-C3B	-2.17	103.42	114.42
39	D	407	PL9	C50-C49-C48	-2.17	116.38	122.65
41	40	212	A86	C-C1-C2	-2.17	119.89	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	41	302	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
35	a	407	LHG	C5-O7-C7	-2.17	112.46	117.79
30	18	311	CLA	O2A-CGA-O1A	-2.17	117.90	123.30
30	36	308	CLA	CHA-C1A-NA	-2.17	121.44	126.40
38	C	517	DGD	O5E-C6E-C5E	-2.17	103.86	111.29
41	20	212	A86	C-C1-C2	-2.17	119.89	122.92
30	C	514	CLA	C2A-C1A-CHA	2.17	127.64	123.86
36	B	620	LMG	C40-C39-C38	-2.17	103.43	114.42
30	32	310	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
36	Q	301	LMG	C3-C4-C5	-2.16	106.38	110.24
36	c	519	LMG	C3-C4-C5	-2.16	106.38	110.24
41	17	314	A86	C-C1-C24	2.16	121.49	118.08
30	b	613	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
30	c	508	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
30	32	312	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
32	B	624	BCR	C38-C26-C27	-2.16	109.46	113.62
30	d	401	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
30	37	309	CLA	CAA-CBA-CGA	-2.16	106.77	112.51
30	C	521	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	b	611	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	39	303	CLA	C3A-C2A-C1A	2.16	104.58	101.34
30	18	305	CLA	CHD-C1D-ND	-2.16	122.47	124.45
36	m	102	LMG	C9-C8-C7	-2.16	106.68	111.79
41	13	316	A86	C28-C27-C26	-2.16	119.90	122.92
38	h	102	DGD	C5B-C4B-C3B	-2.16	103.46	114.42
32	c	521	BCR	C20-C21-C22	-2.16	124.23	127.31
30	14	306	CLA	C2A-C1A-CHA	2.16	127.63	123.86
30	16	302	CLA	O2D-CGD-CBD	2.16	115.10	111.27
30	b	606	CLA	C6-C7-C8	-2.16	108.94	115.92
30	C	503	CLA	CMB-C2B-C3B	2.16	128.72	124.68
30	b	603	CLA	O1D-CGD-CBD	2.16	128.90	124.48
39	d	405	PL9	O2-C1-C6	2.16	124.33	120.59
41	11	316	A86	C28-C27-C26	-2.16	119.90	122.92
30	38	309	CLA	CHA-C1A-NA	-2.16	121.46	126.40
30	19	302	CLA	C2A-C1A-CHA	2.16	127.63	123.86
39	d	408	PL9	C50-C49-C48	-2.16	116.42	122.65
41	31	316	A86	C28-C27-C26	-2.16	119.90	122.92
30	36	302	CLA	O2D-CGD-CBD	2.16	115.10	111.27
30	B	613	CLA	CAA-C2A-C3A	-2.16	106.88	112.78
41	18	302	A86	C28-C27-C26	-2.16	119.90	122.92
41	32	317	A86	C34-O4-C38	-2.16	113.88	117.90
30	15	301	CLA	CAA-CBA-CGA	-2.15	106.96	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	17	311	A86	C7-C6-C8	2.15	121.47	118.08
41	37	314	A86	C-C1-C24	2.15	121.47	118.08
41	13	301	A86	C28-C27-C26	-2.15	119.91	122.92
30	41	302	CLA	CHA-C1A-NA	-2.15	121.46	126.40
30	c	511	CLA	C2A-C1A-CHA	2.15	127.63	123.86
33	B	621	SQD	O48-C23-C24	2.15	118.67	111.91
30	35	301	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
30	37	301	CLA	CHB-C4A-NA	2.15	127.49	124.51
30	12	306	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
30	17	306	CLA	C3A-C2A-C1A	2.15	104.56	101.34
30	a	402	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
30	38	307	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
30	40	206	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
30	A	404	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
32	a	408	BCR	C27-C26-C25	2.15	125.85	122.73
30	18	312	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
30	31	306	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
36	m	102	LMG	C1-O6-C5	-2.15	109.47	113.69
30	32	307	CLA	CAA-C2A-C1A	2.15	119.02	111.97
32	B	618	BCR	C27-C26-C25	2.15	125.85	122.73
32	c	515	BCR	C16-C15-C14	-2.15	119.07	123.47
36	m	102	LMG	C1-C2-C3	-2.15	105.52	110.00
30	33	310	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
30	b	611	CLA	CHD-C1D-ND	-2.15	122.48	124.45
41	14	313	A86	C-C1-C24	2.15	121.46	118.08
30	c	523	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
40	e	101	HEM	C4A-C3A-C2A	2.15	108.49	107.00
32	Z	101	BCR	C16-C15-C14	-2.15	119.08	123.47
30	17	309	CLA	CAA-CBA-CGA	-2.15	106.81	112.51
30	31	308	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
30	17	301	CLA	CHB-C4A-NA	2.15	127.48	124.51
41	15	315	A86	C28-C27-C26	-2.15	119.92	122.92
30	18	309	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
30	b	603	CLA	CAA-CBA-CGA	-2.15	106.98	113.25
30	21	307	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
41	34	313	A86	C-C1-C24	2.14	121.46	118.08
36	m	102	LMG	O1-C7-C8	-2.14	105.72	110.90
30	38	311	CLA	O2D-CGD-CBD	2.14	115.08	111.27
36	M	102	LMG	C9-C8-C7	-2.14	106.72	111.79
30	B	611	CLA	CHD-C1D-ND	-2.14	122.48	124.45
30	D	401	CLA	O2D-CGD-CBD	2.14	115.08	111.27
41	32	317	A86	C-C1-C24	2.14	121.45	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	37	311	A86	C7-C6-C8	2.14	121.45	118.08
30	37	301	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
38	C	517	DGD	C8B-C7B-C6B	-2.14	103.55	114.42
30	37	307	CLA	CMC-C2C-C1C	-2.14	121.78	125.04
32	c	516	BCR	C30-C25-C26	-2.14	119.60	122.61
30	31	306	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
30	41	307	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
38	j	101	DGD	O6E-C1E-O5D	-2.14	104.91	109.97
30	20	206	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
41	18	315	A86	C-C1-C24	2.14	121.45	118.08
30	A	402	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
41	11	313	A86	C-C1-C24	2.14	121.44	118.08
41	39	311	A86	C4-C3-C2	-2.14	119.10	123.47
30	B	603	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
30	33	305	CLA	CAA-C2A-C1A	2.14	118.98	111.97
30	C	506	CLA	CMC-C2C-C3C	2.14	131.92	126.12
30	Z	102	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
32	B	618	BCR	C40-C30-C25	2.14	113.76	110.30
30	34	307	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
30	18	311	CLA	O2D-CGD-CBD	2.13	115.06	111.27
41	38	302	A86	C28-C27-C26	-2.13	119.93	122.92
30	19	303	CLA	C3A-C2A-C1A	2.13	104.53	101.34
41	31	313	A86	C34-O4-C38	-2.13	113.92	117.90
30	17	301	CLA	C1-C2-C3	-2.13	122.36	126.04
30	37	301	CLA	C1-C2-C3	-2.13	122.36	126.04
30	17	301	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
30	11	305	CLA	C2A-C1A-CHA	2.13	127.58	123.86
36	c	519	LMG	C1-C2-C3	-2.13	105.56	110.00
30	b	615	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
30	B	615	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
41	31	313	A86	C-C1-C24	2.13	121.43	118.08
30	36	302	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
30	b	602	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
30	21	302	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	37	308	CLA	C2A-C1A-CHA	2.13	127.58	123.86
32	A	409	BCR	C27-C26-C25	2.13	125.82	122.73
30	b	603	CLA	C4-C3-C5	2.13	118.85	115.27
30	35	308	CLA	CHA-C1A-NA	-2.13	121.53	126.40
32	B	616	BCR	C33-C5-C6	-2.13	122.14	124.53
41	41	313	A86	C41-C32-C31	-2.13	108.57	110.47
30	c	524	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
41	12	318	A86	C-C1-C24	2.13	121.43	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	17	307	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
30	33	305	CLA	C2A-C1A-CHA	2.13	127.58	123.86
39	d	405	PL9	O1-C4-C3	-2.13	118.38	120.72
30	Z	102	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
39	d	408	PL9	C27-C28-C29	-2.13	122.54	127.66
30	C	505	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
41	35	316	A86	C28-C27-C26	-2.12	119.95	122.92
40	e	101	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
30	B	615	CLA	CMA-C3A-C4A	-2.12	106.06	111.77
41	15	313	A86	C34-O4-C38	-2.12	113.94	117.90
30	34	307	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
30	C	512	CLA	CHA-C1A-NA	-2.12	121.53	126.40
41	32	304	A86	C8-C6-C5	2.12	122.20	118.94
36	M	102	LMG	O1-C7-C8	-2.12	105.78	110.90
30	c	502	CLA	C11-C12-C13	-2.12	109.06	115.92
30	36	305	CLA	C3A-C2A-C1A	2.12	104.52	101.34
30	c	503	CLA	CMB-C2B-C3B	2.12	128.65	124.68
32	b	616	BCR	C38-C26-C27	-2.12	109.54	113.62
30	33	307	CLA	C2A-C1A-CHA	2.12	127.57	123.86
35	L	102	LHG	C27-C26-C25	-2.12	103.65	114.42
40	E	101	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
30	37	307	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
30	c	511	CLA	C1-C2-C3	-2.12	122.37	126.04
30	C	521	CLA	C3A-C2A-C1A	2.12	104.52	101.34
30	c	524	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
30	20	205	CLA	C2D-C1D-ND	-2.12	108.54	110.10
30	38	303	CLA	C1-C2-C3	-2.12	122.38	126.04
30	a	403	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
41	19	311	A86	C4-C3-C2	-2.12	119.13	123.47
41	38	315	A86	C34-O4-C38	-2.12	113.95	117.90
30	16	309	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
30	38	310	CLA	C2D-C1D-ND	-2.12	108.54	110.10
30	40	205	CLA	C2D-C1D-ND	-2.12	108.54	110.10
41	15	316	A86	C28-C27-C26	-2.12	119.95	122.92
41	11	316	A86	C8-C6-C5	2.12	122.19	118.94
41	12	318	A86	C34-O4-C38	-2.12	113.95	117.90
41	21	310	A86	C-C1-C2	-2.12	119.96	122.92
30	C	511	CLA	C1-C2-C3	-2.12	122.38	126.04
30	17	308	CLA	C2A-C1A-CHA	2.12	127.56	123.86
30	21	309	CLA	CAA-CBA-CGA	-2.12	106.89	112.51
30	B	603	CLA	C4-C3-C5	2.12	118.83	115.27
30	31	303	CLA	CAA-C2A-C1A	2.12	118.91	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	38	310	CLA	C2A-C1A-CHA	2.12	127.56	123.86
30	W	102	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
30	16	301	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
41	32	316	A86	C-C1-C24	2.12	121.41	118.08
41	33	316	A86	C28-C27-C26	-2.12	119.96	122.92
41	12	304	A86	C8-C6-C5	2.12	122.19	118.94
30	c	514	CLA	C2A-C1A-CHA	2.12	127.56	123.86
41	17	315	A86	C23-C16-C22	-2.12	104.25	107.37
41	14	314	A86	C-C1-C24	2.12	121.41	118.08
38	c	518	DGD	C8B-C7B-C6B	-2.12	103.69	114.42
41	40	212	A86	C12-C11-C13	2.11	119.58	116.02
36	b	618	LMG	O2-C2-C1	-2.11	104.91	110.05
30	16	305	CLA	C3A-C2A-C1A	2.11	104.51	101.34
30	18	308	CLA	C2A-C1A-CHA	2.11	127.56	123.86
32	B	617	BCR	C38-C26-C27	-2.11	109.56	113.62
30	B	623	CLA	CHA-C1A-NA	-2.11	121.56	126.40
30	c	523	CLA	C3A-C2A-C1A	2.11	104.50	101.34
31	A	403	PHO	C1B-NB-C4B	2.11	111.43	107.09
30	32	310	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
41	11	313	A86	C34-O4-C38	-2.11	113.96	117.90
41	33	314	A86	C-C1-C24	2.11	121.41	118.08
41	40	213	A86	C34-O4-C38	-2.11	113.96	117.90
41	31	316	A86	C8-C6-C5	2.11	122.18	118.94
30	c	508	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
30	B	614	CLA	C3A-C2A-C1A	2.11	104.50	101.34
41	34	314	A86	C-C1-C24	2.11	121.40	118.08
31	d	404	PHO	C1B-NB-C4B	2.11	111.43	107.09
30	15	308	CLA	CHA-C1A-NA	-2.11	121.56	126.40
41	37	315	A86	C23-C16-C22	-2.11	104.26	107.37
41	12	317	A86	C-C1-C24	2.11	121.40	118.08
41	15	312	A86	C-C1-C24	2.11	121.40	118.08
30	40	206	CLA	CHA-C1A-NA	-2.11	121.57	126.40
30	b	606	CLA	C2D-C1D-ND	-2.11	108.55	110.10
30	33	303	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
30	38	301	CLA	C2A-C1A-CHA	2.11	127.55	123.86
39	d	405	PL9	O2-C1-C2	-2.11	116.95	121.78
41	20	212	A86	C12-C11-C13	2.11	119.56	116.02
30	18	310	CLA	C2D-C1D-ND	-2.11	108.55	110.10
41	15	313	A86	C-C1-C24	2.11	121.40	118.08
35	l	102	LHG	C27-C26-C25	-2.11	103.73	114.42
30	D	402	CLA	CHD-C1D-ND	-2.11	122.52	124.45
30	C	511	CLA	C2A-C1A-CHA	2.11	127.54	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	617	BCR	C40-C30-C25	2.11	113.72	110.30
30	41	309	CLA	CAA-CBA-CGA	-2.11	106.92	112.51
30	17	305	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
30	16	303	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
41	19	310	A86	C7-C6-C5	-2.11	119.97	122.92
38	j	101	DGD	C7B-C6B-C5B	-2.11	103.73	114.42
30	12	303	CLA	C2A-C1A-CHA	2.11	127.54	123.86
41	13	314	A86	C-C1-C24	2.11	121.39	118.08
30	32	303	CLA	C2A-C1A-CHA	2.11	127.54	123.86
41	34	314	A86	C34-O4-C38	-2.11	113.97	117.90
39	D	404	PL9	O2-C1-C2	-2.10	116.96	121.78
36	M	102	LMG	C1-O6-C5	-2.10	109.56	113.69
36	B	619	LMG	O2-C2-C1	-2.10	104.93	110.05
30	C	502	CLA	C11-C12-C13	-2.10	109.12	115.92
30	13	304	CLA	CAA-C2A-C1A	2.10	118.87	111.97
30	16	302	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
41	36	312	A86	C-C1-C24	2.10	121.39	118.08
32	c	520	BCR	C15-C16-C17	-2.10	119.17	123.47
30	37	305	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
32	B	617	BCR	C16-C15-C14	-2.10	119.17	123.47
41	33	315	A86	C34-O4-C38	-2.10	113.98	117.90
41	21	313	A86	C41-C32-C31	-2.10	108.59	110.47
41	35	313	A86	C-C1-C24	2.10	121.39	118.08
30	34	302	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
41	14	314	A86	C34-O4-C38	-2.10	113.98	117.90
30	C	512	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
41	13	313	A86	C-C1-C24	2.10	121.39	118.08
30	18	303	CLA	C1-C2-C3	-2.10	122.41	126.04
30	31	315	CLA	C2A-C1A-CHA	2.10	127.53	123.86
41	33	302	A86	C8-C6-C5	2.10	122.17	118.94
30	C	508	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
30	B	602	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
30	34	306	CLA	C2A-C1A-CHA	2.10	127.53	123.86
30	c	505	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
30	36	301	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
41	17	314	A86	C34-O4-C38	-2.10	113.98	117.90
32	c	520	BCR	C16-C17-C18	-2.10	124.31	127.31
32	b	616	BCR	C16-C15-C14	-2.10	119.17	123.47
41	35	312	A86	C-C1-C24	2.10	121.39	118.08
41	37	313	A86	C-C1-C24	2.10	121.39	118.08
30	38	311	CLA	CHA-C1A-NA	-2.10	121.59	126.40
30	41	302	CLA	O2A-CGA-O1A	-2.10	118.07	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	18	301	CLA	C2A-C1A-CHA	2.10	127.53	123.86
30	C	507	CLA	CHA-C1A-NA	-2.10	121.59	126.40
30	B	623	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
41	17	313	A86	C-C1-C24	2.10	121.38	118.08
41	13	314	A86	C34-O4-C38	-2.10	113.99	117.90
30	31	301	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
30	A	404	CLA	C3B-C4B-NB	-2.10	106.50	109.21
30	15	301	CLA	CMC-C2C-C1C	2.10	128.23	125.04
30	12	309	CLA	C2A-C1A-CHA	2.10	127.53	123.86
30	31	305	CLA	C2A-C1A-CHA	2.10	127.53	123.86
38	J	101	DGD	C7B-C6B-C5B	-2.10	103.78	114.42
41	41	310	A86	C-C1-C2	-2.10	119.99	122.92
30	36	303	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
36	32	301	LMG	O2-C2-C3	-2.10	105.50	110.35
30	b	608	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
41	37	314	A86	C34-O4-C38	-2.09	113.99	117.90
30	20	203	CLA	C2A-C1A-CHA	2.09	127.52	123.86
30	20	204	CLA	C2A-C1A-CHA	2.09	127.52	123.86
42	32	302	LMU	C2'-C3'-C4'	2.09	114.46	109.68
30	32	307	CLA	C2A-C1A-CHA	2.09	127.52	123.86
30	33	308	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
30	32	308	CLA	CHA-C1A-NA	-2.09	121.60	126.40
30	36	308	CLA	O1A-CGA-CBA	2.09	129.81	123.08
32	A	405	BCR	C7-C8-C9	-2.09	123.07	126.23
30	32	309	CLA	C2A-C1A-CHA	2.09	127.52	123.86
41	35	316	A86	C8-C6-C5	2.09	122.15	118.94
30	C	506	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
30	40	203	CLA	C2A-C1A-CHA	2.09	127.52	123.86
31	D	403	PHO	C1B-NB-C4B	2.09	111.39	107.09
30	16	308	CLA	O1A-CGA-CBA	2.09	129.80	123.08
30	b	615	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
30	36	303	CLA	C2D-C1D-ND	-2.09	108.56	110.10
30	16	306	CLA	C2A-C1A-CHA	2.09	127.52	123.86
32	Y	101	BCR	C15-C16-C17	-2.09	119.19	123.47
30	37	307	CLA	CHC-C1C-NC	2.09	127.38	124.20
41	20	213	A86	C34-O4-C38	-2.09	114.00	117.90
30	35	301	CLA	CMC-C2C-C1C	2.09	128.22	125.04
30	14	304	CLA	CAA-C2A-C1A	2.09	118.82	111.97
36	Q	301	LMG	C1-C2-C3	-2.09	105.64	110.00
41	35	313	A86	C34-O4-C38	-2.09	114.00	117.90
30	21	302	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
30	38	308	CLA	O2A-CGA-O1A	-2.09	118.09	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	D	404	PL9	C36-C37-C38	-2.09	105.01	111.88
41	31	312	A86	C-C1-C24	2.09	121.37	118.08
41	21	313	A86	C19-C18-C17	-2.09	106.74	110.77
41	16	312	A86	C-C1-C24	2.09	121.37	118.08
30	36	309	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
30	32	305	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
30	12	307	CLA	CAA-C2A-C1A	2.09	118.82	111.97
30	40	202	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	35	303	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
32	F	101	BCR	C24-C23-C22	-2.09	123.08	126.23
30	11	301	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
40	v	201	HEM	CBA-CAA-C2A	-2.09	109.06	112.62
30	34	304	CLA	CAA-C2A-C1A	2.09	118.81	111.97
30	B	603	CLA	O1D-CGD-CBD	2.09	128.75	124.48
30	B	608	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
41	15	316	A86	C8-C6-C5	2.09	122.14	118.94
41	18	315	A86	C34-O4-C38	-2.09	114.01	117.90
30	39	307	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
30	15	303	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
30	b	622	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
30	17	308	CLA	CHA-C1A-NA	-2.08	121.62	126.40
30	c	506	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
30	C	502	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	C	503	CLA	C3C-C4C-NC	-2.08	108.23	110.57
30	w	102	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
30	38	308	CLA	C2A-C1A-CHA	2.08	127.50	123.86
30	16	302	CLA	C3A-C2A-C1A	2.08	104.46	101.34
30	13	306	CLA	C2A-C1A-CHA	2.08	127.50	123.86
30	19	307	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
30	36	306	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
41	37	316	A86	C19-C18-C17	-2.08	106.75	110.77
30	40	204	CLA	C2A-C1A-CHA	2.08	127.50	123.86
40	E	101	HEM	C4A-C3A-C2A	2.08	108.44	107.00
30	b	614	CLA	C3A-C2A-C1A	2.08	104.46	101.34
30	C	511	CLA	CHA-C4D-ND	2.08	136.85	132.50
32	C	515	BCR	C30-C25-C26	-2.08	119.68	122.61
30	37	308	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	33	301	CLA	C2A-C1A-CHA	2.08	127.50	123.86
41	17	316	A86	C19-C18-C17	-2.08	106.76	110.77
30	17	310	CLA	C2A-C1A-CHA	2.08	127.50	123.86
30	34	304	CLA	C2A-C1A-CHA	2.08	127.50	123.86
30	20	207	CLA	CAA-C2A-C1A	2.08	118.79	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	18	311	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	C	502	CLA	C1-C2-C3	-2.08	122.45	126.04
30	41	304	CLA	CHB-C4A-NA	2.08	127.39	124.51
41	41	314	A86	C34-O4-C38	-2.08	114.02	117.90
30	35	307	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
30	21	303	CLA	C2A-C1A-CHA	2.08	127.49	123.86
41	39	311	A86	C28-C27-C26	-2.08	120.01	122.92
41	11	312	A86	C-C1-C24	2.08	121.35	118.08
39	D	407	PL9	C27-C28-C29	-2.08	122.66	127.66
32	a	404	BCR	C7-C8-C9	-2.08	123.10	126.23
38	J	101	DGD	O6E-C1E-O5D	-2.08	105.06	109.97
30	21	306	CLA	C2A-C1A-CHA	2.08	127.49	123.86
30	20	207	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
41	13	316	A86	C8-C6-C5	2.08	122.13	118.94
41	15	315	A86	C8-C6-C5	2.08	122.13	118.94
41	33	316	A86	C8-C6-C5	2.08	122.13	118.94
30	c	506	CLA	CMC-C2C-C3C	2.08	131.75	126.12
30	A	402	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
30	40	207	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
30	c	512	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
33	L	103	SQD	O48-C23-O10	-2.08	118.35	123.59
41	21	314	A86	C34-O4-C38	-2.08	114.03	117.90
30	13	302	CLA	CAA-CBA-CGA	-2.08	107.19	113.25
32	Y	101	BCR	C16-C17-C18	-2.08	124.35	127.31
30	20	209	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	17	307	CLA	CHC-C1C-NC	2.07	127.35	124.20
30	37	310	CLA	C2A-C1A-CHA	2.07	127.49	123.86
30	40	207	CLA	CAA-C2A-C1A	2.07	118.77	111.97
41	13	301	A86	C8-C6-C5	2.07	122.12	118.94
30	18	308	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
30	20	206	CLA	CHA-C1A-NA	-2.07	121.65	126.40
30	B	612	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
30	c	507	CLA	CHA-C1A-NA	-2.07	121.65	126.40
35	d	409	LHG	C5-O7-C7	-2.07	112.69	117.79
30	a	402	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
30	37	307	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	18	310	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
30	38	310	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
30	W	103	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
30	36	302	CLA	C3A-C2A-C1A	2.07	104.44	101.34
30	c	503	CLA	C3C-C4C-NC	-2.07	108.25	110.57
30	20	208	CLA	CHA-C1A-NA	-2.07	121.66	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	605	CLA	C1-C2-C3	-2.07	122.47	126.04
30	C	513	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	36	306	CLA	C2A-C1A-CHA	2.07	127.47	123.86
30	41	305	CLA	C2A-C1A-CHA	2.07	127.47	123.86
30	d	402	CLA	CHD-C1D-ND	-2.07	122.55	124.45
30	16	301	CLA	C2A-C1A-CHA	2.07	127.47	123.86
39	d	405	PL9	C22-C23-C24	-2.07	122.68	127.66
32	B	624	BCR	C15-C16-C17	-2.07	119.24	123.47
30	B	606	CLA	C2D-C1D-ND	-2.07	108.58	110.10
30	19	302	CLA	C2D-C1D-ND	-2.07	108.58	110.10
32	C	515	BCR	C24-C23-C22	-2.07	123.11	126.23
30	40	209	CLA	CHA-C1A-NA	-2.07	121.67	126.40
30	12	312	CLA	C2A-C1A-CHA	2.07	127.47	123.86
30	B	604	CLA	C1D-ND-C4D	2.07	107.80	106.33
30	b	604	CLA	C1D-ND-C4D	2.07	107.80	106.33
35	b	621	LHG	C27-C26-C25	-2.06	103.94	114.42
39	D	407	PL9	C46-C47-C48	-2.06	105.09	111.88
30	38	303	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	14	301	CLA	C2A-C1A-CHA	2.06	127.47	123.86
41	35	315	A86	C8-C6-C5	2.06	122.11	118.94
30	b	612	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
30	11	303	CLA	CAA-C2A-C1A	2.06	118.74	111.97
39	d	408	PL9	C20-C19-C21	2.06	118.74	115.27
30	36	307	CLA	CHD-C1D-ND	-2.06	122.56	124.45
41	39	310	A86	C7-C6-C5	-2.06	120.03	122.92
30	40	208	CLA	CHA-C1A-NA	-2.06	121.68	126.40
30	41	303	CLA	C2A-C1A-CHA	2.06	127.46	123.86
30	20	202	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
30	B	612	CLA	C2A-C1A-CHA	2.06	127.46	123.86
30	35	304	CLA	C2A-C1A-CHA	2.06	127.46	123.86
41	40	212	A86	C35-C34-C33	2.06	113.47	109.88
41	37	315	A86	C9-C10-C11	-2.06	120.55	126.61
39	d	405	PL9	C36-C37-C38	-2.06	105.11	111.88
40	V	201	HEM	CBA-CAA-C2A	-2.06	109.11	112.62
30	c	512	CLA	C7-C6-C5	-2.06	107.77	113.36
41	19	311	A86	C28-C27-C26	-2.06	120.04	122.92
30	c	511	CLA	CHA-C4D-ND	2.06	136.80	132.50
30	17	303	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
30	15	307	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
39	D	404	PL9	C22-C23-C24	-2.06	122.71	127.66
35	B	622	LHG	C27-C26-C25	-2.06	103.98	114.42
31	d	403	PHO	CMA-C3A-C4A	-2.06	109.87	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	302	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
41	38	302	A86	C8-C6-C5	2.06	122.10	118.94
41	18	302	A86	C8-C6-C5	2.06	122.09	118.94
35	L	101	LHG	C5-O7-C7	-2.05	112.73	117.79
30	36	301	CLA	C2A-C1A-CHA	2.05	127.45	123.86
41	41	313	A86	C19-C18-C17	-2.05	106.81	110.77
41	41	313	A86	C-C1-C24	2.05	121.31	118.08
30	b	612	CLA	C2A-C1A-CHA	2.05	127.45	123.86
38	C	516	DGD	CBB-CAB-C9B	-2.05	104.00	114.42
30	Z	102	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
30	16	307	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	18	303	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	37	303	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
31	A	403	PHO	CMA-C3A-C4A	-2.05	109.88	114.38
41	17	315	A86	C9-C10-C11	-2.05	120.58	126.61
30	12	307	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	b	615	CLA	O2D-CGD-CBD	2.05	114.91	111.27
41	12	319	A86	C8-C6-C5	-2.05	115.80	118.94
41	17	302	A86	C-C1-C24	2.05	121.31	118.08
30	c	524	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
30	14	304	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	31	303	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	16	302	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	39	305	CLA	O1A-CGA-CBA	2.05	129.66	123.08
30	12	305	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
32	c	520	BCR	C37-C22-C21	-2.05	120.05	122.92
31	d	403	PHO	C1B-NB-C4B	2.05	111.30	107.09
30	17	307	CLA	C2A-C1A-CHA	2.05	127.44	123.86
30	36	302	CLA	CHD-C1D-ND	-2.05	122.57	124.45
41	20	212	A86	C35-C34-C33	2.05	113.45	109.88
30	41	306	CLA	C2A-C1A-CHA	2.05	127.44	123.86
33	l	101	SQD	O48-C23-O10	-2.05	118.43	123.59
30	11	308	CLA	C2D-C1D-ND	-2.04	108.60	110.10
30	b	602	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
30	20	203	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
38	C	516	DGD	C4E-C3E-C2E	-2.04	107.25	110.82
30	35	301	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
41	19	309	A86	C7-C6-C8	2.04	121.30	118.08
30	c	507	CLA	CHB-C4A-NA	2.04	127.34	124.51
30	14	307	CLA	CHA-C1A-NA	-2.04	121.72	126.40
41	37	302	A86	C-C1-C24	2.04	121.30	118.08
32	b	617	BCR	C1-C6-C5	-2.04	119.74	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	12	301	LMG	O6-C1-O1	-2.04	105.14	109.97
30	35	303	CLA	C3A-C2A-C1A	2.04	104.40	101.34
30	21	305	CLA	C2A-C1A-CHA	2.04	127.43	123.86
30	C	502	CLA	C3C-C4C-NC	-2.04	108.28	110.57
39	D	404	PL9	C31-C32-C33	-2.04	105.17	111.88
41	21	313	A86	C-C1-C24	2.04	121.29	118.08
41	20	210	A86	C34-O4-C38	-2.04	114.09	117.90
30	18	307	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
30	20	206	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
30	19	304	CLA	O1A-CGA-CBA	2.04	129.63	123.08
41	15	314	A86	C19-C18-C17	-2.04	106.83	110.77
41	31	312	A86	C7-C6-C5	-2.04	120.07	122.92
30	39	302	CLA	C2D-C1D-ND	-2.04	108.60	110.10
30	11	315	CLA	C2A-C1A-CHA	2.04	127.42	123.86
30	21	304	CLA	CHB-C4A-NA	2.04	127.33	124.51
30	38	307	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
30	15	304	CLA	CHA-C4D-ND	2.04	136.76	132.50
30	B	602	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
30	15	306	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
30	18	309	CLA	C1-C2-C3	-2.04	122.52	126.04
30	16	306	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
30	34	305	CLA	CHA-C1A-NA	-2.04	121.73	126.40
30	15	301	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	40	203	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
38	j	101	DGD	C5B-C4B-C3B	-2.04	104.09	114.42
30	35	304	CLA	CHA-C4D-ND	2.04	136.76	132.50
41	13	317	A86	C19-C18-C17	-2.04	106.84	110.77
30	12	310	CLA	O2A-CGA-O1A	-2.04	118.23	123.30
41	37	311	A86	C26-C25-C24	-2.04	116.87	123.22
30	39	304	CLA	O1A-CGA-CBA	2.04	129.62	123.08
38	c	517	DGD	CBB-CAB-C9B	-2.03	104.09	114.42
30	32	310	CLA	CHA-C1A-NA	-2.03	121.74	126.40
30	31	306	CLA	CHA-C1A-NA	-2.03	121.74	126.40
30	12	308	CLA	C1D-ND-C4D	2.03	107.78	106.33
41	20	210	A86	C28-C27-C26	-2.03	120.07	122.92
41	17	302	A86	C35-C34-C33	2.03	113.42	109.88
30	35	306	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
30	38	310	CLA	CMB-C2B-C3B	2.03	128.48	124.68
30	w	103	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
30	15	303	CLA	C3A-C2A-C1A	2.03	104.38	101.34
41	20	201	A86	C23-C16-C17	-2.03	105.45	108.98
41	40	201	A86	C23-C16-C17	-2.03	105.45	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	615	CLA	O2D-CGD-CBD	2.03	114.88	111.27
39	D	404	PL9	O1-C4-C3	-2.03	118.48	120.72
30	a	403	CLA	C3B-C4B-NB	-2.03	106.58	109.21
32	C	515	BCR	C21-C20-C19	-2.03	116.88	123.22
32	h	101	BCR	C33-C5-C6	-2.03	122.25	124.53
36	b	618	LMG	C6-C5-C4	-2.03	108.25	113.00
41	37	311	A86	C3-C4-C5	-2.03	119.31	123.47
41	35	314	A86	C19-C18-C17	-2.03	106.85	110.77
30	34	307	CLA	CHA-C1A-NA	-2.03	121.75	126.40
41	17	311	A86	C26-C25-C24	-2.03	116.88	123.22
30	36	302	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
30	19	301	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
41	11	314	A86	C19-C18-C17	-2.03	106.85	110.77
41	40	210	A86	C4-C3-C2	-2.03	119.32	123.47
41	35	314	A86	C8-C6-C5	-2.03	115.83	118.94
30	c	502	CLA	C3C-C4C-NC	-2.03	108.30	110.57
39	d	408	PL9	C46-C47-C48	-2.03	105.22	111.88
30	14	310	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
41	31	314	A86	C19-C18-C17	-2.03	106.86	110.77
41	33	317	A86	C19-C18-C17	-2.03	106.86	110.77
41	32	319	A86	C19-C18-C17	-2.03	106.86	110.77
30	32	308	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
41	40	210	A86	C34-O4-C38	-2.03	114.12	117.90
39	d	405	PL9	C31-C32-C33	-2.03	105.22	111.88
30	37	305	CLA	C2A-C1A-CHA	2.03	127.40	123.86
38	C	516	DGD	O3E-C3E-C2E	-2.03	105.67	110.35
30	A	402	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
30	35	304	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
30	19	305	CLA	O1A-CGA-CBA	2.03	129.59	123.08
30	38	301	CLA	CHA-C1A-NA	-2.02	121.76	126.40
30	16	303	CLA	C2D-C1D-ND	-2.02	108.61	110.10
41	35	312	A86	C7-C6-C5	-2.02	120.09	122.92
38	c	517	DGD	O3E-C3E-C2E	-2.02	105.67	110.35
30	B	601	CLA	C3A-C2A-C1A	2.02	104.37	101.34
30	40	206	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
30	34	305	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
30	b	603	CLA	CHC-C1C-NC	2.02	127.27	124.20
30	17	305	CLA	C2A-C1A-CHA	2.02	127.39	123.86
32	f	101	BCR	C40-C30-C25	2.02	113.58	110.30
30	20	207	CLA	CHA-C1A-NA	-2.02	121.77	126.40
41	32	318	A86	C19-C18-C17	-2.02	106.87	110.77
30	c	502	CLA	C1-C2-C3	-2.02	122.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	314	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
30	35	307	CLA	CHA-C1A-NA	-2.02	121.77	126.40
30	40	207	CLA	CHA-C1A-NA	-2.02	121.77	126.40
38	J	101	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
30	15	304	CLA	C2A-C1A-CHA	2.02	127.39	123.86
30	C	512	CLA	C7-C6-C5	-2.02	107.87	113.36
38	c	517	DGD	C4E-C3E-C2E	-2.02	107.30	110.82
41	20	210	A86	C4-C3-C2	-2.02	119.33	123.47
41	13	315	A86	C19-C18-C17	-2.02	106.87	110.77
39	D	407	PL9	C20-C19-C21	2.02	118.67	115.27
30	c	513	CLA	C2A-C1A-CHA	2.02	127.39	123.86
30	31	304	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
30	d	401	CLA	C3A-C2A-C1A	2.02	104.36	101.34
41	12	319	A86	C19-C18-C17	-2.02	106.87	110.77
41	37	302	A86	C35-C34-C33	2.02	113.40	109.88
38	C	516	DGD	C7A-C6A-C5A	-2.02	104.18	114.42
30	17	301	CLA	C7-C6-C5	-2.02	107.88	113.36
32	F	101	BCR	C40-C30-C25	2.02	113.57	110.30
30	B	603	CLA	C2D-C1D-ND	-2.02	108.62	110.10
41	39	309	A86	C7-C6-C8	2.02	121.26	118.08
41	15	314	A86	C8-C6-C5	-2.02	115.84	118.94
30	16	302	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
30	18	310	CLA	CMB-C2B-C3B	2.02	128.45	124.68
40	V	201	HEM	CHD-C1D-ND	2.02	126.62	124.43
38	c	517	DGD	C7A-C6A-C5A	-2.02	104.19	114.42
30	20	204	CLA	O1D-CGD-CBD	2.02	128.61	124.48
30	a	403	CLA	O2D-CGD-CBD	2.02	114.85	111.27
30	C	506	CLA	CHC-C1C-NC	2.02	127.26	124.20
41	11	312	A86	C7-C6-C5	-2.02	120.10	122.92
30	15	307	CLA	CHA-C1A-NA	-2.02	121.78	126.40
39	d	408	PL9	C7-C3-C2	-2.02	120.65	123.30
30	38	309	CLA	C1-C2-C3	-2.02	122.56	126.04
36	32	301	LMG	O7-C10-O9	-2.01	118.83	123.70
30	C	514	CLA	O1D-CGD-CBD	2.01	128.60	124.48
41	40	210	A86	C28-C27-C26	-2.01	120.10	122.92
30	A	404	CLA	O2D-CGD-CBD	2.01	114.85	111.27
38	H	102	DGD	O6E-C1E-O5D	-2.01	105.21	109.97
40	V	201	HEM	CAD-C3D-C2D	-2.01	124.13	127.88
38	c	518	DGD	C7B-C6B-C5B	-2.01	104.21	114.42
30	12	310	CLA	CHA-C1A-NA	-2.01	121.79	126.40
30	37	301	CLA	C7-C6-C5	-2.01	107.90	113.36
32	a	408	BCR	C24-C23-C22	-2.01	123.20	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	605	CLA	C1-C2-C3	-2.01	122.56	126.04
30	c	509	CLA	C16-C15-C13	-2.01	109.42	115.92
30	D	401	CLA	C2A-C1A-CHA	2.01	127.38	123.86
35	a	407	LHG	C27-C26-C25	-2.01	104.22	114.42
30	15	304	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
36	c	519	LMG	C22-C21-C20	-2.01	104.22	114.42
30	20	208	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
30	C	509	CLA	C16-C15-C13	-2.01	109.42	115.92
30	D	405	CLA	C1-C2-C3	-2.01	122.57	126.04
30	17	307	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
30	18	301	CLA	CHA-C1A-NA	-2.01	121.80	126.40
30	40	208	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
35	a	407	LHG	O8-C23-O10	-2.01	118.52	123.59
36	Q	301	LMG	C22-C21-C20	-2.01	104.23	114.42
38	C	517	DGD	C7B-C6B-C5B	-2.01	104.23	114.42
32	H	101	BCR	C20-C21-C22	-2.01	124.44	127.31
41	17	311	A86	C3-C4-C5	-2.01	119.36	123.47
30	b	601	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
30	B	613	CLA	O1D-CGD-CBD	2.01	128.59	124.48
30	D	405	CLA	C11-C12-C13	-2.01	109.43	115.92
30	18	304	CLA	CHA-C1A-NA	-2.01	121.80	126.40
32	b	623	BCR	C15-C16-C17	-2.01	119.36	123.47
32	m	103	BCR	C16-C15-C14	-2.01	119.36	123.47
30	39	301	CLA	C6-C7-C8	-2.01	109.44	115.92
41	11	314	A86	C8-C6-C5	-2.01	115.86	118.94
41	32	318	A86	C8-C6-C5	-2.01	115.86	118.94
41	32	304	A86	C23-C16-C17	-2.01	105.50	108.98
30	z	101	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
30	13	304	CLA	C2A-C1A-CHA	2.01	127.37	123.86
30	d	406	CLA	C11-C12-C13	-2.01	109.44	115.92
30	17	310	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
41	16	313	A86	C19-C18-C17	-2.00	106.90	110.77
30	40	203	CLA	CBC-CAC-C3C	-2.00	106.90	112.43
30	14	302	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
30	B	609	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	b	602	CLA	C4-C3-C5	2.00	118.64	115.27
30	c	511	CLA	C3A-C2A-C1A	2.00	104.34	101.34
32	f	101	BCR	C33-C5-C6	-2.00	122.28	124.53
36	B	619	LMG	C6-C5-C4	-2.00	108.31	113.00
30	c	506	CLA	C7-C6-C5	-2.00	107.92	113.36
30	D	401	CLA	C3A-C2A-C1A	2.00	104.34	101.34
38	C	517	DGD	C5B-C4B-C3B	-2.00	104.26	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c	518	DGD	C5B-C4B-C3B	-2.00	104.27	114.42
30	38	304	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	11	303	CLA	C2A-C1A-CHA	2.00	127.36	123.86
30	C	507	CLA	CHB-C4A-NA	2.00	127.28	124.51
30	37	307	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
30	35	302	CLA	CHA-C1A-NA	-2.00	121.82	126.40
30	11	301	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
35	A	408	LHG	C27-C26-C25	-2.00	104.27	114.42

All (254) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	A	402	CLA	ND
30	A	404	CLA	ND
30	B	601	CLA	ND
30	B	602	CLA	ND
30	B	603	CLA	ND
30	B	604	CLA	ND
30	B	605	CLA	ND
30	B	606	CLA	ND
30	B	607	CLA	ND
30	B	608	CLA	ND
30	B	609	CLA	ND
30	B	610	CLA	ND
30	B	611	CLA	ND
30	B	612	CLA	ND
30	B	613	CLA	ND
30	B	614	CLA	ND
30	B	615	CLA	ND
30	B	623	CLA	ND
30	C	502	CLA	ND
30	C	503	CLA	ND
30	C	504	CLA	ND
30	C	505	CLA	ND
30	C	506	CLA	ND
30	C	507	CLA	ND
30	C	508	CLA	ND
30	C	509	CLA	ND
30	C	510	CLA	ND
30	C	511	CLA	ND
30	C	512	CLA	ND
30	C	513	CLA	ND

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Mol	Chain	Res	Type	Atom
30	C	514	CLA	ND
30	C	520	CLA	ND
30	C	521	CLA	ND
30	D	401	CLA	ND
30	D	402	CLA	ND
30	D	405	CLA	ND
30	D	406	CLA	ND
30	M	101	CLA	ND
30	Z	102	CLA	ND
30	W	102	CLA	ND
30	a	402	CLA	ND
30	a	403	CLA	ND
30	b	601	CLA	ND
30	b	602	CLA	ND
30	b	603	CLA	ND
30	b	604	CLA	ND
30	b	605	CLA	ND
30	b	606	CLA	ND
30	b	607	CLA	ND
30	b	608	CLA	ND
30	b	609	CLA	ND
30	b	610	CLA	ND
30	b	611	CLA	ND
30	b	612	CLA	ND
30	b	613	CLA	ND
30	b	614	CLA	ND
30	b	615	CLA	ND
30	b	622	CLA	ND
30	c	502	CLA	ND
30	c	503	CLA	ND
30	c	504	CLA	ND
30	c	505	CLA	ND
30	c	506	CLA	ND
30	c	507	CLA	ND
30	c	508	CLA	ND
30	c	509	CLA	ND
30	c	510	CLA	ND
30	c	511	CLA	ND
30	c	512	CLA	ND
30	c	513	CLA	ND
30	c	514	CLA	ND
30	c	522	CLA	ND

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Mol	Chain	Res	Type	Atom
30	c	523	CLA	ND
30	c	524	CLA	ND
30	d	401	CLA	ND
30	d	402	CLA	ND
30	d	406	CLA	ND
30	d	407	CLA	ND
30	m	101	CLA	ND
30	w	102	CLA	ND
30	11	301	CLA	ND
30	11	302	CLA	ND
30	11	303	CLA	ND
30	11	304	CLA	ND
30	11	305	CLA	ND
30	11	306	CLA	ND
30	11	307	CLA	ND
30	11	309	CLA	ND
30	11	315	CLA	ND
30	12	303	CLA	ND
30	12	305	CLA	ND
30	12	306	CLA	ND
30	12	307	CLA	ND
30	12	308	CLA	ND
30	12	309	CLA	ND
30	12	310	CLA	ND
30	12	311	CLA	ND
30	12	312	CLA	ND
30	12	314	CLA	ND
30	13	302	CLA	ND
30	13	303	CLA	ND
30	13	304	CLA	ND
30	13	305	CLA	ND
30	13	306	CLA	ND
30	13	307	CLA	ND
30	13	308	CLA	ND
30	13	310	CLA	ND
30	14	301	CLA	ND
30	14	302	CLA	ND
30	14	303	CLA	ND
30	14	304	CLA	ND
30	14	305	CLA	ND
30	14	306	CLA	ND
30	14	307	CLA	ND

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Mol	Chain	Res	Type	Atom
30	14	308	CLA	ND
30	14	310	CLA	ND
30	15	301	CLA	ND
30	15	302	CLA	ND
30	15	303	CLA	ND
30	15	305	CLA	ND
30	15	306	CLA	ND
30	15	307	CLA	ND
30	15	308	CLA	ND
30	15	309	CLA	ND
30	16	301	CLA	ND
30	16	302	CLA	ND
30	16	303	CLA	ND
30	16	304	CLA	ND
30	16	306	CLA	ND
30	16	307	CLA	ND
30	16	309	CLA	ND
30	17	301	CLA	ND
30	17	303	CLA	ND
30	17	305	CLA	ND
30	17	307	CLA	ND
30	17	308	CLA	ND
30	17	309	CLA	ND
30	17	310	CLA	ND
30	18	301	CLA	ND
30	18	303	CLA	ND
30	18	304	CLA	ND
30	18	305	CLA	ND
30	18	307	CLA	ND
30	18	308	CLA	ND
30	18	309	CLA	ND
30	18	310	CLA	ND
30	18	311	CLA	ND
30	18	312	CLA	ND
30	19	302	CLA	ND
30	19	303	CLA	ND
30	19	304	CLA	ND
30	19	305	CLA	ND
30	19	306	CLA	ND
30	19	307	CLA	ND
30	19	308	CLA	ND
30	20	203	CLA	ND

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Mol	Chain	Res	Type	Atom
30	20	204	CLA	ND
30	20	206	CLA	ND
30	20	207	CLA	ND
30	20	209	CLA	ND
30	21	303	CLA	ND
30	21	304	CLA	ND
30	21	305	CLA	ND
30	21	306	CLA	ND
30	21	307	CLA	ND
30	21	308	CLA	ND
30	21	309	CLA	ND
30	31	301	CLA	ND
30	31	302	CLA	ND
30	31	303	CLA	ND
30	31	304	CLA	ND
30	31	305	CLA	ND
30	31	306	CLA	ND
30	31	307	CLA	ND
30	31	309	CLA	ND
30	31	315	CLA	ND
30	32	303	CLA	ND
30	32	305	CLA	ND
30	32	306	CLA	ND
30	32	307	CLA	ND
30	32	308	CLA	ND
30	32	309	CLA	ND
30	32	310	CLA	ND
30	32	311	CLA	ND
30	32	313	CLA	ND
30	33	301	CLA	ND
30	33	303	CLA	ND
30	33	304	CLA	ND
30	33	305	CLA	ND
30	33	306	CLA	ND
30	33	307	CLA	ND
30	33	308	CLA	ND
30	33	309	CLA	ND
30	33	311	CLA	ND
30	34	301	CLA	ND
30	34	302	CLA	ND
30	34	303	CLA	ND
30	34	304	CLA	ND

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Mol	Chain	Res	Type	Atom
30	34	305	CLA	ND
30	34	306	CLA	ND
30	34	307	CLA	ND
30	34	308	CLA	ND
30	34	310	CLA	ND
30	35	301	CLA	ND
30	35	302	CLA	ND
30	35	303	CLA	ND
30	35	305	CLA	ND
30	35	306	CLA	ND
30	35	307	CLA	ND
30	35	308	CLA	ND
30	35	309	CLA	ND
30	36	301	CLA	ND
30	36	302	CLA	ND
30	36	303	CLA	ND
30	36	304	CLA	ND
30	36	306	CLA	ND
30	36	307	CLA	ND
30	36	309	CLA	ND
30	37	301	CLA	ND
30	37	303	CLA	ND
30	37	305	CLA	ND
30	37	307	CLA	ND
30	37	308	CLA	ND
30	37	309	CLA	ND
30	37	310	CLA	ND
30	38	301	CLA	ND
30	38	303	CLA	ND
30	38	304	CLA	ND
30	38	305	CLA	ND
30	38	307	CLA	ND
30	38	308	CLA	ND
30	38	309	CLA	ND
30	38	310	CLA	ND
30	38	311	CLA	ND
30	38	312	CLA	ND
30	39	302	CLA	ND
30	39	303	CLA	ND
30	39	304	CLA	ND
30	39	305	CLA	ND
30	39	306	CLA	ND

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Mol	Chain	Res	Type	Atom
30	39	307	CLA	ND
30	39	308	CLA	ND
30	40	203	CLA	ND
30	40	204	CLA	ND
30	40	206	CLA	ND
30	40	207	CLA	ND
30	40	209	CLA	ND
30	41	303	CLA	ND
30	41	304	CLA	ND
30	41	305	CLA	ND
30	41	306	CLA	ND
30	41	307	CLA	ND
30	41	308	CLA	ND
30	41	309	CLA	ND

All (5224) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	402	CLA	CBD-CGD-O2D-CED
30	B	601	CLA	C1A-C2A-CAA-CBA
30	B	601	CLA	CHA-CBD-CGD-O1D
30	B	601	CLA	CHA-CBD-CGD-O2D
30	B	601	CLA	CAD-CBD-CGD-O1D
30	B	602	CLA	C2-C3-C5-C6
30	B	602	CLA	C4-C3-C5-C6
30	B	603	CLA	CAD-CBD-CGD-O1D
30	B	603	CLA	CAD-CBD-CGD-O2D
30	B	603	CLA	C4-C3-C5-C6
30	B	604	CLA	CHA-CBD-CGD-O1D
30	B	604	CLA	CHA-CBD-CGD-O2D
30	B	605	CLA	C2-C3-C5-C6
30	B	605	CLA	C4-C3-C5-C6
30	B	608	CLA	CHA-CBD-CGD-O1D
30	B	608	CLA	CHA-CBD-CGD-O2D
30	B	610	CLA	CHA-CBD-CGD-O2D
30	B	611	CLA	CHA-CBD-CGD-O1D
30	B	611	CLA	CHA-CBD-CGD-O2D
30	B	611	CLA	CBD-CGD-O2D-CED
30	B	612	CLA	C1A-C2A-CAA-CBA
30	B	612	CLA	C3A-C2A-CAA-CBA
30	B	613	CLA	C2-C3-C5-C6
30	B	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	B	614	CLA	CHA-CBD-CGD-O1D
30	B	614	CLA	CHA-CBD-CGD-O2D
30	B	615	CLA	CHA-CBD-CGD-O2D
30	C	502	CLA	C1A-C2A-CAA-CBA
30	C	504	CLA	CBD-CGD-O2D-CED
30	C	505	CLA	CHA-CBD-CGD-O1D
30	C	505	CLA	CHA-CBD-CGD-O2D
30	C	506	CLA	CHA-CBD-CGD-O1D
30	C	506	CLA	CHA-CBD-CGD-O2D
30	C	510	CLA	CBD-CGD-O2D-CED
30	C	510	CLA	C6-C7-C8-C9
30	C	512	CLA	CHA-CBD-CGD-O1D
30	C	514	CLA	CBD-CGD-O2D-CED
30	D	401	CLA	CHA-CBD-CGD-O1D
30	D	401	CLA	CHA-CBD-CGD-O2D
30	D	402	CLA	CHA-CBD-CGD-O1D
30	D	402	CLA	CHA-CBD-CGD-O2D
30	D	405	CLA	C1A-C2A-CAA-CBA
30	M	101	CLA	CHA-CBD-CGD-O1D
30	M	101	CLA	CHA-CBD-CGD-O2D
30	M	101	CLA	CAD-CBD-CGD-O1D
30	M	101	CLA	CAD-CBD-CGD-O2D
30	M	101	CLA	C2-C3-C5-C6
30	M	101	CLA	C4-C3-C5-C6
30	W	102	CLA	C1A-C2A-CAA-CBA
30	a	402	CLA	CBD-CGD-O2D-CED
30	b	601	CLA	C1A-C2A-CAA-CBA
30	b	601	CLA	CHA-CBD-CGD-O1D
30	b	601	CLA	CHA-CBD-CGD-O2D
30	b	601	CLA	CAD-CBD-CGD-O1D
30	b	602	CLA	C2-C3-C5-C6
30	b	602	CLA	C4-C3-C5-C6
30	b	603	CLA	CAD-CBD-CGD-O1D
30	b	603	CLA	CAD-CBD-CGD-O2D
30	b	603	CLA	C4-C3-C5-C6
30	b	604	CLA	CHA-CBD-CGD-O1D
30	b	604	CLA	CHA-CBD-CGD-O2D
30	b	605	CLA	C2-C3-C5-C6
30	b	605	CLA	C4-C3-C5-C6
30	b	608	CLA	CHA-CBD-CGD-O1D
30	b	608	CLA	CHA-CBD-CGD-O2D
30	b	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	b	611	CLA	CHA-CBD-CGD-O1D
30	b	611	CLA	CHA-CBD-CGD-O2D
30	b	611	CLA	CBD-CGD-O2D-CED
30	b	612	CLA	C1A-C2A-CAA-CBA
30	b	612	CLA	C3A-C2A-CAA-CBA
30	b	613	CLA	C2-C3-C5-C6
30	b	613	CLA	C4-C3-C5-C6
30	b	614	CLA	CHA-CBD-CGD-O1D
30	b	614	CLA	CHA-CBD-CGD-O2D
30	b	615	CLA	CHA-CBD-CGD-O2D
30	c	502	CLA	C1A-C2A-CAA-CBA
30	c	504	CLA	CBD-CGD-O2D-CED
30	c	505	CLA	CHA-CBD-CGD-O1D
30	c	505	CLA	CHA-CBD-CGD-O2D
30	c	506	CLA	CHA-CBD-CGD-O1D
30	c	506	CLA	CHA-CBD-CGD-O2D
30	c	510	CLA	CBD-CGD-O2D-CED
30	c	510	CLA	C6-C7-C8-C9
30	c	512	CLA	CHA-CBD-CGD-O1D
30	c	513	CLA	C1A-C2A-CAA-CBA
30	c	514	CLA	CBD-CGD-O2D-CED
30	d	401	CLA	CHA-CBD-CGD-O1D
30	d	401	CLA	CHA-CBD-CGD-O2D
30	d	402	CLA	CHA-CBD-CGD-O1D
30	d	402	CLA	CHA-CBD-CGD-O2D
30	d	406	CLA	C1A-C2A-CAA-CBA
30	m	101	CLA	CHA-CBD-CGD-O1D
30	m	101	CLA	CHA-CBD-CGD-O2D
30	m	101	CLA	CAD-CBD-CGD-O1D
30	m	101	CLA	CAD-CBD-CGD-O2D
30	m	101	CLA	C2-C3-C5-C6
30	m	101	CLA	C4-C3-C5-C6
30	w	102	CLA	C1A-C2A-CAA-CBA
30	11	301	CLA	C3A-C2A-CAA-CBA
30	11	303	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	CHA-CBD-CGD-O1D
30	11	304	CLA	CHA-CBD-CGD-O2D
30	11	305	CLA	C1A-C2A-CAA-CBA
30	11	305	CLA	C3A-C2A-CAA-CBA
30	11	305	CLA	CHA-CBD-CGD-O1D
30	11	308	CLA	C1A-C2A-CAA-CBA
30	11	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	11	315	CLA	CHA-CBD-CGD-O1D
30	11	315	CLA	CHA-CBD-CGD-O2D
30	12	303	CLA	CHA-CBD-CGD-O1D
30	12	303	CLA	CHA-CBD-CGD-O2D
30	12	305	CLA	C3A-C2A-CAA-CBA
30	12	307	CLA	C1A-C2A-CAA-CBA
30	12	308	CLA	CHA-CBD-CGD-O1D
30	12	308	CLA	CHA-CBD-CGD-O2D
30	12	309	CLA	C1A-C2A-CAA-CBA
30	12	309	CLA	C3A-C2A-CAA-CBA
30	12	309	CLA	CHA-CBD-CGD-O1D
30	12	312	CLA	CHA-CBD-CGD-O1D
30	12	312	CLA	CHA-CBD-CGD-O2D
30	12	313	CLA	C1A-C2A-CAA-CBA
30	12	314	CLA	C1A-C2A-CAA-CBA
30	13	302	CLA	C3A-C2A-CAA-CBA
30	13	304	CLA	C1A-C2A-CAA-CBA
30	13	305	CLA	CHA-CBD-CGD-O1D
30	13	305	CLA	CHA-CBD-CGD-O2D
30	13	306	CLA	C1A-C2A-CAA-CBA
30	13	306	CLA	C3A-C2A-CAA-CBA
30	13	306	CLA	CHA-CBD-CGD-O1D
30	13	309	CLA	C1A-C2A-CAA-CBA
30	13	310	CLA	C1A-C2A-CAA-CBA
30	14	301	CLA	CHA-CBD-CGD-O1D
30	14	301	CLA	CHA-CBD-CGD-O2D
30	14	302	CLA	C3A-C2A-CAA-CBA
30	14	304	CLA	C1A-C2A-CAA-CBA
30	14	305	CLA	CHA-CBD-CGD-O1D
30	14	305	CLA	CHA-CBD-CGD-O2D
30	14	306	CLA	C1A-C2A-CAA-CBA
30	14	306	CLA	C3A-C2A-CAA-CBA
30	14	306	CLA	CHA-CBD-CGD-O1D
30	14	309	CLA	C1A-C2A-CAA-CBA
30	14	310	CLA	C1A-C2A-CAA-CBA
30	15	301	CLA	C1A-C2A-CAA-CBA
30	15	301	CLA	C3A-C2A-CAA-CBA
30	15	302	CLA	C1A-C2A-CAA-CBA
30	15	302	CLA	CBD-CGD-O2D-CED
30	15	303	CLA	C1A-C2A-CAA-CBA
30	15	303	CLA	CHA-CBD-CGD-O1D
30	15	303	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	15	307	CLA	C1A-C2A-CAA-CBA
30	15	307	CLA	C3A-C2A-CAA-CBA
30	16	302	CLA	CBD-CGD-O2D-CED
30	16	303	CLA	C1A-C2A-CAA-CBA
30	16	303	CLA	CBD-CGD-O2D-CED
30	16	304	CLA	C1A-C2A-CAA-CBA
30	16	304	CLA	CHA-CBD-CGD-O1D
30	16	304	CLA	CHA-CBD-CGD-O2D
30	16	304	CLA	CAD-CBD-CGD-O1D
30	16	307	CLA	C1A-C2A-CAA-CBA
30	16	307	CLA	C3A-C2A-CAA-CBA
30	16	308	CLA	C1A-C2A-CAA-CBA
30	16	308	CLA	C3A-C2A-CAA-CBA
30	16	309	CLA	C1A-C2A-CAA-CBA
30	17	301	CLA	CHA-CBD-CGD-O1D
30	17	301	CLA	CHA-CBD-CGD-O2D
30	17	303	CLA	C1A-C2A-CAA-CBA
30	17	303	CLA	C3A-C2A-CAA-CBA
30	17	303	CLA	CHA-CBD-CGD-O1D
30	17	303	CLA	CHA-CBD-CGD-O2D
30	17	304	CLA	C1A-C2A-CAA-CBA
30	17	304	CLA	CBD-CGD-O2D-CED
30	17	305	CLA	C1A-C2A-CAA-CBA
30	17	305	CLA	CHA-CBD-CGD-O1D
30	17	305	CLA	CHA-CBD-CGD-O2D
30	17	306	CLA	CBD-CGD-O2D-CED
30	17	308	CLA	C1A-C2A-CAA-CBA
30	17	308	CLA	C3A-C2A-CAA-CBA
30	17	309	CLA	CHA-CBD-CGD-O2D
30	17	310	CLA	C1A-C2A-CAA-CBA
30	18	301	CLA	CHA-CBD-CGD-O1D
30	18	301	CLA	CHA-CBD-CGD-O2D
30	18	303	CLA	C1A-C2A-CAA-CBA
30	18	303	CLA	C3A-C2A-CAA-CBA
30	18	304	CLA	CBD-CGD-O2D-CED
30	18	305	CLA	C1A-C2A-CAA-CBA
30	18	305	CLA	CHA-CBD-CGD-O1D
30	18	305	CLA	CHA-CBD-CGD-O2D
30	18	309	CLA	C3A-C2A-CAA-CBA
30	18	311	CLA	CHA-CBD-CGD-O1D
30	18	311	CLA	CHA-CBD-CGD-O2D
30	19	301	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	19	301	CLA	C3A-C2A-CAA-CBA
30	19	302	CLA	CBD-CGD-O2D-CED
30	19	305	CLA	C1A-C2A-CAA-CBA
30	19	305	CLA	C3A-C2A-CAA-CBA
30	19	308	CLA	C1A-C2A-CAA-CBA
30	19	308	CLA	C3A-C2A-CAA-CBA
30	20	202	CLA	C1A-C2A-CAA-CBA
30	20	202	CLA	C3A-C2A-CAA-CBA
30	20	202	CLA	CHA-CBD-CGD-O1D
30	20	202	CLA	CHA-CBD-CGD-O2D
30	20	204	CLA	C1A-C2A-CAA-CBA
30	20	207	CLA	C1A-C2A-CAA-CBA
30	20	208	CLA	C1A-C2A-CAA-CBA
30	20	209	CLA	C1A-C2A-CAA-CBA
30	20	209	CLA	C3A-C2A-CAA-CBA
30	21	301	CLA	C1A-C2A-CAA-CBA
30	21	302	CLA	C1A-C2A-CAA-CBA
30	21	302	CLA	CBD-CGD-O2D-CED
30	21	303	CLA	C1A-C2A-CAA-CBA
30	21	306	CLA	C1A-C2A-CAA-CBA
30	21	306	CLA	C3A-C2A-CAA-CBA
30	31	301	CLA	C3A-C2A-CAA-CBA
30	31	303	CLA	C1A-C2A-CAA-CBA
30	31	304	CLA	CHA-CBD-CGD-O1D
30	31	304	CLA	CHA-CBD-CGD-O2D
30	31	305	CLA	C1A-C2A-CAA-CBA
30	31	305	CLA	C3A-C2A-CAA-CBA
30	31	305	CLA	CHA-CBD-CGD-O1D
30	31	308	CLA	C1A-C2A-CAA-CBA
30	31	309	CLA	C1A-C2A-CAA-CBA
30	31	315	CLA	CHA-CBD-CGD-O1D
30	31	315	CLA	CHA-CBD-CGD-O2D
30	32	303	CLA	CHA-CBD-CGD-O1D
30	32	303	CLA	CHA-CBD-CGD-O2D
30	32	305	CLA	C3A-C2A-CAA-CBA
30	32	307	CLA	C1A-C2A-CAA-CBA
30	32	308	CLA	CHA-CBD-CGD-O1D
30	32	308	CLA	CHA-CBD-CGD-O2D
30	32	309	CLA	C1A-C2A-CAA-CBA
30	32	309	CLA	C3A-C2A-CAA-CBA
30	32	309	CLA	CHA-CBD-CGD-O1D
30	32	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	32	312	CLA	C1A-C2A-CAA-CBA
30	32	313	CLA	C1A-C2A-CAA-CBA
30	33	301	CLA	CHA-CBD-CGD-O1D
30	33	301	CLA	CHA-CBD-CGD-O2D
30	33	303	CLA	C3A-C2A-CAA-CBA
30	33	305	CLA	C1A-C2A-CAA-CBA
30	33	306	CLA	CHA-CBD-CGD-O1D
30	33	306	CLA	CHA-CBD-CGD-O2D
30	33	307	CLA	C1A-C2A-CAA-CBA
30	33	307	CLA	C3A-C2A-CAA-CBA
30	33	307	CLA	CHA-CBD-CGD-O1D
30	33	310	CLA	C1A-C2A-CAA-CBA
30	33	311	CLA	C1A-C2A-CAA-CBA
30	34	301	CLA	CHA-CBD-CGD-O1D
30	34	301	CLA	CHA-CBD-CGD-O2D
30	34	302	CLA	C3A-C2A-CAA-CBA
30	34	304	CLA	C1A-C2A-CAA-CBA
30	34	305	CLA	CHA-CBD-CGD-O1D
30	34	305	CLA	CHA-CBD-CGD-O2D
30	34	306	CLA	C1A-C2A-CAA-CBA
30	34	306	CLA	C3A-C2A-CAA-CBA
30	34	306	CLA	CHA-CBD-CGD-O1D
30	34	309	CLA	C1A-C2A-CAA-CBA
30	34	310	CLA	C1A-C2A-CAA-CBA
30	35	301	CLA	C1A-C2A-CAA-CBA
30	35	301	CLA	C3A-C2A-CAA-CBA
30	35	302	CLA	C1A-C2A-CAA-CBA
30	35	302	CLA	CBD-CGD-O2D-CED
30	35	303	CLA	C1A-C2A-CAA-CBA
30	35	303	CLA	CHA-CBD-CGD-O1D
30	35	303	CLA	CHA-CBD-CGD-O2D
30	35	307	CLA	C1A-C2A-CAA-CBA
30	35	307	CLA	C3A-C2A-CAA-CBA
30	36	302	CLA	CBD-CGD-O2D-CED
30	36	303	CLA	C1A-C2A-CAA-CBA
30	36	303	CLA	CBD-CGD-O2D-CED
30	36	304	CLA	C1A-C2A-CAA-CBA
30	36	304	CLA	CHA-CBD-CGD-O1D
30	36	304	CLA	CHA-CBD-CGD-O2D
30	36	304	CLA	CAD-CBD-CGD-O1D
30	36	307	CLA	C1A-C2A-CAA-CBA
30	36	307	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	36	308	CLA	C1A-C2A-CAA-CBA
30	36	308	CLA	C3A-C2A-CAA-CBA
30	36	309	CLA	C1A-C2A-CAA-CBA
30	37	301	CLA	CHA-CBD-CGD-O1D
30	37	301	CLA	CHA-CBD-CGD-O2D
30	37	303	CLA	C1A-C2A-CAA-CBA
30	37	303	CLA	C3A-C2A-CAA-CBA
30	37	303	CLA	CHA-CBD-CGD-O1D
30	37	303	CLA	CHA-CBD-CGD-O2D
30	37	304	CLA	C1A-C2A-CAA-CBA
30	37	304	CLA	CBD-CGD-O2D-CED
30	37	305	CLA	C1A-C2A-CAA-CBA
30	37	305	CLA	CHA-CBD-CGD-O1D
30	37	305	CLA	CHA-CBD-CGD-O2D
30	37	306	CLA	CBD-CGD-O2D-CED
30	37	308	CLA	C1A-C2A-CAA-CBA
30	37	308	CLA	C3A-C2A-CAA-CBA
30	37	309	CLA	CHA-CBD-CGD-O2D
30	37	310	CLA	C1A-C2A-CAA-CBA
30	38	301	CLA	CHA-CBD-CGD-O1D
30	38	301	CLA	CHA-CBD-CGD-O2D
30	38	303	CLA	C1A-C2A-CAA-CBA
30	38	303	CLA	C3A-C2A-CAA-CBA
30	38	304	CLA	CBD-CGD-O2D-CED
30	38	305	CLA	C1A-C2A-CAA-CBA
30	38	305	CLA	CHA-CBD-CGD-O1D
30	38	305	CLA	CHA-CBD-CGD-O2D
30	38	309	CLA	C3A-C2A-CAA-CBA
30	38	311	CLA	CHA-CBD-CGD-O1D
30	38	311	CLA	CHA-CBD-CGD-O2D
30	39	301	CLA	C1A-C2A-CAA-CBA
30	39	301	CLA	C3A-C2A-CAA-CBA
30	39	302	CLA	CBD-CGD-O2D-CED
30	39	305	CLA	C1A-C2A-CAA-CBA
30	39	305	CLA	C3A-C2A-CAA-CBA
30	39	308	CLA	C1A-C2A-CAA-CBA
30	39	308	CLA	C3A-C2A-CAA-CBA
30	40	202	CLA	C1A-C2A-CAA-CBA
30	40	202	CLA	C3A-C2A-CAA-CBA
30	40	202	CLA	CHA-CBD-CGD-O1D
30	40	202	CLA	CHA-CBD-CGD-O2D
30	40	204	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	40	207	CLA	C1A-C2A-CAA-CBA
30	40	208	CLA	C1A-C2A-CAA-CBA
30	40	209	CLA	C1A-C2A-CAA-CBA
30	40	209	CLA	C3A-C2A-CAA-CBA
30	41	301	CLA	C1A-C2A-CAA-CBA
30	41	302	CLA	C1A-C2A-CAA-CBA
30	41	302	CLA	CBD-CGD-O2D-CED
30	41	303	CLA	C1A-C2A-CAA-CBA
30	41	306	CLA	C1A-C2A-CAA-CBA
30	41	306	CLA	C3A-C2A-CAA-CBA
32	A	405	BCR	C7-C8-C9-C10
32	A	405	BCR	C35-C13-C14-C15
32	A	405	BCR	C14-C15-C16-C17
32	A	405	BCR	C16-C17-C18-C19
32	A	405	BCR	C16-C17-C18-C36
32	A	405	BCR	C18-C19-C20-C21
32	A	409	BCR	C6-C7-C8-C9
32	A	409	BCR	C7-C8-C9-C10
32	A	409	BCR	C7-C8-C9-C34
32	B	616	BCR	C23-C24-C25-C30
32	B	617	BCR	C1-C6-C7-C8
32	B	617	BCR	C7-C8-C9-C10
32	B	617	BCR	C20-C21-C22-C37
32	B	618	BCR	C1-C6-C7-C8
32	B	618	BCR	C7-C8-C9-C10
32	B	624	BCR	C6-C7-C8-C9
32	B	624	BCR	C7-C8-C9-C10
32	B	624	BCR	C10-C11-C12-C13
32	B	624	BCR	C11-C12-C13-C35
32	B	624	BCR	C16-C17-C18-C36
32	B	624	BCR	C20-C21-C22-C23
32	B	624	BCR	C20-C21-C22-C37
32	C	515	BCR	C1-C6-C7-C8
32	C	515	BCR	C22-C23-C24-C25
32	C	518	BCR	C1-C6-C7-C8
32	C	518	BCR	C21-C22-C23-C24
32	F	101	BCR	C7-C8-C9-C10
32	F	101	BCR	C11-C10-C9-C34
32	F	101	BCR	C35-C13-C14-C15
32	F	101	BCR	C16-C17-C18-C36
32	F	101	BCR	C21-C22-C23-C24
32	F	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
32	F	101	BCR	C22-C23-C24-C25
32	H	101	BCR	C1-C6-C7-C8
32	H	101	BCR	C20-C21-C22-C37
32	H	101	BCR	C37-C22-C23-C24
32	Y	101	BCR	C7-C8-C9-C34
32	Y	101	BCR	C11-C12-C13-C35
32	Y	101	BCR	C17-C18-C19-C20
32	Y	101	BCR	C18-C19-C20-C21
32	Y	101	BCR	C21-C22-C23-C24
32	Z	101	BCR	C11-C12-C13-C14
32	Z	101	BCR	C11-C12-C13-C35
32	Z	101	BCR	C16-C17-C18-C36
32	Z	101	BCR	C21-C22-C23-C24
32	Z	101	BCR	C23-C24-C25-C30
32	a	404	BCR	C7-C8-C9-C10
32	a	404	BCR	C35-C13-C14-C15
32	a	404	BCR	C14-C15-C16-C17
32	a	404	BCR	C16-C17-C18-C19
32	a	404	BCR	C16-C17-C18-C36
32	a	404	BCR	C18-C19-C20-C21
32	a	408	BCR	C6-C7-C8-C9
32	a	408	BCR	C7-C8-C9-C10
32	a	408	BCR	C7-C8-C9-C34
32	b	616	BCR	C1-C6-C7-C8
32	b	616	BCR	C7-C8-C9-C10
32	b	616	BCR	C20-C21-C22-C37
32	b	617	BCR	C1-C6-C7-C8
32	b	617	BCR	C7-C8-C9-C10
32	b	623	BCR	C6-C7-C8-C9
32	b	623	BCR	C7-C8-C9-C10
32	b	623	BCR	C10-C11-C12-C13
32	b	623	BCR	C11-C12-C13-C35
32	b	623	BCR	C16-C17-C18-C36
32	b	623	BCR	C20-C21-C22-C23
32	b	623	BCR	C20-C21-C22-C37
32	c	515	BCR	C11-C12-C13-C14
32	c	515	BCR	C11-C12-C13-C35
32	c	515	BCR	C16-C17-C18-C36
32	c	515	BCR	C21-C22-C23-C24
32	c	515	BCR	C23-C24-C25-C30
32	c	516	BCR	C1-C6-C7-C8
32	c	516	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
32	c	520	BCR	C7-C8-C9-C34
32	c	520	BCR	C11-C12-C13-C35
32	c	520	BCR	C17-C18-C19-C20
32	c	520	BCR	C18-C19-C20-C21
32	c	520	BCR	C21-C22-C23-C24
32	c	521	BCR	C1-C6-C7-C8
32	c	521	BCR	C21-C22-C23-C24
32	f	101	BCR	C7-C8-C9-C10
32	f	101	BCR	C11-C10-C9-C34
32	f	101	BCR	C35-C13-C14-C15
32	f	101	BCR	C16-C17-C18-C36
32	f	101	BCR	C21-C22-C23-C24
32	f	101	BCR	C37-C22-C23-C24
32	f	101	BCR	C22-C23-C24-C25
32	h	101	BCR	C1-C6-C7-C8
32	h	101	BCR	C20-C21-C22-C37
32	h	101	BCR	C37-C22-C23-C24
32	m	103	BCR	C23-C24-C25-C30
33	A	406	SQD	C5-C6-S-O7
33	B	621	SQD	C2-C1-O6-C44
33	L	103	SQD	O5-C1-O6-C44
33	L	103	SQD	C8-C7-O47-C45
33	L	103	SQD	O5-C5-C6-S
33	a	405	SQD	C5-C6-S-O7
33	b	620	SQD	C2-C1-O6-C44
33	l	101	SQD	O5-C1-O6-C44
33	l	101	SQD	C8-C7-O47-C45
33	l	101	SQD	O5-C5-C6-S
35	A	408	LHG	C3-O3-P-O5
35	A	408	LHG	C4-O6-P-O3
35	B	622	LHG	C3-O3-P-O4
35	B	622	LHG	C4-O6-P-O4
35	L	101	LHG	O1-C1-C2-C3
35	L	101	LHG	C3-O3-P-O4
35	L	101	LHG	C3-O3-P-O6
35	L	102	LHG	C4-O6-P-O5
35	a	407	LHG	C3-O3-P-O5
35	a	407	LHG	C4-O6-P-O3
35	b	621	LHG	C3-O3-P-O4
35	b	621	LHG	C4-O6-P-O4
35	d	409	LHG	O1-C1-C2-C3
35	d	409	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
35	d	409	LHG	C3-O3-P-O6
35	l	102	LHG	C4-O6-P-O5
36	M	102	LMG	O9-C10-O7-C8
36	W	101	LMG	O6-C1-O1-C7
36	W	101	LMG	O1-C7-C8-O7
36	m	102	LMG	O9-C10-O7-C8
36	w	101	LMG	O6-C1-O1-C7
36	w	101	LMG	O1-C7-C8-O7
36	12	301	LMG	O6-C1-O1-C7
36	32	301	LMG	O6-C1-O1-C7
39	D	404	PL9	C7-C8-C9-C11
39	D	404	PL9	C24-C26-C27-C28
39	D	404	PL9	C37-C38-C39-C40
39	D	404	PL9	C44-C46-C47-C48
39	D	407	PL9	C12-C13-C14-C16
39	D	407	PL9	C42-C43-C44-C45
39	d	405	PL9	C7-C8-C9-C11
39	d	405	PL9	C24-C26-C27-C28
39	d	405	PL9	C37-C38-C39-C40
39	d	405	PL9	C44-C46-C47-C48
39	d	408	PL9	C12-C13-C14-C16
39	d	408	PL9	C42-C43-C44-C45
40	E	101	HEM	C1A-C2A-CAA-CBA
40	E	101	HEM	C3A-C2A-CAA-CBA
40	e	101	HEM	C1A-C2A-CAA-CBA
40	e	101	HEM	C3A-C2A-CAA-CBA
41	11	310	A86	C39-C38-O4-C34
41	11	310	A86	C5-C6-C8-C9
41	11	310	A86	C7-C6-C8-C9
41	11	312	A86	C26-C27-C29-C30
41	11	312	A86	C28-C27-C29-C30
41	11	312	A86	C35-C34-O4-C38
41	11	313	A86	C2-C1-C24-C25
41	11	313	A86	C12-C11-C13-O
41	11	314	A86	C24-C25-C26-C27
41	11	314	A86	C39-C38-O4-C34
41	11	314	A86	O5-C38-O4-C34
41	11	316	A86	C11-C13-C14-C15
41	11	316	A86	C13-C14-C15-C16
41	11	316	A86	C39-C38-O4-C34
41	11	316	A86	O5-C38-O4-C34
41	12	304	A86	C11-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
41	12	304	A86	C13-C14-C15-C16
41	12	304	A86	C39-C38-O4-C34
41	12	304	A86	O5-C38-O4-C34
41	12	315	A86	C39-C38-O4-C34
41	12	315	A86	C5-C6-C8-C9
41	12	315	A86	C7-C6-C8-C9
41	12	317	A86	C26-C27-C29-C30
41	12	317	A86	C28-C27-C29-C30
41	12	317	A86	C35-C34-O4-C38
41	12	318	A86	C2-C1-C24-C25
41	12	318	A86	C12-C11-C13-O
41	12	319	A86	C24-C25-C26-C27
41	12	319	A86	C39-C38-O4-C34
41	12	319	A86	O5-C38-O4-C34
41	13	301	A86	C11-C13-C14-C15
41	13	301	A86	C13-C14-C15-C16
41	13	301	A86	C39-C38-O4-C34
41	13	301	A86	O5-C38-O4-C34
41	13	311	A86	C39-C38-O4-C34
41	13	311	A86	C5-C6-C8-C9
41	13	311	A86	C7-C6-C8-C9
41	13	313	A86	C26-C27-C29-C30
41	13	313	A86	C28-C27-C29-C30
41	13	313	A86	C35-C34-O4-C38
41	13	314	A86	C2-C1-C24-C25
41	13	314	A86	C12-C11-C13-O
41	13	315	A86	C24-C25-C26-C27
41	13	315	A86	C39-C38-O4-C34
41	13	315	A86	O5-C38-O4-C34
41	13	316	A86	C11-C13-C14-C15
41	13	316	A86	C13-C14-C15-C16
41	13	316	A86	C39-C38-O4-C34
41	13	316	A86	O5-C38-O4-C34
41	13	317	A86	C24-C25-C26-C27
41	13	317	A86	C39-C38-O4-C34
41	13	317	A86	O5-C38-O4-C34
41	14	311	A86	C39-C38-O4-C34
41	14	311	A86	C5-C6-C8-C9
41	14	311	A86	C7-C6-C8-C9
41	14	313	A86	C26-C27-C29-C30
41	14	313	A86	C28-C27-C29-C30
41	14	313	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
41	14	314	A86	C2-C1-C24-C25
41	14	314	A86	C12-C11-C13-O
41	15	310	A86	C39-C38-O4-C34
41	15	310	A86	C5-C6-C8-C9
41	15	310	A86	C7-C6-C8-C9
41	15	312	A86	C26-C27-C29-C30
41	15	312	A86	C28-C27-C29-C30
41	15	312	A86	C35-C34-O4-C38
41	15	313	A86	C2-C1-C24-C25
41	15	313	A86	C12-C11-C13-O
41	15	314	A86	C24-C25-C26-C27
41	15	314	A86	C39-C38-O4-C34
41	15	314	A86	O5-C38-O4-C34
41	15	315	A86	C11-C13-C14-C15
41	15	315	A86	C13-C14-C15-C16
41	15	315	A86	C39-C38-O4-C34
41	15	315	A86	O5-C38-O4-C34
41	15	316	A86	C11-C13-C14-C15
41	15	316	A86	C13-C14-C15-C16
41	15	316	A86	C39-C38-O4-C34
41	15	316	A86	O5-C38-O4-C34
41	16	310	A86	C13-C14-C15-C16
41	16	310	A86	C26-C27-C29-C30
41	16	310	A86	C28-C27-C29-C30
41	16	312	A86	C26-C27-C29-C30
41	16	312	A86	C28-C27-C29-C30
41	16	312	A86	C35-C34-O4-C38
41	16	313	A86	C24-C25-C26-C27
41	16	313	A86	C39-C38-O4-C34
41	16	313	A86	O5-C38-O4-C34
41	17	302	A86	C-C1-C24-C25
41	17	302	A86	C2-C1-C24-C25
41	17	302	A86	C10-C11-C13-O
41	17	302	A86	C12-C11-C13-O
41	17	302	A86	C11-C13-C14-C15
41	17	302	A86	C1-C2-C3-C4
41	17	302	A86	C39-C38-O4-C34
41	17	302	A86	O5-C38-O4-C34
41	17	311	A86	C28-C27-C29-C30
41	17	311	A86	C39-C38-O4-C34
41	17	311	A86	O5-C38-O4-C34
41	17	311	A86	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
41	17	311	A86	C7-C6-C8-C9
41	17	313	A86	C26-C27-C29-C30
41	17	313	A86	C28-C27-C29-C30
41	17	313	A86	C35-C34-O4-C38
41	17	314	A86	C2-C1-C24-C25
41	17	314	A86	C12-C11-C13-O
41	17	315	A86	C13-C14-C15-C16
41	17	315	A86	C1-C2-C3-C4
41	17	315	A86	C39-C38-O4-C34
41	17	316	A86	C24-C25-C26-C27
41	17	316	A86	C39-C38-O4-C34
41	17	316	A86	O5-C38-O4-C34
41	18	302	A86	C11-C13-C14-C15
41	18	302	A86	C13-C14-C15-C16
41	18	302	A86	C39-C38-O4-C34
41	18	302	A86	O5-C38-O4-C34
41	18	313	A86	C39-C38-O4-C34
41	18	313	A86	C5-C6-C8-C9
41	18	313	A86	C7-C6-C8-C9
41	18	315	A86	C2-C1-C24-C25
41	18	315	A86	C12-C11-C13-O
41	19	309	A86	C13-C14-C15-C16
41	19	309	A86	C1-C2-C3-C4
41	19	309	A86	O5-C38-O4-C34
41	19	309	A86	C5-C6-C8-C9
41	19	309	A86	C7-C6-C8-C9
41	19	310	A86	C12-C11-C13-C14
41	19	310	A86	O-C13-C14-C15
41	19	310	A86	C11-C13-C14-C15
41	19	310	A86	C13-C14-C15-C16
41	19	310	A86	C13-C14-C15-C20
41	19	310	A86	C13-C14-C15-O1
41	19	310	A86	C33-C34-O4-C38
41	19	311	A86	C11-C10-C9-C8
41	19	311	A86	C26-C27-C29-C30
41	19	311	A86	C28-C27-C29-C30
41	19	311	A86	C5-C6-C8-C9
41	19	311	A86	C7-C6-C8-C9
41	20	201	A86	C1-C2-C3-C4
41	20	210	A86	C-C1-C24-C25
41	20	210	A86	C2-C1-C24-C25
41	20	210	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
41	20	210	A86	C26-C27-C29-C30
41	20	210	A86	C28-C27-C29-C30
41	20	210	A86	C39-C38-O4-C34
41	20	210	A86	C3-C4-C5-C6
41	20	210	A86	C5-C6-C8-C9
41	20	211	A86	C13-C14-C15-C16
41	20	212	A86	C11-C13-C14-C15
41	20	212	A86	C13-C14-C15-O1
41	20	212	A86	C35-C34-O4-C38
41	20	213	A86	C2-C1-C24-C25
41	20	213	A86	C13-C14-C15-O1
41	20	213	A86	C1-C2-C3-C4
41	20	213	A86	C39-C38-O4-C34
41	20	213	A86	O5-C38-O4-C34
41	20	213	A86	C5-C6-C8-C9
41	20	213	A86	C7-C6-C8-C9
41	21	310	A86	C24-C25-C26-C27
41	21	310	A86	C39-C38-O4-C34
41	21	310	A86	O5-C38-O4-C34
41	21	311	A86	C13-C14-C15-C16
41	21	312	A86	C35-C34-O4-C38
41	21	312	A86	C5-C6-C8-C9
41	21	312	A86	C7-C6-C8-C9
41	21	313	A86	C13-C14-C15-C16
41	21	313	A86	C24-C25-C26-C27
41	21	313	A86	C26-C27-C29-C30
41	21	313	A86	C28-C27-C29-C30
41	21	313	A86	C39-C38-O4-C34
41	21	313	A86	C5-C6-C8-C9
41	21	313	A86	C7-C6-C8-C9
41	21	314	A86	C2-C1-C24-C25
41	21	314	A86	C13-C14-C15-O1
41	21	314	A86	C1-C2-C3-C4
41	21	314	A86	C39-C38-O4-C34
41	21	314	A86	O5-C38-O4-C34
41	21	314	A86	C5-C6-C8-C9
41	21	314	A86	C7-C6-C8-C9
41	31	310	A86	C39-C38-O4-C34
41	31	310	A86	C5-C6-C8-C9
41	31	310	A86	C7-C6-C8-C9
41	31	312	A86	C26-C27-C29-C30
41	31	312	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
41	31	312	A86	C35-C34-O4-C38
41	31	313	A86	C2-C1-C24-C25
41	31	313	A86	C12-C11-C13-O
41	31	314	A86	C24-C25-C26-C27
41	31	314	A86	C39-C38-O4-C34
41	31	314	A86	O5-C38-O4-C34
41	31	316	A86	C11-C13-C14-C15
41	31	316	A86	C13-C14-C15-C16
41	31	316	A86	C39-C38-O4-C34
41	31	316	A86	O5-C38-O4-C34
41	32	304	A86	C11-C13-C14-C15
41	32	304	A86	C13-C14-C15-C16
41	32	304	A86	C39-C38-O4-C34
41	32	304	A86	O5-C38-O4-C34
41	32	314	A86	C39-C38-O4-C34
41	32	314	A86	C5-C6-C8-C9
41	32	314	A86	C7-C6-C8-C9
41	32	316	A86	C26-C27-C29-C30
41	32	316	A86	C28-C27-C29-C30
41	32	316	A86	C35-C34-O4-C38
41	32	317	A86	C2-C1-C24-C25
41	32	317	A86	C12-C11-C13-O
41	32	318	A86	C24-C25-C26-C27
41	32	318	A86	C39-C38-O4-C34
41	32	318	A86	O5-C38-O4-C34
41	32	319	A86	C24-C25-C26-C27
41	32	319	A86	C39-C38-O4-C34
41	32	319	A86	O5-C38-O4-C34
41	33	302	A86	C11-C13-C14-C15
41	33	302	A86	C13-C14-C15-C16
41	33	302	A86	C39-C38-O4-C34
41	33	302	A86	O5-C38-O4-C34
41	33	312	A86	C39-C38-O4-C34
41	33	312	A86	C5-C6-C8-C9
41	33	312	A86	C7-C6-C8-C9
41	33	314	A86	C26-C27-C29-C30
41	33	314	A86	C28-C27-C29-C30
41	33	314	A86	C35-C34-O4-C38
41	33	315	A86	C2-C1-C24-C25
41	33	315	A86	C12-C11-C13-O
41	33	316	A86	C11-C13-C14-C15
41	33	316	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
41	33	316	A86	C39-C38-O4-C34
41	33	316	A86	O5-C38-O4-C34
41	33	317	A86	C24-C25-C26-C27
41	33	317	A86	C39-C38-O4-C34
41	33	317	A86	O5-C38-O4-C34
41	34	311	A86	C39-C38-O4-C34
41	34	311	A86	C5-C6-C8-C9
41	34	311	A86	C7-C6-C8-C9
41	34	313	A86	C26-C27-C29-C30
41	34	313	A86	C28-C27-C29-C30
41	34	313	A86	C35-C34-O4-C38
41	34	314	A86	C2-C1-C24-C25
41	34	314	A86	C12-C11-C13-O
41	35	310	A86	C39-C38-O4-C34
41	35	310	A86	C5-C6-C8-C9
41	35	310	A86	C7-C6-C8-C9
41	35	312	A86	C26-C27-C29-C30
41	35	312	A86	C28-C27-C29-C30
41	35	312	A86	C35-C34-O4-C38
41	35	313	A86	C2-C1-C24-C25
41	35	313	A86	C12-C11-C13-O
41	35	314	A86	C24-C25-C26-C27
41	35	314	A86	C39-C38-O4-C34
41	35	314	A86	O5-C38-O4-C34
41	35	315	A86	C11-C13-C14-C15
41	35	315	A86	C13-C14-C15-C16
41	35	315	A86	C39-C38-O4-C34
41	35	315	A86	O5-C38-O4-C34
41	35	316	A86	C11-C13-C14-C15
41	35	316	A86	C13-C14-C15-C16
41	35	316	A86	C39-C38-O4-C34
41	35	316	A86	O5-C38-O4-C34
41	36	310	A86	C13-C14-C15-C16
41	36	310	A86	C26-C27-C29-C30
41	36	310	A86	C28-C27-C29-C30
41	36	312	A86	C26-C27-C29-C30
41	36	312	A86	C28-C27-C29-C30
41	36	312	A86	C35-C34-O4-C38
41	36	313	A86	C24-C25-C26-C27
41	36	313	A86	C39-C38-O4-C34
41	36	313	A86	O5-C38-O4-C34
41	37	302	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
41	37	302	A86	C2-C1-C24-C25
41	37	302	A86	C10-C11-C13-O
41	37	302	A86	C12-C11-C13-O
41	37	302	A86	C11-C13-C14-C15
41	37	302	A86	C1-C2-C3-C4
41	37	302	A86	C39-C38-O4-C34
41	37	302	A86	O5-C38-O4-C34
41	37	311	A86	C28-C27-C29-C30
41	37	311	A86	C39-C38-O4-C34
41	37	311	A86	O5-C38-O4-C34
41	37	311	A86	C5-C6-C8-C9
41	37	311	A86	C7-C6-C8-C9
41	37	313	A86	C26-C27-C29-C30
41	37	313	A86	C28-C27-C29-C30
41	37	313	A86	C35-C34-O4-C38
41	37	314	A86	C2-C1-C24-C25
41	37	314	A86	C12-C11-C13-O
41	37	315	A86	C13-C14-C15-C16
41	37	315	A86	C1-C2-C3-C4
41	37	315	A86	C39-C38-O4-C34
41	37	316	A86	C24-C25-C26-C27
41	37	316	A86	C39-C38-O4-C34
41	37	316	A86	O5-C38-O4-C34
41	38	302	A86	C11-C13-C14-C15
41	38	302	A86	C13-C14-C15-C16
41	38	302	A86	C39-C38-O4-C34
41	38	302	A86	O5-C38-O4-C34
41	38	313	A86	C39-C38-O4-C34
41	38	313	A86	C5-C6-C8-C9
41	38	313	A86	C7-C6-C8-C9
41	38	315	A86	C2-C1-C24-C25
41	38	315	A86	C12-C11-C13-O
41	39	309	A86	C13-C14-C15-C16
41	39	309	A86	C1-C2-C3-C4
41	39	309	A86	O5-C38-O4-C34
41	39	309	A86	C5-C6-C8-C9
41	39	309	A86	C7-C6-C8-C9
41	39	310	A86	C12-C11-C13-C14
41	39	310	A86	O-C13-C14-C15
41	39	310	A86	C11-C13-C14-C15
41	39	310	A86	C13-C14-C15-C16
41	39	310	A86	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
41	39	310	A86	C33-C34-O4-C38
41	39	311	A86	C11-C10-C9-C8
41	39	311	A86	C26-C27-C29-C30
41	39	311	A86	C28-C27-C29-C30
41	39	311	A86	C5-C6-C8-C9
41	39	311	A86	C7-C6-C8-C9
41	40	201	A86	C1-C2-C3-C4
41	40	210	A86	C-C1-C24-C25
41	40	210	A86	C2-C1-C24-C25
41	40	210	A86	C13-C14-C15-C16
41	40	210	A86	C26-C27-C29-C30
41	40	210	A86	C28-C27-C29-C30
41	40	210	A86	C39-C38-O4-C34
41	40	210	A86	C3-C4-C5-C6
41	40	210	A86	C5-C6-C8-C9
41	40	211	A86	C13-C14-C15-C16
41	40	212	A86	C11-C13-C14-C15
41	40	212	A86	C13-C14-C15-O1
41	40	212	A86	C35-C34-O4-C38
41	40	213	A86	C2-C1-C24-C25
41	40	213	A86	C13-C14-C15-O1
41	40	213	A86	C1-C2-C3-C4
41	40	213	A86	C39-C38-O4-C34
41	40	213	A86	O5-C38-O4-C34
41	40	213	A86	C5-C6-C8-C9
41	40	213	A86	C7-C6-C8-C9
41	41	310	A86	C24-C25-C26-C27
41	41	310	A86	C39-C38-O4-C34
41	41	310	A86	O5-C38-O4-C34
41	41	311	A86	C13-C14-C15-C16
41	41	312	A86	C35-C34-O4-C38
41	41	312	A86	C5-C6-C8-C9
41	41	312	A86	C7-C6-C8-C9
41	41	313	A86	C13-C14-C15-C16
41	41	313	A86	C24-C25-C26-C27
41	41	313	A86	C26-C27-C29-C30
41	41	313	A86	C28-C27-C29-C30
41	41	313	A86	C39-C38-O4-C34
41	41	313	A86	C5-C6-C8-C9
41	41	313	A86	C7-C6-C8-C9
41	41	314	A86	C2-C1-C24-C25
41	41	314	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
41	41	314	A86	C1-C2-C3-C4
41	41	314	A86	C39-C38-O4-C34
41	41	314	A86	O5-C38-O4-C34
41	41	314	A86	C5-C6-C8-C9
41	41	314	A86	C7-C6-C8-C9
42	12	302	LMU	C2-C1-O1'-C1'
41	11	311	A86	C39-C38-O4-C34
41	11	312	A86	C39-C38-O4-C34
41	12	316	A86	C39-C38-O4-C34
41	12	317	A86	C39-C38-O4-C34
41	13	312	A86	C39-C38-O4-C34
41	13	313	A86	C39-C38-O4-C34
41	14	312	A86	C39-C38-O4-C34
41	14	313	A86	C39-C38-O4-C34
41	15	311	A86	C39-C38-O4-C34
41	15	312	A86	C39-C38-O4-C34
41	16	311	A86	C39-C38-O4-C34
41	16	312	A86	C39-C38-O4-C34
41	17	312	A86	C39-C38-O4-C34
41	17	313	A86	C39-C38-O4-C34
41	17	315	A86	O5-C38-O4-C34
41	18	314	A86	C39-C38-O4-C34
41	19	309	A86	C39-C38-O4-C34
41	20	201	A86	C39-C38-O4-C34
41	31	311	A86	C39-C38-O4-C34
41	31	312	A86	C39-C38-O4-C34
41	32	315	A86	C39-C38-O4-C34
41	32	316	A86	C39-C38-O4-C34
41	33	313	A86	C39-C38-O4-C34
41	33	314	A86	C39-C38-O4-C34
41	34	312	A86	C39-C38-O4-C34
41	34	313	A86	C39-C38-O4-C34
41	35	311	A86	C39-C38-O4-C34
41	35	312	A86	C39-C38-O4-C34
41	36	311	A86	C39-C38-O4-C34
41	36	312	A86	C39-C38-O4-C34
41	37	312	A86	C39-C38-O4-C34
41	37	313	A86	C39-C38-O4-C34
41	37	315	A86	O5-C38-O4-C34
41	38	314	A86	C39-C38-O4-C34
41	39	309	A86	C39-C38-O4-C34
41	40	201	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
30	16	302	CLA	O1D-CGD-O2D-CED
30	16	303	CLA	O1D-CGD-O2D-CED
30	18	304	CLA	O1D-CGD-O2D-CED
30	19	302	CLA	O1D-CGD-O2D-CED
30	19	304	CLA	O1D-CGD-O2D-CED
30	20	208	CLA	O1D-CGD-O2D-CED
30	36	302	CLA	O1D-CGD-O2D-CED
30	36	303	CLA	O1D-CGD-O2D-CED
30	38	304	CLA	O1D-CGD-O2D-CED
30	39	302	CLA	O1D-CGD-O2D-CED
30	39	304	CLA	O1D-CGD-O2D-CED
30	40	208	CLA	O1D-CGD-O2D-CED
41	11	310	A86	O5-C38-O4-C34
41	12	315	A86	O5-C38-O4-C34
41	13	311	A86	O5-C38-O4-C34
41	14	311	A86	O5-C38-O4-C34
41	15	310	A86	O5-C38-O4-C34
41	16	310	A86	C39-C38-O4-C34
41	18	313	A86	O5-C38-O4-C34
41	20	210	A86	O5-C38-O4-C34
41	21	313	A86	O5-C38-O4-C34
41	31	310	A86	O5-C38-O4-C34
41	32	314	A86	O5-C38-O4-C34
41	33	312	A86	O5-C38-O4-C34
41	34	311	A86	O5-C38-O4-C34
41	35	310	A86	O5-C38-O4-C34
41	36	310	A86	C39-C38-O4-C34
41	38	313	A86	O5-C38-O4-C34
41	40	210	A86	O5-C38-O4-C34
41	41	313	A86	O5-C38-O4-C34
30	A	402	CLA	O1D-CGD-O2D-CED
30	C	510	CLA	O1D-CGD-O2D-CED
30	a	402	CLA	O1D-CGD-O2D-CED
30	c	510	CLA	O1D-CGD-O2D-CED
30	11	304	CLA	O1D-CGD-O2D-CED
30	11	305	CLA	O1D-CGD-O2D-CED
30	12	308	CLA	O1D-CGD-O2D-CED
30	12	309	CLA	O1D-CGD-O2D-CED
30	13	305	CLA	O1D-CGD-O2D-CED
30	13	306	CLA	O1D-CGD-O2D-CED
30	14	305	CLA	O1D-CGD-O2D-CED
30	14	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	15	302	CLA	O1D-CGD-O2D-CED
30	15	303	CLA	O1D-CGD-O2D-CED
30	17	304	CLA	O1D-CGD-O2D-CED
30	17	309	CLA	O1D-CGD-O2D-CED
30	18	305	CLA	O1D-CGD-O2D-CED
30	18	306	CLA	O1D-CGD-O2D-CED
30	18	311	CLA	O1D-CGD-O2D-CED
30	20	204	CLA	O1D-CGD-O2D-CED
30	31	304	CLA	O1D-CGD-O2D-CED
30	31	305	CLA	O1D-CGD-O2D-CED
30	32	308	CLA	O1D-CGD-O2D-CED
30	32	309	CLA	O1D-CGD-O2D-CED
30	33	306	CLA	O1D-CGD-O2D-CED
30	33	307	CLA	O1D-CGD-O2D-CED
30	34	305	CLA	O1D-CGD-O2D-CED
30	34	306	CLA	O1D-CGD-O2D-CED
30	35	302	CLA	O1D-CGD-O2D-CED
30	35	303	CLA	O1D-CGD-O2D-CED
30	37	304	CLA	O1D-CGD-O2D-CED
30	37	309	CLA	O1D-CGD-O2D-CED
30	38	305	CLA	O1D-CGD-O2D-CED
30	38	306	CLA	O1D-CGD-O2D-CED
30	38	311	CLA	O1D-CGD-O2D-CED
30	40	204	CLA	O1D-CGD-O2D-CED
30	B	603	CLA	CBD-CGD-O2D-CED
30	B	604	CLA	CBD-CGD-O2D-CED
30	C	508	CLA	CBD-CGD-O2D-CED
30	C	521	CLA	CBD-CGD-O2D-CED
30	W	103	CLA	CBD-CGD-O2D-CED
30	b	603	CLA	CBD-CGD-O2D-CED
30	b	604	CLA	CBD-CGD-O2D-CED
30	c	508	CLA	CBD-CGD-O2D-CED
30	c	523	CLA	CBD-CGD-O2D-CED
30	w	103	CLA	CBD-CGD-O2D-CED
30	11	301	CLA	CBD-CGD-O2D-CED
30	11	304	CLA	CBD-CGD-O2D-CED
30	11	305	CLA	CBD-CGD-O2D-CED
30	12	305	CLA	CBD-CGD-O2D-CED
30	12	308	CLA	CBD-CGD-O2D-CED
30	12	309	CLA	CBD-CGD-O2D-CED
30	13	302	CLA	CBD-CGD-O2D-CED
30	13	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	13	306	CLA	CBD-CGD-O2D-CED
30	14	302	CLA	CBD-CGD-O2D-CED
30	14	305	CLA	CBD-CGD-O2D-CED
30	14	306	CLA	CBD-CGD-O2D-CED
30	15	303	CLA	CBD-CGD-O2D-CED
30	15	304	CLA	CBD-CGD-O2D-CED
30	15	306	CLA	CBD-CGD-O2D-CED
30	15	307	CLA	CBD-CGD-O2D-CED
30	16	305	CLA	CBD-CGD-O2D-CED
30	16	306	CLA	CBD-CGD-O2D-CED
30	17	303	CLA	CBD-CGD-O2D-CED
30	17	309	CLA	CBD-CGD-O2D-CED
30	18	305	CLA	CBD-CGD-O2D-CED
30	18	306	CLA	CBD-CGD-O2D-CED
30	18	311	CLA	CBD-CGD-O2D-CED
30	19	301	CLA	CBD-CGD-O2D-CED
30	19	304	CLA	CBD-CGD-O2D-CED
30	20	204	CLA	CBD-CGD-O2D-CED
30	20	205	CLA	CBD-CGD-O2D-CED
30	20	208	CLA	CBD-CGD-O2D-CED
30	21	301	CLA	CBD-CGD-O2D-CED
30	21	304	CLA	CBD-CGD-O2D-CED
30	21	307	CLA	CBD-CGD-O2D-CED
30	31	301	CLA	CBD-CGD-O2D-CED
30	31	304	CLA	CBD-CGD-O2D-CED
30	31	305	CLA	CBD-CGD-O2D-CED
30	32	305	CLA	CBD-CGD-O2D-CED
30	32	308	CLA	CBD-CGD-O2D-CED
30	32	309	CLA	CBD-CGD-O2D-CED
30	33	303	CLA	CBD-CGD-O2D-CED
30	33	306	CLA	CBD-CGD-O2D-CED
30	33	307	CLA	CBD-CGD-O2D-CED
30	34	302	CLA	CBD-CGD-O2D-CED
30	34	305	CLA	CBD-CGD-O2D-CED
30	34	306	CLA	CBD-CGD-O2D-CED
30	35	303	CLA	CBD-CGD-O2D-CED
30	35	304	CLA	CBD-CGD-O2D-CED
30	35	306	CLA	CBD-CGD-O2D-CED
30	35	307	CLA	CBD-CGD-O2D-CED
30	36	305	CLA	CBD-CGD-O2D-CED
30	36	306	CLA	CBD-CGD-O2D-CED
30	37	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	37	309	CLA	CBD-CGD-O2D-CED
30	38	305	CLA	CBD-CGD-O2D-CED
30	38	306	CLA	CBD-CGD-O2D-CED
30	38	311	CLA	CBD-CGD-O2D-CED
30	39	301	CLA	CBD-CGD-O2D-CED
30	39	304	CLA	CBD-CGD-O2D-CED
30	40	204	CLA	CBD-CGD-O2D-CED
30	40	205	CLA	CBD-CGD-O2D-CED
30	40	208	CLA	CBD-CGD-O2D-CED
30	41	301	CLA	CBD-CGD-O2D-CED
30	41	304	CLA	CBD-CGD-O2D-CED
30	41	307	CLA	CBD-CGD-O2D-CED
30	15	307	CLA	O1A-CGA-O2A-C1
30	21	301	CLA	O1A-CGA-O2A-C1
30	35	307	CLA	O1A-CGA-O2A-C1
30	41	301	CLA	O1A-CGA-O2A-C1
30	15	304	CLA	O1D-CGD-O2D-CED
30	19	301	CLA	O1D-CGD-O2D-CED
30	35	304	CLA	O1D-CGD-O2D-CED
30	39	301	CLA	O1D-CGD-O2D-CED
30	B	611	CLA	O1D-CGD-O2D-CED
30	C	504	CLA	O1D-CGD-O2D-CED
30	C	514	CLA	O1D-CGD-O2D-CED
30	W	103	CLA	O1D-CGD-O2D-CED
30	b	611	CLA	O1D-CGD-O2D-CED
30	c	504	CLA	O1D-CGD-O2D-CED
30	c	514	CLA	O1D-CGD-O2D-CED
30	w	103	CLA	O1D-CGD-O2D-CED
30	17	303	CLA	O1D-CGD-O2D-CED
30	21	302	CLA	O1D-CGD-O2D-CED
30	21	304	CLA	O1D-CGD-O2D-CED
30	37	303	CLA	O1D-CGD-O2D-CED
30	41	302	CLA	O1D-CGD-O2D-CED
30	41	304	CLA	O1D-CGD-O2D-CED
30	21	301	CLA	CBA-CGA-O2A-C1
30	41	301	CLA	CBA-CGA-O2A-C1
39	D	404	PL9	C47-C48-C49-C50
39	D	404	PL9	C47-C48-C49-C51
39	d	405	PL9	C47-C48-C49-C50
39	d	405	PL9	C47-C48-C49-C51
30	B	602	CLA	CBD-CGD-O2D-CED
30	B	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	B	614	CLA	CBD-CGD-O2D-CED
30	C	507	CLA	CBD-CGD-O2D-CED
30	b	602	CLA	CBD-CGD-O2D-CED
30	b	609	CLA	CBD-CGD-O2D-CED
30	b	614	CLA	CBD-CGD-O2D-CED
30	c	507	CLA	CBD-CGD-O2D-CED
30	11	303	CLA	CBD-CGD-O2D-CED
30	11	309	CLA	CBD-CGD-O2D-CED
30	12	307	CLA	CBD-CGD-O2D-CED
30	12	314	CLA	CBD-CGD-O2D-CED
30	13	304	CLA	CBD-CGD-O2D-CED
30	13	310	CLA	CBD-CGD-O2D-CED
30	14	304	CLA	CBD-CGD-O2D-CED
30	14	310	CLA	CBD-CGD-O2D-CED
30	15	301	CLA	CBD-CGD-O2D-CED
30	15	309	CLA	CBD-CGD-O2D-CED
30	16	301	CLA	CBD-CGD-O2D-CED
30	16	308	CLA	CBD-CGD-O2D-CED
30	17	310	CLA	CBD-CGD-O2D-CED
30	18	308	CLA	CBD-CGD-O2D-CED
30	18	312	CLA	CBD-CGD-O2D-CED
30	19	305	CLA	CBD-CGD-O2D-CED
30	21	308	CLA	CBD-CGD-O2D-CED
30	31	303	CLA	CBD-CGD-O2D-CED
30	32	307	CLA	CBD-CGD-O2D-CED
30	33	305	CLA	CBD-CGD-O2D-CED
30	34	304	CLA	CBD-CGD-O2D-CED
30	35	301	CLA	CBD-CGD-O2D-CED
30	35	309	CLA	CBD-CGD-O2D-CED
30	36	301	CLA	CBD-CGD-O2D-CED
30	36	308	CLA	CBD-CGD-O2D-CED
30	37	310	CLA	CBD-CGD-O2D-CED
30	38	308	CLA	CBD-CGD-O2D-CED
30	38	312	CLA	CBD-CGD-O2D-CED
30	39	305	CLA	CBD-CGD-O2D-CED
30	41	308	CLA	CBD-CGD-O2D-CED
41	20	201	A86	O5-C38-O4-C34
41	40	201	A86	O5-C38-O4-C34
30	B	615	CLA	O1A-CGA-O2A-C1
30	b	615	CLA	O1A-CGA-O2A-C1
30	15	301	CLA	O1A-CGA-O2A-C1
30	15	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	17	305	CLA	O1A-CGA-O2A-C1
30	17	308	CLA	O1A-CGA-O2A-C1
30	18	303	CLA	O1A-CGA-O2A-C1
30	18	309	CLA	O1A-CGA-O2A-C1
30	20	204	CLA	O1A-CGA-O2A-C1
30	21	306	CLA	O1A-CGA-O2A-C1
30	35	301	CLA	O1A-CGA-O2A-C1
30	35	303	CLA	O1A-CGA-O2A-C1
30	37	305	CLA	O1A-CGA-O2A-C1
30	37	308	CLA	O1A-CGA-O2A-C1
30	38	303	CLA	O1A-CGA-O2A-C1
30	38	309	CLA	O1A-CGA-O2A-C1
30	40	204	CLA	O1A-CGA-O2A-C1
30	41	306	CLA	O1A-CGA-O2A-C1
30	17	306	CLA	O1D-CGD-O2D-CED
30	37	306	CLA	O1D-CGD-O2D-CED
41	11	312	A86	O5-C38-O4-C34
41	12	317	A86	O5-C38-O4-C34
41	13	313	A86	O5-C38-O4-C34
41	14	313	A86	O5-C38-O4-C34
41	15	312	A86	O5-C38-O4-C34
41	16	312	A86	O5-C38-O4-C34
41	17	313	A86	O5-C38-O4-C34
41	31	312	A86	O5-C38-O4-C34
41	32	316	A86	O5-C38-O4-C34
41	33	314	A86	O5-C38-O4-C34
41	34	313	A86	O5-C38-O4-C34
41	35	312	A86	O5-C38-O4-C34
41	36	312	A86	O5-C38-O4-C34
41	37	313	A86	O5-C38-O4-C34
30	B	607	CLA	CBD-CGD-O2D-CED
30	C	502	CLA	CBD-CGD-O2D-CED
30	Z	102	CLA	CBD-CGD-O2D-CED
30	b	607	CLA	CBD-CGD-O2D-CED
30	c	502	CLA	CBD-CGD-O2D-CED
30	c	524	CLA	CBD-CGD-O2D-CED
30	17	305	CLA	CBD-CGD-O2D-CED
30	31	309	CLA	CBD-CGD-O2D-CED
30	32	313	CLA	CBD-CGD-O2D-CED
30	33	311	CLA	CBD-CGD-O2D-CED
30	34	310	CLA	CBD-CGD-O2D-CED
30	37	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	40	209	CLA	CBD-CGD-O2D-CED
30	21	301	CLA	O1D-CGD-O2D-CED
30	41	301	CLA	O1D-CGD-O2D-CED
33	L	103	SQD	O49-C7-O47-C45
33	l	101	SQD	O49-C7-O47-C45
41	12	318	A86	C39-C38-O4-C34
30	B	607	CLA	C3-C5-C6-C7
30	C	513	CLA	C3-C5-C6-C7
30	M	101	CLA	C3-C5-C6-C7
30	b	607	CLA	C3-C5-C6-C7
30	c	513	CLA	C3-C5-C6-C7
30	m	101	CLA	C3-C5-C6-C7
30	17	303	CLA	C3-C5-C6-C7
30	19	301	CLA	C3-C5-C6-C7
30	20	204	CLA	C3-C5-C6-C7
30	37	303	CLA	C3-C5-C6-C7
30	39	301	CLA	C3-C5-C6-C7
30	40	204	CLA	C3-C5-C6-C7
30	B	615	CLA	CBA-CGA-O2A-C1
30	C	519	CLA	CBA-CGA-O2A-C1
30	b	615	CLA	CBA-CGA-O2A-C1
30	z	101	CLA	CBA-CGA-O2A-C1
30	15	301	CLA	CBA-CGA-O2A-C1
30	15	303	CLA	CBA-CGA-O2A-C1
30	15	307	CLA	CBA-CGA-O2A-C1
30	17	308	CLA	CBA-CGA-O2A-C1
30	18	303	CLA	CBA-CGA-O2A-C1
30	18	309	CLA	CBA-CGA-O2A-C1
30	20	204	CLA	CBA-CGA-O2A-C1
30	21	306	CLA	CBA-CGA-O2A-C1
30	35	301	CLA	CBA-CGA-O2A-C1
30	35	303	CLA	CBA-CGA-O2A-C1
30	35	307	CLA	CBA-CGA-O2A-C1
30	37	308	CLA	CBA-CGA-O2A-C1
30	38	303	CLA	CBA-CGA-O2A-C1
30	38	309	CLA	CBA-CGA-O2A-C1
30	40	204	CLA	CBA-CGA-O2A-C1
30	41	306	CLA	CBA-CGA-O2A-C1
41	11	313	A86	C39-C38-O4-C34
41	13	314	A86	C39-C38-O4-C34
41	14	314	A86	C39-C38-O4-C34
41	15	313	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
41	17	314	A86	C39-C38-O4-C34
41	18	315	A86	C39-C38-O4-C34
41	31	313	A86	C39-C38-O4-C34
41	32	317	A86	C39-C38-O4-C34
41	33	315	A86	C39-C38-O4-C34
41	34	314	A86	C39-C38-O4-C34
41	35	313	A86	C39-C38-O4-C34
41	37	314	A86	C39-C38-O4-C34
41	38	315	A86	C39-C38-O4-C34
36	M	102	LMG	C11-C10-O7-C8
36	m	102	LMG	C11-C10-O7-C8
30	C	508	CLA	O1D-CGD-O2D-CED
30	c	508	CLA	O1D-CGD-O2D-CED
30	16	305	CLA	O1D-CGD-O2D-CED
30	20	205	CLA	O1D-CGD-O2D-CED
30	36	305	CLA	O1D-CGD-O2D-CED
30	40	205	CLA	O1D-CGD-O2D-CED
30	C	520	CLA	CBD-CGD-O2D-CED
30	c	522	CLA	CBD-CGD-O2D-CED
30	20	209	CLA	CBD-CGD-O2D-CED
30	C	502	CLA	C4-C3-C5-C6
30	c	502	CLA	C4-C3-C5-C6
30	C	512	CLA	CBD-CGD-O2D-CED
30	c	512	CLA	CBD-CGD-O2D-CED
30	A	402	CLA	C2A-CAA-CBA-CGA
30	B	601	CLA	C2A-CAA-CBA-CGA
30	B	606	CLA	C2A-CAA-CBA-CGA
30	B	610	CLA	C2A-CAA-CBA-CGA
30	C	503	CLA	C2A-CAA-CBA-CGA
30	C	513	CLA	C2A-CAA-CBA-CGA
30	C	521	CLA	C2A-CAA-CBA-CGA
30	W	103	CLA	C2A-CAA-CBA-CGA
30	a	402	CLA	C2A-CAA-CBA-CGA
30	b	601	CLA	C2A-CAA-CBA-CGA
30	b	606	CLA	C2A-CAA-CBA-CGA
30	b	610	CLA	C2A-CAA-CBA-CGA
30	c	503	CLA	C2A-CAA-CBA-CGA
30	c	513	CLA	C2A-CAA-CBA-CGA
30	c	523	CLA	C2A-CAA-CBA-CGA
30	w	103	CLA	C2A-CAA-CBA-CGA
30	11	301	CLA	C2A-CAA-CBA-CGA
30	11	307	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	12	305	CLA	C2A-CAA-CBA-CGA
30	12	311	CLA	C2A-CAA-CBA-CGA
30	13	302	CLA	C2A-CAA-CBA-CGA
30	13	308	CLA	C2A-CAA-CBA-CGA
30	14	302	CLA	C2A-CAA-CBA-CGA
30	14	308	CLA	C2A-CAA-CBA-CGA
30	15	301	CLA	C2A-CAA-CBA-CGA
30	15	304	CLA	C2A-CAA-CBA-CGA
30	15	306	CLA	C2A-CAA-CBA-CGA
30	16	302	CLA	C2A-CAA-CBA-CGA
30	16	305	CLA	C2A-CAA-CBA-CGA
30	16	306	CLA	C2A-CAA-CBA-CGA
30	16	308	CLA	C2A-CAA-CBA-CGA
30	17	304	CLA	C2A-CAA-CBA-CGA
30	18	306	CLA	C2A-CAA-CBA-CGA
30	20	205	CLA	C2A-CAA-CBA-CGA
30	21	304	CLA	C2A-CAA-CBA-CGA
30	21	308	CLA	C2A-CAA-CBA-CGA
30	31	301	CLA	C2A-CAA-CBA-CGA
30	31	307	CLA	C2A-CAA-CBA-CGA
30	32	305	CLA	C2A-CAA-CBA-CGA
30	33	303	CLA	C2A-CAA-CBA-CGA
30	33	309	CLA	C2A-CAA-CBA-CGA
30	34	302	CLA	C2A-CAA-CBA-CGA
30	34	308	CLA	C2A-CAA-CBA-CGA
30	35	301	CLA	C2A-CAA-CBA-CGA
30	35	304	CLA	C2A-CAA-CBA-CGA
30	35	306	CLA	C2A-CAA-CBA-CGA
30	36	302	CLA	C2A-CAA-CBA-CGA
30	36	305	CLA	C2A-CAA-CBA-CGA
30	36	306	CLA	C2A-CAA-CBA-CGA
30	36	308	CLA	C2A-CAA-CBA-CGA
30	37	304	CLA	C2A-CAA-CBA-CGA
30	38	306	CLA	C2A-CAA-CBA-CGA
30	40	205	CLA	C2A-CAA-CBA-CGA
30	41	304	CLA	C2A-CAA-CBA-CGA
30	41	308	CLA	C2A-CAA-CBA-CGA
30	C	505	CLA	C3-C5-C6-C7
30	c	505	CLA	C3-C5-C6-C7
31	A	403	PHO	C3-C5-C6-C7
31	d	403	PHO	C3-C5-C6-C7
30	C	508	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	C	513	CLA	CBA-CGA-O2A-C1
30	c	508	CLA	CBA-CGA-O2A-C1
30	16	304	CLA	CBA-CGA-O2A-C1
30	17	305	CLA	CBA-CGA-O2A-C1
30	31	301	CLA	CBA-CGA-O2A-C1
30	32	305	CLA	CBA-CGA-O2A-C1
30	33	303	CLA	CBA-CGA-O2A-C1
30	34	302	CLA	CBA-CGA-O2A-C1
30	36	304	CLA	CBA-CGA-O2A-C1
30	37	305	CLA	CBA-CGA-O2A-C1
36	W	101	LMG	O6-C5-C6-O5
36	w	101	LMG	O6-C5-C6-O5
41	11	311	A86	O5-C38-O4-C34
41	12	316	A86	O5-C38-O4-C34
41	13	312	A86	O5-C38-O4-C34
41	14	312	A86	O5-C38-O4-C34
41	15	311	A86	O5-C38-O4-C34
41	16	311	A86	O5-C38-O4-C34
41	17	312	A86	O5-C38-O4-C34
41	18	314	A86	O5-C38-O4-C34
41	31	311	A86	O5-C38-O4-C34
41	32	315	A86	O5-C38-O4-C34
41	33	313	A86	O5-C38-O4-C34
41	34	312	A86	O5-C38-O4-C34
41	35	311	A86	O5-C38-O4-C34
41	36	311	A86	O5-C38-O4-C34
41	37	312	A86	O5-C38-O4-C34
41	38	314	A86	O5-C38-O4-C34
38	H	102	DGD	C4D-C5D-C6D-O5D
38	h	102	DGD	C4D-C5D-C6D-O5D
41	21	311	A86	C39-C38-O4-C34
30	11	301	CLA	O1D-CGD-O2D-CED
30	12	305	CLA	O1D-CGD-O2D-CED
30	13	302	CLA	O1D-CGD-O2D-CED
30	14	302	CLA	O1D-CGD-O2D-CED
30	15	306	CLA	O1D-CGD-O2D-CED
30	35	306	CLA	O1D-CGD-O2D-CED
39	D	404	PL9	C37-C38-C39-C41
39	D	407	PL9	C7-C8-C9-C11
39	D	407	PL9	C42-C43-C44-C46
39	d	405	PL9	C37-C38-C39-C41
39	d	408	PL9	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
39	d	408	PL9	C42-C43-C44-C46
30	C	519	CLA	O1A-CGA-O2A-C1
30	z	101	CLA	O1A-CGA-O2A-C1
30	11	301	CLA	O1A-CGA-O2A-C1
30	12	305	CLA	O1A-CGA-O2A-C1
30	13	302	CLA	O1A-CGA-O2A-C1
30	14	302	CLA	O1A-CGA-O2A-C1
30	16	304	CLA	O1A-CGA-O2A-C1
30	31	301	CLA	O1A-CGA-O2A-C1
30	32	305	CLA	O1A-CGA-O2A-C1
30	33	303	CLA	O1A-CGA-O2A-C1
30	34	302	CLA	O1A-CGA-O2A-C1
30	36	304	CLA	O1A-CGA-O2A-C1
41	16	310	A86	O5-C38-O4-C34
41	20	211	A86	C39-C38-O4-C34
41	36	310	A86	O5-C38-O4-C34
41	40	211	A86	C39-C38-O4-C34
41	41	311	A86	C39-C38-O4-C34
30	15	307	CLA	O1D-CGD-O2D-CED
30	35	307	CLA	O1D-CGD-O2D-CED
41	11	311	A86	C24-C25-C26-C27
41	12	316	A86	C24-C25-C26-C27
41	13	312	A86	C24-C25-C26-C27
41	14	312	A86	C24-C25-C26-C27
41	15	311	A86	C24-C25-C26-C27
41	16	311	A86	C24-C25-C26-C27
41	17	311	A86	C1-C2-C3-C4
41	17	311	A86	C3-C4-C5-C6
41	17	312	A86	C24-C25-C26-C27
41	18	314	A86	C24-C25-C26-C27
41	19	309	A86	C24-C25-C26-C27
41	19	309	A86	C3-C4-C5-C6
41	20	201	A86	C3-C4-C5-C6
41	20	211	A86	C3-C4-C5-C6
41	20	212	A86	C24-C25-C26-C27
41	21	310	A86	C1-C2-C3-C4
41	21	311	A86	C3-C4-C5-C6
41	21	312	A86	C1-C2-C3-C4
41	31	311	A86	C24-C25-C26-C27
41	32	315	A86	C24-C25-C26-C27
41	33	313	A86	C24-C25-C26-C27
41	34	312	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
41	35	311	A86	C24-C25-C26-C27
41	36	311	A86	C24-C25-C26-C27
41	37	311	A86	C1-C2-C3-C4
41	37	311	A86	C3-C4-C5-C6
41	37	312	A86	C24-C25-C26-C27
41	38	314	A86	C24-C25-C26-C27
41	39	309	A86	C24-C25-C26-C27
41	39	309	A86	C3-C4-C5-C6
41	40	201	A86	C3-C4-C5-C6
41	40	211	A86	C3-C4-C5-C6
41	40	212	A86	C24-C25-C26-C27
41	41	310	A86	C1-C2-C3-C4
41	41	311	A86	C3-C4-C5-C6
41	41	312	A86	C1-C2-C3-C4
41	41	314	A86	C24-C25-C26-C27
30	B	610	CLA	CBD-CGD-O2D-CED
30	B	623	CLA	CBD-CGD-O2D-CED
30	M	101	CLA	CBD-CGD-O2D-CED
30	b	610	CLA	CBD-CGD-O2D-CED
30	b	622	CLA	CBD-CGD-O2D-CED
30	m	101	CLA	CBD-CGD-O2D-CED
30	15	305	CLA	CBD-CGD-O2D-CED
30	16	307	CLA	CBD-CGD-O2D-CED
30	17	301	CLA	CBD-CGD-O2D-CED
30	18	310	CLA	CBD-CGD-O2D-CED
30	20	207	CLA	CBD-CGD-O2D-CED
30	35	305	CLA	CBD-CGD-O2D-CED
30	36	307	CLA	CBD-CGD-O2D-CED
30	37	301	CLA	CBD-CGD-O2D-CED
30	38	310	CLA	CBD-CGD-O2D-CED
30	40	207	CLA	CBD-CGD-O2D-CED
30	B	603	CLA	O1D-CGD-O2D-CED
30	b	603	CLA	O1D-CGD-O2D-CED
30	C	512	CLA	CBA-CGA-O2A-C1
30	c	512	CLA	CBA-CGA-O2A-C1
30	c	513	CLA	CBA-CGA-O2A-C1
30	11	301	CLA	CBA-CGA-O2A-C1
30	12	305	CLA	CBA-CGA-O2A-C1
30	13	302	CLA	CBA-CGA-O2A-C1
30	14	302	CLA	CBA-CGA-O2A-C1
30	16	306	CLA	O1D-CGD-O2D-CED
30	21	307	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	36	306	CLA	O1D-CGD-O2D-CED
30	41	307	CLA	O1D-CGD-O2D-CED
31	A	403	PHO	C10-C11-C12-C13
31	d	403	PHO	C10-C11-C12-C13
30	b	604	CLA	O1D-CGD-O2D-CED
30	C	503	CLA	CBD-CGD-O2D-CED
30	19	306	CLA	CBD-CGD-O2D-CED
30	19	308	CLA	CBD-CGD-O2D-CED
30	39	306	CLA	CBD-CGD-O2D-CED
30	39	308	CLA	CBD-CGD-O2D-CED
30	B	604	CLA	O1D-CGD-O2D-CED
36	B	619	LMG	O6-C5-C6-O5
36	b	618	LMG	O6-C5-C6-O5
36	W	101	LMG	C4-C5-C6-O5
36	w	101	LMG	C4-C5-C6-O5
30	31	301	CLA	O1D-CGD-O2D-CED
30	32	305	CLA	O1D-CGD-O2D-CED
30	33	303	CLA	O1D-CGD-O2D-CED
30	34	302	CLA	O1D-CGD-O2D-CED
30	c	503	CLA	CBD-CGD-O2D-CED
30	B	623	CLA	C3-C5-C6-C7
30	D	401	CLA	C3-C5-C6-C7
30	b	622	CLA	C3-C5-C6-C7
30	d	401	CLA	C3-C5-C6-C7
30	C	508	CLA	O1A-CGA-O2A-C1
30	C	513	CLA	O1A-CGA-O2A-C1
30	c	508	CLA	O1A-CGA-O2A-C1
42	12	302	LMU	O5B-C5B-C6B-O6B
42	32	302	LMU	O5B-C5B-C6B-O6B
30	17	308	CLA	C4-C3-C5-C6
30	37	308	CLA	C4-C3-C5-C6
30	B	603	CLA	C2-C3-C5-C6
30	b	603	CLA	C2-C3-C5-C6
30	17	308	CLA	C2-C3-C5-C6
30	37	308	CLA	C2-C3-C5-C6
30	17	306	CLA	C2A-CAA-CBA-CGA
30	20	202	CLA	C2A-CAA-CBA-CGA
30	37	306	CLA	C2A-CAA-CBA-CGA
30	40	202	CLA	C2A-CAA-CBA-CGA
36	12	301	LMG	O6-C5-C6-O5
30	c	513	CLA	O1A-CGA-O2A-C1
38	C	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
39	D	404	PL9	C19-C21-C22-C23
39	d	405	PL9	C19-C21-C22-C23
30	A	402	CLA	CBA-CGA-O2A-C1
30	C	511	CLA	CBA-CGA-O2A-C1
30	c	511	CLA	CBA-CGA-O2A-C1
30	18	305	CLA	CBA-CGA-O2A-C1
30	19	301	CLA	CBA-CGA-O2A-C1
30	38	305	CLA	CBA-CGA-O2A-C1
30	39	301	CLA	CBA-CGA-O2A-C1
33	B	621	SQD	C24-C23-O48-C46
33	b	620	SQD	C24-C23-O48-C46
38	H	102	DGD	O6E-C5E-C6E-O5E
38	h	102	DGD	O6E-C5E-C6E-O5E
30	C	507	CLA	O1D-CGD-O2D-CED
30	C	521	CLA	O1D-CGD-O2D-CED
30	b	602	CLA	O1D-CGD-O2D-CED
30	c	507	CLA	O1D-CGD-O2D-CED
30	c	523	CLA	O1D-CGD-O2D-CED
30	C	512	CLA	O1A-CGA-O2A-C1
30	c	512	CLA	O1A-CGA-O2A-C1
30	18	305	CLA	O1A-CGA-O2A-C1
30	38	305	CLA	O1A-CGA-O2A-C1
30	B	602	CLA	O1D-CGD-O2D-CED
30	15	301	CLA	O1D-CGD-O2D-CED
30	15	309	CLA	O1D-CGD-O2D-CED
30	16	301	CLA	O1D-CGD-O2D-CED
30	17	310	CLA	O1D-CGD-O2D-CED
30	18	312	CLA	O1D-CGD-O2D-CED
30	19	305	CLA	O1D-CGD-O2D-CED
30	21	308	CLA	O1D-CGD-O2D-CED
30	35	301	CLA	O1D-CGD-O2D-CED
30	35	309	CLA	O1D-CGD-O2D-CED
30	36	301	CLA	O1D-CGD-O2D-CED
30	37	310	CLA	O1D-CGD-O2D-CED
30	38	312	CLA	O1D-CGD-O2D-CED
30	39	305	CLA	O1D-CGD-O2D-CED
30	41	308	CLA	O1D-CGD-O2D-CED
30	B	614	CLA	O1D-CGD-O2D-CED
30	b	614	CLA	O1D-CGD-O2D-CED
30	19	301	CLA	O1A-CGA-O2A-C1
30	39	301	CLA	O1A-CGA-O2A-C1
30	B	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	b	602	CLA	C3-C5-C6-C7
30	15	303	CLA	C3-C5-C6-C7
30	16	302	CLA	C3-C5-C6-C7
30	35	303	CLA	C3-C5-C6-C7
30	36	302	CLA	C3-C5-C6-C7
30	C	505	CLA	CBA-CGA-O2A-C1
30	C	506	CLA	CBA-CGA-O2A-C1
30	a	402	CLA	CBA-CGA-O2A-C1
30	c	505	CLA	CBA-CGA-O2A-C1
30	c	506	CLA	CBA-CGA-O2A-C1
30	20	202	CLA	CBA-CGA-O2A-C1
30	40	202	CLA	CBA-CGA-O2A-C1
30	11	306	CLA	CBD-CGD-O2D-CED
30	12	310	CLA	CBD-CGD-O2D-CED
30	13	307	CLA	CBD-CGD-O2D-CED
30	14	307	CLA	CBD-CGD-O2D-CED
32	B	624	BCR	C15-C16-C17-C18
32	b	623	BCR	C15-C16-C17-C18
41	11	310	A86	C24-C25-C26-C27
41	11	312	A86	C24-C25-C26-C27
41	12	315	A86	C24-C25-C26-C27
41	12	317	A86	C24-C25-C26-C27
41	13	311	A86	C24-C25-C26-C27
41	13	313	A86	C24-C25-C26-C27
41	14	311	A86	C24-C25-C26-C27
41	14	313	A86	C24-C25-C26-C27
41	15	310	A86	C24-C25-C26-C27
41	15	312	A86	C24-C25-C26-C27
41	16	312	A86	C24-C25-C26-C27
41	17	313	A86	C24-C25-C26-C27
41	18	313	A86	C24-C25-C26-C27
41	19	310	A86	C1-C2-C3-C4
41	19	311	A86	C24-C25-C26-C27
41	20	201	A86	C24-C25-C26-C27
41	20	210	A86	C24-C25-C26-C27
41	20	211	A86	C1-C2-C3-C4
41	20	213	A86	C24-C25-C26-C27
41	21	311	A86	C1-C2-C3-C4
41	21	314	A86	C24-C25-C26-C27
41	31	310	A86	C24-C25-C26-C27
41	31	312	A86	C24-C25-C26-C27
41	32	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
41	32	316	A86	C24-C25-C26-C27
41	33	312	A86	C24-C25-C26-C27
41	33	314	A86	C24-C25-C26-C27
41	34	311	A86	C24-C25-C26-C27
41	34	313	A86	C24-C25-C26-C27
41	35	310	A86	C24-C25-C26-C27
41	35	312	A86	C24-C25-C26-C27
41	36	312	A86	C24-C25-C26-C27
41	37	313	A86	C24-C25-C26-C27
41	38	313	A86	C24-C25-C26-C27
41	39	310	A86	C1-C2-C3-C4
41	39	311	A86	C24-C25-C26-C27
41	40	201	A86	C24-C25-C26-C27
41	40	210	A86	C24-C25-C26-C27
41	40	211	A86	C1-C2-C3-C4
41	40	213	A86	C24-C25-C26-C27
41	41	311	A86	C1-C2-C3-C4
30	B	610	CLA	C15-C16-C17-C18
30	B	623	CLA	C5-C6-C7-C8
30	b	610	CLA	C15-C16-C17-C18
30	b	622	CLA	C5-C6-C7-C8
30	11	307	CLA	C8-C10-C11-C12
30	12	311	CLA	C8-C10-C11-C12
30	13	308	CLA	C8-C10-C11-C12
30	14	308	CLA	C8-C10-C11-C12
30	B	601	CLA	C8-C10-C11-C12
30	B	611	CLA	C10-C11-C12-C13
30	M	101	CLA	C13-C15-C16-C17
30	W	103	CLA	C13-C15-C16-C17
30	b	601	CLA	C8-C10-C11-C12
30	b	611	CLA	C10-C11-C12-C13
30	m	101	CLA	C13-C15-C16-C17
30	w	103	CLA	C13-C15-C16-C17
30	C	511	CLA	O1A-CGA-O2A-C1
30	c	511	CLA	O1A-CGA-O2A-C1
36	32	301	LMG	O6-C5-C6-O5
36	B	619	LMG	C4-C5-C6-O5
36	b	618	LMG	C4-C5-C6-O5
30	C	502	CLA	C2-C3-C5-C6
30	c	502	CLA	C2-C3-C5-C6
30	B	601	CLA	C11-C10-C8-C9
30	B	604	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	610	CLA	C11-C12-C13-C14
30	C	506	CLA	C11-C12-C13-C14
30	C	511	CLA	C11-C12-C13-C14
30	C	519	CLA	C11-C12-C13-C14
30	C	520	CLA	C11-C10-C8-C9
30	M	101	CLA	C6-C7-C8-C9
30	b	601	CLA	C11-C10-C8-C9
30	b	604	CLA	C11-C10-C8-C9
30	b	610	CLA	C11-C12-C13-C14
30	c	506	CLA	C11-C12-C13-C14
30	c	511	CLA	C11-C12-C13-C14
30	c	522	CLA	C11-C10-C8-C9
30	m	101	CLA	C6-C7-C8-C9
30	z	101	CLA	C11-C12-C13-C14
30	16	302	CLA	C6-C7-C8-C9
30	36	302	CLA	C6-C7-C8-C9
31	A	403	PHO	C11-C10-C8-C9
31	D	403	PHO	C6-C7-C8-C9
31	d	403	PHO	C11-C10-C8-C9
31	d	404	PHO	C6-C7-C8-C9
30	B	609	CLA	O1D-CGD-O2D-CED
30	b	609	CLA	O1D-CGD-O2D-CED
30	31	307	CLA	C8-C10-C11-C12
30	32	311	CLA	C8-C10-C11-C12
30	34	308	CLA	C8-C10-C11-C12
32	B	624	BCR	C7-C8-C9-C34
32	B	624	BCR	C37-C22-C23-C24
32	C	515	BCR	C11-C12-C13-C35
32	C	515	BCR	C37-C22-C23-C24
32	C	518	BCR	C37-C22-C23-C24
32	F	101	BCR	C7-C8-C9-C34
32	Y	101	BCR	C37-C22-C23-C24
32	Z	101	BCR	C37-C22-C23-C24
32	b	623	BCR	C7-C8-C9-C34
32	b	623	BCR	C37-C22-C23-C24
32	c	515	BCR	C37-C22-C23-C24
32	c	516	BCR	C11-C12-C13-C35
32	c	516	BCR	C37-C22-C23-C24
32	c	520	BCR	C37-C22-C23-C24
32	c	521	BCR	C37-C22-C23-C24
32	f	101	BCR	C7-C8-C9-C34
41	11	313	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
41	12	318	A86	C-C1-C24-C25
41	13	314	A86	C-C1-C24-C25
41	14	314	A86	C-C1-C24-C25
41	15	313	A86	C-C1-C24-C25
41	17	302	A86	C7-C6-C8-C9
41	17	314	A86	C-C1-C24-C25
41	18	315	A86	C-C1-C24-C25
41	20	201	A86	C7-C6-C8-C9
41	20	210	A86	C7-C6-C8-C9
41	21	313	A86	C-C1-C24-C25
41	31	313	A86	C-C1-C24-C25
41	32	317	A86	C-C1-C24-C25
41	33	315	A86	C-C1-C24-C25
41	34	314	A86	C-C1-C24-C25
41	35	313	A86	C-C1-C24-C25
41	37	302	A86	C7-C6-C8-C9
41	37	314	A86	C-C1-C24-C25
41	38	315	A86	C-C1-C24-C25
41	40	201	A86	C7-C6-C8-C9
41	40	210	A86	C7-C6-C8-C9
41	41	313	A86	C-C1-C24-C25
41	17	302	A86	C5-C6-C8-C9
41	20	201	A86	C5-C6-C8-C9
41	21	313	A86	C2-C1-C24-C25
41	37	302	A86	C5-C6-C8-C9
41	40	201	A86	C5-C6-C8-C9
41	41	313	A86	C2-C1-C24-C25
35	L	101	LHG	C8-C7-O7-C5
35	d	409	LHG	C8-C7-O7-C5
36	12	301	LMG	C4-C5-C6-O5
38	H	102	DGD	C4E-C5E-C6E-O5E
38	h	102	DGD	C4E-C5E-C6E-O5E
30	C	506	CLA	O1A-CGA-O2A-C1
30	c	506	CLA	O1A-CGA-O2A-C1
30	B	608	CLA	C15-C16-C17-C18
30	B	615	CLA	C8-C10-C11-C12
30	b	608	CLA	C15-C16-C17-C18
30	b	615	CLA	C8-C10-C11-C12
30	16	304	CLA	C10-C11-C12-C13
30	16	304	CLA	C15-C16-C17-C18
30	33	309	CLA	C8-C10-C11-C12
30	36	304	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	36	304	CLA	C15-C16-C17-C18
30	34	304	CLA	O1D-CGD-O2D-CED
36	Q	301	LMG	O6-C5-C6-O5
36	c	519	LMG	O6-C5-C6-O5
30	11	303	CLA	O1D-CGD-O2D-CED
30	17	305	CLA	C3-C5-C6-C7
30	17	308	CLA	C3-C5-C6-C7
30	37	305	CLA	C3-C5-C6-C7
30	37	308	CLA	C3-C5-C6-C7
30	11	307	CLA	CBA-CGA-O2A-C1
30	12	311	CLA	CBA-CGA-O2A-C1
30	13	308	CLA	CBA-CGA-O2A-C1
30	14	308	CLA	CBA-CGA-O2A-C1
30	31	307	CLA	CBA-CGA-O2A-C1
30	32	311	CLA	CBA-CGA-O2A-C1
30	33	309	CLA	CBA-CGA-O2A-C1
30	34	308	CLA	CBA-CGA-O2A-C1
30	B	615	CLA	C13-C15-C16-C17
30	C	508	CLA	C8-C10-C11-C12
30	C	514	CLA	C8-C10-C11-C12
30	C	519	CLA	C8-C10-C11-C12
30	b	615	CLA	C13-C15-C16-C17
30	b	622	CLA	C13-C15-C16-C17
30	c	514	CLA	C8-C10-C11-C12
30	z	101	CLA	C8-C10-C11-C12
30	17	303	CLA	C15-C16-C17-C18
30	17	308	CLA	C5-C6-C7-C8
30	37	303	CLA	C15-C16-C17-C18
30	37	308	CLA	C5-C6-C7-C8
31	A	403	PHO	C15-C16-C17-C18
31	d	403	PHO	C15-C16-C17-C18
36	32	301	LMG	C10-C11-C12-C13
30	12	307	CLA	O1D-CGD-O2D-CED
30	13	304	CLA	O1D-CGD-O2D-CED
30	14	304	CLA	O1D-CGD-O2D-CED
30	31	303	CLA	O1D-CGD-O2D-CED
30	32	307	CLA	O1D-CGD-O2D-CED
30	33	305	CLA	O1D-CGD-O2D-CED
30	C	513	CLA	CBD-CGD-O2D-CED
30	c	513	CLA	CBD-CGD-O2D-CED
30	B	604	CLA	C8-C10-C11-C12
30	B	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	B	613	CLA	C10-C11-C12-C13
30	B	623	CLA	C13-C15-C16-C17
30	C	509	CLA	C8-C10-C11-C12
30	C	521	CLA	C5-C6-C7-C8
30	C	521	CLA	C10-C11-C12-C13
30	D	402	CLA	C15-C16-C17-C18
30	W	102	CLA	C10-C11-C12-C13
30	W	103	CLA	C10-C11-C12-C13
30	b	604	CLA	C8-C10-C11-C12
30	b	606	CLA	C10-C11-C12-C13
30	b	613	CLA	C10-C11-C12-C13
30	c	508	CLA	C8-C10-C11-C12
30	c	509	CLA	C8-C10-C11-C12
30	c	523	CLA	C5-C6-C7-C8
30	c	523	CLA	C10-C11-C12-C13
30	d	402	CLA	C15-C16-C17-C18
30	w	102	CLA	C10-C11-C12-C13
30	w	103	CLA	C10-C11-C12-C13
30	15	307	CLA	C8-C10-C11-C12
30	35	307	CLA	C8-C10-C11-C12
30	16	308	CLA	O1D-CGD-O2D-CED
30	36	308	CLA	O1D-CGD-O2D-CED
39	D	407	PL9	C7-C8-C9-C10
35	B	622	LHG	C23-C24-C25-C26
35	L	101	LHG	C7-C8-C9-C10
35	b	621	LHG	C23-C24-C25-C26
35	d	409	LHG	C7-C8-C9-C10
36	12	301	LMG	C10-C11-C12-C13
30	A	404	CLA	C8-C10-C11-C12
30	B	601	CLA	C5-C6-C7-C8
30	C	511	CLA	C8-C10-C11-C12
30	a	403	CLA	C8-C10-C11-C12
30	b	601	CLA	C5-C6-C7-C8
30	c	511	CLA	C8-C10-C11-C12
30	17	308	CLA	C10-C11-C12-C13
30	37	308	CLA	C10-C11-C12-C13
30	12	314	CLA	O1D-CGD-O2D-CED
36	B	619	LMG	C28-C29-C30-C31
36	b	618	LMG	C28-C29-C30-C31
30	31	306	CLA	CBD-CGD-O2D-CED
30	32	310	CLA	CBD-CGD-O2D-CED
30	33	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	34	307	CLA	CBD-CGD-O2D-CED
30	C	504	CLA	C5-C6-C7-C8
30	C	505	CLA	C15-C16-C17-C18
30	C	513	CLA	C8-C10-C11-C12
30	c	504	CLA	C5-C6-C7-C8
30	c	505	CLA	C15-C16-C17-C18
30	c	513	CLA	C8-C10-C11-C12
30	B	615	CLA	C6-C7-C8-C10
30	C	504	CLA	C6-C7-C8-C10
30	C	505	CLA	C6-C7-C8-C10
30	Z	102	CLA	C12-C13-C15-C16
30	W	103	CLA	C12-C13-C15-C16
30	b	615	CLA	C6-C7-C8-C10
30	c	504	CLA	C6-C7-C8-C10
30	c	505	CLA	C6-C7-C8-C10
30	c	524	CLA	C12-C13-C15-C16
30	w	103	CLA	C12-C13-C15-C16
30	11	307	CLA	C6-C7-C8-C10
30	12	311	CLA	C6-C7-C8-C10
30	13	308	CLA	C6-C7-C8-C10
30	14	308	CLA	C6-C7-C8-C10
30	31	307	CLA	C6-C7-C8-C10
30	32	311	CLA	C6-C7-C8-C10
30	33	309	CLA	C6-C7-C8-C10
30	34	308	CLA	C6-C7-C8-C10
30	C	505	CLA	O1A-CGA-O2A-C1
30	c	505	CLA	O1A-CGA-O2A-C1
41	11	313	A86	C24-C25-C26-C27
41	11	316	A86	C11-C10-C9-C8
41	12	304	A86	C11-C10-C9-C8
41	12	318	A86	C24-C25-C26-C27
41	13	301	A86	C11-C10-C9-C8
41	13	314	A86	C24-C25-C26-C27
41	13	316	A86	C11-C10-C9-C8
41	14	314	A86	C24-C25-C26-C27
41	15	313	A86	C24-C25-C26-C27
41	15	315	A86	C11-C10-C9-C8
41	15	316	A86	C11-C10-C9-C8
41	16	310	A86	C1-C2-C3-C4
41	16	310	A86	C24-C25-C26-C27
41	17	311	A86	C11-C10-C9-C8
41	17	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
41	17	315	A86	C3-C4-C5-C6
41	18	302	A86	C11-C10-C9-C8
41	18	315	A86	C24-C25-C26-C27
41	20	210	A86	C11-C10-C9-C8
41	21	310	A86	C3-C4-C5-C6
41	21	312	A86	C24-C25-C26-C27
41	31	313	A86	C24-C25-C26-C27
41	31	316	A86	C11-C10-C9-C8
41	32	304	A86	C11-C10-C9-C8
41	32	317	A86	C24-C25-C26-C27
41	33	302	A86	C11-C10-C9-C8
41	33	315	A86	C24-C25-C26-C27
41	33	316	A86	C11-C10-C9-C8
41	34	314	A86	C24-C25-C26-C27
41	35	313	A86	C24-C25-C26-C27
41	35	315	A86	C11-C10-C9-C8
41	35	316	A86	C11-C10-C9-C8
41	36	310	A86	C1-C2-C3-C4
41	36	310	A86	C24-C25-C26-C27
41	37	311	A86	C11-C10-C9-C8
41	37	314	A86	C24-C25-C26-C27
41	37	315	A86	C3-C4-C5-C6
41	38	302	A86	C11-C10-C9-C8
41	38	315	A86	C24-C25-C26-C27
41	40	210	A86	C11-C10-C9-C8
41	41	310	A86	C3-C4-C5-C6
41	41	312	A86	C24-C25-C26-C27
30	11	306	CLA	C2A-CAA-CBA-CGA
30	12	310	CLA	C2A-CAA-CBA-CGA
30	13	307	CLA	C2A-CAA-CBA-CGA
30	14	307	CLA	C2A-CAA-CBA-CGA
30	18	308	CLA	C2A-CAA-CBA-CGA
30	38	308	CLA	C2A-CAA-CBA-CGA
30	C	502	CLA	O1D-CGD-O2D-CED
30	Z	102	CLA	O1D-CGD-O2D-CED
30	c	502	CLA	O1D-CGD-O2D-CED
30	c	524	CLA	O1D-CGD-O2D-CED
30	11	309	CLA	O1D-CGD-O2D-CED
30	13	310	CLA	O1D-CGD-O2D-CED
30	14	310	CLA	O1D-CGD-O2D-CED
30	31	309	CLA	O1D-CGD-O2D-CED
30	32	313	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	33	311	CLA	O1D-CGD-O2D-CED
30	34	310	CLA	O1D-CGD-O2D-CED
30	B	602	CLA	C5-C6-C7-C8
30	16	302	CLA	C10-C11-C12-C13
30	17	308	CLA	C8-C10-C11-C12
30	19	301	CLA	C15-C16-C17-C18
30	20	209	CLA	C5-C6-C7-C8
30	36	302	CLA	C10-C11-C12-C13
30	37	308	CLA	C8-C10-C11-C12
30	39	301	CLA	C15-C16-C17-C18
30	40	209	CLA	C5-C6-C7-C8
30	20	202	CLA	O1A-CGA-O2A-C1
30	40	202	CLA	O1A-CGA-O2A-C1
30	W	102	CLA	CBD-CGD-O2D-CED
33	B	621	SQD	O5-C1-O6-C44
33	b	620	SQD	O5-C1-O6-C44
38	c	518	DGD	O6E-C1E-O5D-C6D
30	b	602	CLA	C5-C6-C7-C8
30	18	308	CLA	O1D-CGD-O2D-CED
30	38	308	CLA	O1D-CGD-O2D-CED
39	D	404	PL9	C9-C11-C12-C13
39	D	404	PL9	C29-C31-C32-C33
39	D	404	PL9	C34-C36-C37-C38
39	D	404	PL9	C39-C41-C42-C43
39	d	405	PL9	C9-C11-C12-C13
39	d	405	PL9	C29-C31-C32-C33
39	d	405	PL9	C34-C36-C37-C38
39	d	405	PL9	C39-C41-C42-C43
32	B	617	BCR	C10-C11-C12-C13
32	F	101	BCR	C10-C11-C12-C13
32	Z	101	BCR	C10-C11-C12-C13
32	b	616	BCR	C10-C11-C12-C13
32	c	515	BCR	C10-C11-C12-C13
32	f	101	BCR	C10-C11-C12-C13
35	a	407	LHG	O9-C7-O7-C5
42	32	302	LMU	C4B-C5B-C6B-O6B
30	B	612	CLA	C10-C11-C12-C13
30	C	505	CLA	C8-C10-C11-C12
30	C	508	CLA	C10-C11-C12-C13
30	D	402	CLA	C10-C11-C12-C13
30	M	101	CLA	C8-C10-C11-C12
30	Z	102	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	b	612	CLA	C10-C11-C12-C13
30	c	505	CLA	C8-C10-C11-C12
30	c	508	CLA	C10-C11-C12-C13
30	c	524	CLA	C10-C11-C12-C13
30	d	402	CLA	C10-C11-C12-C13
30	m	101	CLA	C8-C10-C11-C12
30	18	309	CLA	C5-C6-C7-C8
30	38	309	CLA	C5-C6-C7-C8
30	20	209	CLA	O1D-CGD-O2D-CED
30	40	209	CLA	O1D-CGD-O2D-CED
30	A	402	CLA	O1A-CGA-O2A-C1
30	a	402	CLA	O1A-CGA-O2A-C1
30	11	307	CLA	O1A-CGA-O2A-C1
30	12	311	CLA	O1A-CGA-O2A-C1
30	13	308	CLA	O1A-CGA-O2A-C1
30	14	308	CLA	O1A-CGA-O2A-C1
30	32	311	CLA	O1A-CGA-O2A-C1
30	33	309	CLA	O1A-CGA-O2A-C1
42	12	302	LMU	C4B-C5B-C6B-O6B
30	C	505	CLA	C13-C15-C16-C17
30	C	507	CLA	C10-C11-C12-C13
30	C	507	CLA	C15-C16-C17-C18
30	C	508	CLA	C15-C16-C17-C18
30	W	102	CLA	C8-C10-C11-C12
30	b	608	CLA	C8-C10-C11-C12
30	c	504	CLA	C10-C11-C12-C13
30	c	505	CLA	C13-C15-C16-C17
30	c	507	CLA	C10-C11-C12-C13
30	c	507	CLA	C15-C16-C17-C18
30	c	508	CLA	C15-C16-C17-C18
30	w	102	CLA	C8-C10-C11-C12
30	18	310	CLA	C15-C16-C17-C18
30	38	310	CLA	C15-C16-C17-C18
41	12	318	A86	O5-C38-O4-C34
41	13	314	A86	O5-C38-O4-C34
41	17	314	A86	O5-C38-O4-C34
41	33	315	A86	O5-C38-O4-C34
41	34	314	A86	O5-C38-O4-C34
30	B	607	CLA	O1D-CGD-O2D-CED
30	b	607	CLA	O1D-CGD-O2D-CED
30	17	305	CLA	O1D-CGD-O2D-CED
30	37	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	w	102	CLA	CBD-CGD-O2D-CED
30	31	307	CLA	O1A-CGA-O2A-C1
30	34	308	CLA	O1A-CGA-O2A-C1
36	W	101	LMG	C11-C10-O7-C8
36	w	101	LMG	C11-C10-O7-C8
41	31	313	A86	O5-C38-O4-C34
30	B	602	CLA	C15-C16-C17-C18
30	B	613	CLA	C5-C6-C7-C8
30	C	504	CLA	C10-C11-C12-C13
30	C	510	CLA	C13-C15-C16-C17
30	C	519	CLA	C13-C15-C16-C17
30	b	602	CLA	C15-C16-C17-C18
30	b	613	CLA	C5-C6-C7-C8
30	z	101	CLA	C13-C15-C16-C17
30	16	301	CLA	C8-C10-C11-C12
30	16	301	CLA	C13-C15-C16-C17
30	36	301	CLA	C8-C10-C11-C12
30	36	301	CLA	C13-C15-C16-C17
35	B	622	LHG	C4-O6-P-O3
35	L	101	LHG	C4-O6-P-O3
35	L	102	LHG	C3-O3-P-O6
35	b	621	LHG	C4-O6-P-O3
35	d	409	LHG	C4-O6-P-O3
35	l	102	LHG	C3-O3-P-O6
41	11	313	A86	O5-C38-O4-C34
41	14	314	A86	O5-C38-O4-C34
41	15	313	A86	O5-C38-O4-C34
41	18	315	A86	O5-C38-O4-C34
41	32	317	A86	O5-C38-O4-C34
41	35	313	A86	O5-C38-O4-C34
41	37	314	A86	O5-C38-O4-C34
41	38	315	A86	O5-C38-O4-C34
30	B	607	CLA	CBA-CGA-O2A-C1
30	D	406	CLA	CBA-CGA-O2A-C1
30	b	607	CLA	CBA-CGA-O2A-C1
30	d	407	CLA	CBA-CGA-O2A-C1
36	W	101	LMG	C29-C28-O8-C9
36	w	101	LMG	C29-C28-O8-C9
38	J	101	DGD	C2A-C1A-O1G-C1G
38	j	101	DGD	C2A-C1A-O1G-C1G
39	d	408	PL9	C7-C8-C9-C10
30	18	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	B	608	CLA	C8-C10-C11-C12
30	c	510	CLA	C13-C15-C16-C17
36	32	301	LMG	C4-C5-C6-O5
30	C	520	CLA	O1D-CGD-O2D-CED
30	c	522	CLA	O1D-CGD-O2D-CED
35	A	408	LHG	O9-C7-O7-C5
30	D	406	CLA	C4-C3-C5-C6
30	d	407	CLA	C4-C3-C5-C6
30	D	401	CLA	C13-C15-C16-C17
30	D	405	CLA	C15-C16-C17-C18
30	d	401	CLA	C13-C15-C16-C17
30	d	406	CLA	C15-C16-C17-C18
41	12	304	A86	C35-C34-O4-C38
41	15	315	A86	C35-C34-O4-C38
41	32	304	A86	C35-C34-O4-C38
30	C	502	CLA	C2A-CAA-CBA-CGA
30	c	502	CLA	C2A-CAA-CBA-CGA
30	19	304	CLA	C2A-CAA-CBA-CGA
30	39	304	CLA	C2A-CAA-CBA-CGA
30	b	611	CLA	C16-C17-C18-C19
30	18	310	CLA	C16-C17-C18-C20
30	38	310	CLA	C16-C17-C18-C20
30	B	615	CLA	C3-C5-C6-C7
30	b	615	CLA	C3-C5-C6-C7
30	W	103	CLA	CBA-CGA-O2A-C1
30	w	103	CLA	CBA-CGA-O2A-C1
36	B	620	LMG	C29-C28-O8-C9
36	b	619	LMG	C29-C28-O8-C9
36	B	620	LMG	C10-C11-C12-C13
36	b	619	LMG	C10-C11-C12-C13
30	c	522	CLA	C13-C15-C16-C17
41	16	310	A86	C3-C4-C5-C6
41	17	302	A86	C3-C4-C5-C6
41	17	311	A86	C24-C25-C26-C27
41	36	310	A86	C3-C4-C5-C6
41	37	302	A86	C3-C4-C5-C6
41	37	311	A86	C24-C25-C26-C27
41	11	316	A86	C35-C34-O4-C38
41	13	301	A86	C35-C34-O4-C38
41	13	316	A86	C35-C34-O4-C38
41	15	316	A86	C35-C34-O4-C38
41	18	302	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
41	31	316	A86	C35-C34-O4-C38
41	33	302	A86	C35-C34-O4-C38
41	33	316	A86	C35-C34-O4-C38
41	35	315	A86	C35-C34-O4-C38
41	35	316	A86	C35-C34-O4-C38
41	38	302	A86	C35-C34-O4-C38
38	H	102	DGD	C1B-C2B-C3B-C4B
36	12	301	LMG	C12-C13-C14-C15
38	h	102	DGD	C7A-C8A-C9A-CAA
30	38	301	CLA	CBD-CGD-O2D-CED
30	C	520	CLA	C13-C15-C16-C17
32	B	616	BCR	C16-C17-C18-C36
32	B	616	BCR	C20-C21-C22-C37
32	B	618	BCR	C16-C17-C18-C36
32	C	515	BCR	C20-C21-C22-C37
32	Y	101	BCR	C11-C10-C9-C34
32	Z	101	BCR	C11-C10-C9-C34
32	Z	101	BCR	C20-C21-C22-C37
32	b	617	BCR	C16-C17-C18-C36
32	c	515	BCR	C11-C10-C9-C34
32	c	515	BCR	C20-C21-C22-C37
32	c	516	BCR	C20-C21-C22-C37
32	c	520	BCR	C11-C10-C9-C34
32	m	103	BCR	C16-C17-C18-C36
32	m	103	BCR	C20-C21-C22-C37
30	18	309	CLA	C3-C5-C6-C7
30	38	309	CLA	C3-C5-C6-C7
33	A	406	SQD	C11-C12-C13-C14
33	a	405	SQD	C11-C12-C13-C14
35	B	622	LHG	C11-C10-C9-C8
35	a	407	LHG	C29-C30-C31-C32
35	b	621	LHG	C11-C10-C9-C8
36	B	619	LMG	C31-C32-C33-C34
36	Q	301	LMG	C32-C33-C34-C35
36	b	618	LMG	C31-C32-C33-C34
36	c	519	LMG	C32-C33-C34-C35
38	H	102	DGD	C7A-C8A-C9A-CAA
42	12	302	LMU	C5-C6-C7-C8
30	B	611	CLA	C16-C17-C18-C19
33	A	406	SQD	C10-C11-C12-C13
33	a	405	SQD	C10-C11-C12-C13
35	A	408	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
35	A	408	LHG	C29-C30-C31-C32
35	a	407	LHG	C15-C16-C17-C18
36	D	408	LMG	C35-C36-C37-C38
36	d	410	LMG	C35-C36-C37-C38
42	32	302	LMU	C5-C6-C7-C8
33	L	103	SQD	C46-C45-O47-C7
33	l	101	SQD	C46-C45-O47-C7
38	h	102	DGD	C1B-C2B-C3B-C4B
30	20	203	CLA	CBD-CGD-O2D-CED
35	L	102	LHG	C16-C17-C18-C19
35	l	102	LHG	C16-C17-C18-C19
36	32	301	LMG	C12-C13-C14-C15
30	C	512	CLA	O1D-CGD-O2D-CED
30	c	512	CLA	O1D-CGD-O2D-CED
30	18	310	CLA	O1D-CGD-O2D-CED
30	38	310	CLA	O1D-CGD-O2D-CED
33	L	103	SQD	C15-C16-C17-C18
33	l	101	SQD	C15-C16-C17-C18
36	W	101	LMG	C20-C21-C22-C23
30	20	207	CLA	O1D-CGD-O2D-CED
33	L	103	SQD	C32-C33-C34-C35
33	l	101	SQD	C32-C33-C34-C35
36	M	102	LMG	C15-C16-C17-C18
36	M	102	LMG	C33-C34-C35-C36
36	m	102	LMG	C15-C16-C17-C18
36	m	102	LMG	C33-C34-C35-C36
36	w	101	LMG	C20-C21-C22-C23
38	c	518	DGD	C2A-C3A-C4A-C5A
35	L	102	LHG	C23-C24-C25-C26
35	l	102	LHG	C23-C24-C25-C26
36	B	620	LMG	C28-C29-C30-C31
36	b	619	LMG	C28-C29-C30-C31
30	40	207	CLA	O1D-CGD-O2D-CED
32	A	405	BCR	C20-C21-C22-C23
32	B	624	BCR	C12-C13-C14-C15
32	B	624	BCR	C16-C17-C18-C19
32	F	101	BCR	C20-C21-C22-C23
32	Y	101	BCR	C12-C13-C14-C15
32	Y	101	BCR	C20-C21-C22-C23
32	Z	101	BCR	C12-C13-C14-C15
32	Z	101	BCR	C16-C17-C18-C19
32	a	404	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
32	b	623	BCR	C12-C13-C14-C15
32	b	623	BCR	C16-C17-C18-C19
32	c	515	BCR	C12-C13-C14-C15
32	c	515	BCR	C16-C17-C18-C19
32	c	520	BCR	C12-C13-C14-C15
32	c	520	BCR	C20-C21-C22-C23
32	f	101	BCR	C20-C21-C22-C23
38	C	517	DGD	C2E-C1E-O5D-C6D
38	J	101	DGD	C2E-C1E-O5D-C6D
38	c	518	DGD	C2E-C1E-O5D-C6D
38	j	101	DGD	C2E-C1E-O5D-C6D
30	B	612	CLA	CBA-CGA-O2A-C1
30	b	612	CLA	CBA-CGA-O2A-C1
38	C	517	DGD	C2A-C3A-C4A-C5A
30	A	404	CLA	C5-C6-C7-C8
30	a	403	CLA	C5-C6-C7-C8
30	B	607	CLA	O1A-CGA-O2A-C1
30	W	103	CLA	O1A-CGA-O2A-C1
30	b	607	CLA	O1A-CGA-O2A-C1
30	w	103	CLA	O1A-CGA-O2A-C1
36	M	102	LMG	O10-C28-O8-C9
36	m	102	LMG	O10-C28-O8-C9
30	B	605	CLA	C16-C17-C18-C20
30	b	605	CLA	C16-C17-C18-C20
30	15	305	CLA	O1D-CGD-O2D-CED
30	35	305	CLA	O1D-CGD-O2D-CED
30	C	507	CLA	C4-C3-C5-C6
30	c	507	CLA	C4-C3-C5-C6
30	C	504	CLA	C6-C7-C8-C9
30	c	504	CLA	C6-C7-C8-C9
35	A	408	LHG	C23-C24-C25-C26
35	a	407	LHG	C23-C24-C25-C26
33	l	101	SQD	C33-C34-C35-C36
35	L	102	LHG	C32-C33-C34-C35
35	a	407	LHG	C28-C29-C30-C31
35	l	102	LHG	C32-C33-C34-C35
36	D	408	LMG	C36-C37-C38-C39
36	d	410	LMG	C36-C37-C38-C39
30	D	406	CLA	O1A-CGA-O2A-C1
30	d	407	CLA	O1A-CGA-O2A-C1
41	17	315	A86	C7-C6-C8-C9
41	19	310	A86	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
41	20	212	A86	C-C1-C24-C25
41	20	213	A86	C-C1-C24-C25
41	21	314	A86	C-C1-C24-C25
41	37	315	A86	C7-C6-C8-C9
41	39	310	A86	C7-C6-C8-C9
41	40	212	A86	C-C1-C24-C25
41	40	213	A86	C-C1-C24-C25
41	41	314	A86	C-C1-C24-C25
33	L	103	SQD	C33-C34-C35-C36
35	A	408	LHG	C28-C29-C30-C31
35	d	409	LHG	C24-C25-C26-C27
36	D	408	LMG	C30-C31-C32-C33
36	W	101	LMG	C19-C20-C21-C22
32	B	616	BCR	C21-C22-C23-C24
32	B	624	BCR	C21-C22-C23-C24
32	Y	101	BCR	C11-C12-C13-C14
32	b	623	BCR	C21-C22-C23-C24
32	c	520	BCR	C11-C12-C13-C14
32	m	103	BCR	C21-C22-C23-C24
41	17	315	A86	C5-C6-C8-C9
41	19	310	A86	C5-C6-C8-C9
41	20	212	A86	C2-C1-C24-C25
41	37	315	A86	C5-C6-C8-C9
41	39	310	A86	C5-C6-C8-C9
41	40	212	A86	C2-C1-C24-C25
30	16	304	CLA	C3-C5-C6-C7
30	36	304	CLA	C3-C5-C6-C7
35	L	101	LHG	C24-C25-C26-C27
35	L	101	LHG	C25-C26-C27-C28
35	d	409	LHG	C25-C26-C27-C28
36	M	102	LMG	C14-C15-C16-C17
36	W	101	LMG	C14-C15-C16-C17
36	d	410	LMG	C30-C31-C32-C33
36	m	102	LMG	C14-C15-C16-C17
36	w	101	LMG	C14-C15-C16-C17
36	w	101	LMG	C19-C20-C21-C22
41	20	211	A86	O5-C38-O4-C34
41	21	311	A86	O5-C38-O4-C34
41	40	211	A86	O5-C38-O4-C34
41	41	311	A86	O5-C38-O4-C34
30	40	203	CLA	CBD-CGD-O2D-CED
30	41	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	A	408	LHG	C7-C8-C9-C10
35	B	622	LHG	C30-C31-C32-C33
35	b	621	LHG	C30-C31-C32-C33
35	l	102	LHG	C28-C29-C30-C31
36	M	102	LMG	C31-C32-C33-C34
36	m	102	LMG	C31-C32-C33-C34
38	C	516	DGD	C3A-C4A-C5A-C6A
30	C	520	CLA	C16-C17-C18-C19
30	C	520	CLA	C16-C17-C18-C20
30	C	521	CLA	C16-C17-C18-C19
30	c	522	CLA	C16-C17-C18-C19
30	c	522	CLA	C16-C17-C18-C20
30	c	523	CLA	C16-C17-C18-C19
30	15	303	CLA	C16-C17-C18-C19
30	35	303	CLA	C16-C17-C18-C19
38	C	516	DGD	O6D-C1D-O3G-C3G
38	J	101	DGD	O6E-C1E-O5D-C6D
38	c	517	DGD	O6D-C1D-O3G-C3G
38	j	101	DGD	O6E-C1E-O5D-C6D
30	C	508	CLA	C13-C15-C16-C17
30	c	508	CLA	C13-C15-C16-C17
35	L	102	LHG	C28-C29-C30-C31
38	c	517	DGD	C3A-C4A-C5A-C6A
30	21	303	CLA	CBD-CGD-O2D-CED
30	b	622	CLA	O1D-CGD-O2D-CED
30	17	301	CLA	O1D-CGD-O2D-CED
30	37	301	CLA	O1D-CGD-O2D-CED
38	C	516	DGD	CCA-CDA-CEA-CFA
38	c	517	DGD	CCA-CDA-CEA-CFA
38	j	101	DGD	C8A-C9A-CAA-CBA
35	a	407	LHG	C7-C8-C9-C10
33	A	406	SQD	C32-C33-C34-C35
33	a	405	SQD	C32-C33-C34-C35
36	Q	301	LMG	C18-C19-C20-C21
36	c	519	LMG	C18-C19-C20-C21
38	J	101	DGD	C8A-C9A-CAA-CBA
38	C	516	DGD	C7B-C8B-C9B-CAB
38	H	102	DGD	C3A-C4A-C5A-C6A
38	c	517	DGD	C7B-C8B-C9B-CAB
38	h	102	DGD	C3A-C4A-C5A-C6A
30	B	610	CLA	O1D-CGD-O2D-CED
30	M	101	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	b	610	CLA	O1D-CGD-O2D-CED
30	m	101	CLA	O1D-CGD-O2D-CED
30	B	623	CLA	C3A-C2A-CAA-CBA
30	D	405	CLA	C3A-C2A-CAA-CBA
30	W	102	CLA	C3A-C2A-CAA-CBA
30	W	103	CLA	C3A-C2A-CAA-CBA
30	d	406	CLA	C3A-C2A-CAA-CBA
30	w	102	CLA	C3A-C2A-CAA-CBA
30	w	103	CLA	C3A-C2A-CAA-CBA
30	11	303	CLA	C3A-C2A-CAA-CBA
30	11	304	CLA	C3A-C2A-CAA-CBA
30	11	306	CLA	C3A-C2A-CAA-CBA
30	11	308	CLA	C3A-C2A-CAA-CBA
30	12	307	CLA	C3A-C2A-CAA-CBA
30	12	308	CLA	C3A-C2A-CAA-CBA
30	12	310	CLA	C3A-C2A-CAA-CBA
30	12	313	CLA	C3A-C2A-CAA-CBA
30	13	304	CLA	C3A-C2A-CAA-CBA
30	13	305	CLA	C3A-C2A-CAA-CBA
30	13	307	CLA	C3A-C2A-CAA-CBA
30	13	309	CLA	C3A-C2A-CAA-CBA
30	14	304	CLA	C3A-C2A-CAA-CBA
30	14	305	CLA	C3A-C2A-CAA-CBA
30	14	307	CLA	C3A-C2A-CAA-CBA
30	14	309	CLA	C3A-C2A-CAA-CBA
30	15	302	CLA	C3A-C2A-CAA-CBA
30	15	304	CLA	C3A-C2A-CAA-CBA
30	15	306	CLA	C3A-C2A-CAA-CBA
30	15	308	CLA	C3A-C2A-CAA-CBA
30	16	303	CLA	C3A-C2A-CAA-CBA
30	16	304	CLA	C3A-C2A-CAA-CBA
30	16	305	CLA	C3A-C2A-CAA-CBA
30	16	306	CLA	C3A-C2A-CAA-CBA
30	17	304	CLA	C3A-C2A-CAA-CBA
30	17	305	CLA	C3A-C2A-CAA-CBA
30	17	306	CLA	C3A-C2A-CAA-CBA
30	17	307	CLA	C3A-C2A-CAA-CBA
30	18	305	CLA	C3A-C2A-CAA-CBA
30	18	306	CLA	C3A-C2A-CAA-CBA
30	18	308	CLA	C3A-C2A-CAA-CBA
30	18	311	CLA	C3A-C2A-CAA-CBA
30	19	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	19	306	CLA	C3A-C2A-CAA-CBA
30	20	205	CLA	C3A-C2A-CAA-CBA
30	20	206	CLA	C3A-C2A-CAA-CBA
30	20	207	CLA	C3A-C2A-CAA-CBA
30	20	208	CLA	C3A-C2A-CAA-CBA
30	21	302	CLA	C3A-C2A-CAA-CBA
30	21	304	CLA	C3A-C2A-CAA-CBA
30	21	305	CLA	C3A-C2A-CAA-CBA
30	21	309	CLA	C3A-C2A-CAA-CBA
30	31	303	CLA	C3A-C2A-CAA-CBA
30	31	304	CLA	C3A-C2A-CAA-CBA
30	31	306	CLA	C3A-C2A-CAA-CBA
30	31	308	CLA	C3A-C2A-CAA-CBA
30	32	307	CLA	C3A-C2A-CAA-CBA
30	32	308	CLA	C3A-C2A-CAA-CBA
30	32	310	CLA	C3A-C2A-CAA-CBA
30	32	312	CLA	C3A-C2A-CAA-CBA
30	33	305	CLA	C3A-C2A-CAA-CBA
30	33	306	CLA	C3A-C2A-CAA-CBA
30	33	308	CLA	C3A-C2A-CAA-CBA
30	33	310	CLA	C3A-C2A-CAA-CBA
30	34	304	CLA	C3A-C2A-CAA-CBA
30	34	305	CLA	C3A-C2A-CAA-CBA
30	34	307	CLA	C3A-C2A-CAA-CBA
30	34	309	CLA	C3A-C2A-CAA-CBA
30	35	302	CLA	C3A-C2A-CAA-CBA
30	35	304	CLA	C3A-C2A-CAA-CBA
30	35	306	CLA	C3A-C2A-CAA-CBA
30	35	308	CLA	C3A-C2A-CAA-CBA
30	36	303	CLA	C3A-C2A-CAA-CBA
30	36	304	CLA	C3A-C2A-CAA-CBA
30	36	305	CLA	C3A-C2A-CAA-CBA
30	36	306	CLA	C3A-C2A-CAA-CBA
30	37	304	CLA	C3A-C2A-CAA-CBA
30	37	305	CLA	C3A-C2A-CAA-CBA
30	37	306	CLA	C3A-C2A-CAA-CBA
30	37	307	CLA	C3A-C2A-CAA-CBA
30	38	305	CLA	C3A-C2A-CAA-CBA
30	38	306	CLA	C3A-C2A-CAA-CBA
30	38	308	CLA	C3A-C2A-CAA-CBA
30	38	311	CLA	C3A-C2A-CAA-CBA
30	39	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	39	306	CLA	C3A-C2A-CAA-CBA
30	40	205	CLA	C3A-C2A-CAA-CBA
30	40	206	CLA	C3A-C2A-CAA-CBA
30	40	207	CLA	C3A-C2A-CAA-CBA
30	40	208	CLA	C3A-C2A-CAA-CBA
30	41	302	CLA	C3A-C2A-CAA-CBA
30	41	304	CLA	C3A-C2A-CAA-CBA
30	41	305	CLA	C3A-C2A-CAA-CBA
30	41	309	CLA	C3A-C2A-CAA-CBA
30	C	504	CLA	C8-C10-C11-C12
30	c	504	CLA	C8-C10-C11-C12
30	11	307	CLA	C5-C6-C7-C8
30	12	311	CLA	C5-C6-C7-C8
30	18	309	CLA	C15-C16-C17-C18
30	31	307	CLA	C5-C6-C7-C8
30	38	309	CLA	C15-C16-C17-C18
42	32	302	LMU	C2-C1-O1'-C1'
36	W	101	LMG	C12-C13-C14-C15
36	w	101	LMG	C12-C13-C14-C15
30	16	307	CLA	O1D-CGD-O2D-CED
30	36	307	CLA	O1D-CGD-O2D-CED
30	B	605	CLA	C16-C17-C18-C19
30	b	605	CLA	C16-C17-C18-C19
30	B	623	CLA	O1D-CGD-O2D-CED
30	C	503	CLA	O1D-CGD-O2D-CED
30	c	505	CLA	CBD-CGD-O2D-CED
30	B	601	CLA	C3-C5-C6-C7
30	b	601	CLA	C3-C5-C6-C7
30	13	308	CLA	C5-C6-C7-C8
30	14	308	CLA	C5-C6-C7-C8
30	32	311	CLA	C5-C6-C7-C8
30	33	309	CLA	C5-C6-C7-C8
30	34	308	CLA	C5-C6-C7-C8
30	C	511	CLA	C4-C3-C5-C6
30	c	511	CLA	C4-C3-C5-C6
30	C	507	CLA	C2-C3-C5-C6
30	C	511	CLA	C2-C3-C5-C6
30	c	507	CLA	C2-C3-C5-C6
30	c	511	CLA	C2-C3-C5-C6
30	C	505	CLA	CBD-CGD-O2D-CED
33	L	103	SQD	C14-C15-C16-C17
35	B	622	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	b	621	LHG	C9-C10-C11-C12
36	W	101	LMG	C37-C38-C39-C40
36	w	101	LMG	C37-C38-C39-C40
41	21	313	A86	C35-C34-O4-C38
41	41	313	A86	C35-C34-O4-C38
30	37	307	CLA	C2A-CAA-CBA-CGA
33	l	101	SQD	C14-C15-C16-C17
35	A	408	LHG	C14-C15-C16-C17
35	L	101	LHG	C31-C32-C33-C34
35	a	407	LHG	C14-C15-C16-C17
35	d	409	LHG	C31-C32-C33-C34
38	C	517	DGD	O6E-C5E-C6E-O5E
38	c	518	DGD	O6E-C5E-C6E-O5E
30	37	301	CLA	C16-C17-C18-C20
33	B	621	SQD	C11-C10-C9-C8
33	L	103	SQD	C31-C32-C33-C34
38	C	517	DGD	CAA-CBA-CCA-CDA
33	b	620	SQD	C11-C10-C9-C8
33	l	101	SQD	C31-C32-C33-C34
35	L	101	LHG	C13-C14-C15-C16
35	L	101	LHG	C29-C30-C31-C32
35	d	409	LHG	C29-C30-C31-C32
36	B	620	LMG	C18-C19-C20-C21
36	b	619	LMG	C18-C19-C20-C21
38	c	518	DGD	CAA-CBA-CCA-CDA
42	12	302	LMU	C2-C3-C4-C5
41	11	316	A86	C33-C34-O4-C38
41	12	304	A86	C33-C34-O4-C38
41	13	301	A86	C33-C34-O4-C38
41	13	316	A86	C33-C34-O4-C38
41	18	302	A86	C33-C34-O4-C38
41	32	304	A86	C33-C34-O4-C38
41	33	302	A86	C33-C34-O4-C38
35	d	409	LHG	C13-C14-C15-C16
36	Q	301	LMG	C19-C20-C21-C22
36	c	519	LMG	C19-C20-C21-C22
36	d	410	LMG	C17-C18-C19-C20
35	L	101	LHG	O9-C7-O7-C5
35	d	409	LHG	O9-C7-O7-C5
30	B	612	CLA	C2-C1-O2A-CGA
30	b	612	CLA	C2-C1-O2A-CGA
33	A	406	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
36	D	408	LMG	C17-C18-C19-C20
30	C	512	CLA	C5-C6-C7-C8
30	c	512	CLA	C5-C6-C7-C8
30	20	202	CLA	C8-C10-C11-C12
30	40	202	CLA	C8-C10-C11-C12
30	B	612	CLA	O1A-CGA-O2A-C1
30	b	612	CLA	O1A-CGA-O2A-C1
36	Q	301	LMG	C4-C5-C6-O5
33	a	405	SQD	C12-C13-C14-C15
30	15	303	CLA	C16-C17-C18-C20
30	17	301	CLA	C16-C17-C18-C20
30	18	310	CLA	C16-C17-C18-C19
30	35	303	CLA	C16-C17-C18-C20
30	38	310	CLA	C16-C17-C18-C19
33	L	103	SQD	C7-C8-C9-C10
33	l	101	SQD	C7-C8-C9-C10
32	A	405	BCR	C1-C6-C7-C8
32	A	405	BCR	C5-C6-C7-C8
32	A	409	BCR	C1-C6-C7-C8
32	A	409	BCR	C5-C6-C7-C8
32	B	616	BCR	C1-C6-C7-C8
32	B	616	BCR	C5-C6-C7-C8
32	B	616	BCR	C23-C24-C25-C26
32	B	617	BCR	C5-C6-C7-C8
32	B	618	BCR	C5-C6-C7-C8
32	B	624	BCR	C1-C6-C7-C8
32	B	624	BCR	C5-C6-C7-C8
32	C	515	BCR	C5-C6-C7-C8
32	C	518	BCR	C5-C6-C7-C8
32	C	518	BCR	C23-C24-C25-C26
32	C	518	BCR	C23-C24-C25-C30
32	F	101	BCR	C1-C6-C7-C8
32	F	101	BCR	C5-C6-C7-C8
32	H	101	BCR	C5-C6-C7-C8
32	Y	101	BCR	C5-C6-C7-C8
32	Z	101	BCR	C1-C6-C7-C8
32	Z	101	BCR	C5-C6-C7-C8
32	Z	101	BCR	C23-C24-C25-C26
32	a	404	BCR	C1-C6-C7-C8
32	a	404	BCR	C5-C6-C7-C8
32	a	408	BCR	C1-C6-C7-C8
32	a	408	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	b	616	BCR	C5-C6-C7-C8
32	b	617	BCR	C5-C6-C7-C8
32	b	623	BCR	C1-C6-C7-C8
32	b	623	BCR	C5-C6-C7-C8
32	c	515	BCR	C1-C6-C7-C8
32	c	515	BCR	C5-C6-C7-C8
32	c	515	BCR	C23-C24-C25-C26
32	c	516	BCR	C5-C6-C7-C8
32	c	520	BCR	C5-C6-C7-C8
32	c	521	BCR	C5-C6-C7-C8
32	c	521	BCR	C23-C24-C25-C26
32	c	521	BCR	C23-C24-C25-C30
32	f	101	BCR	C1-C6-C7-C8
32	f	101	BCR	C5-C6-C7-C8
32	h	101	BCR	C5-C6-C7-C8
32	m	103	BCR	C1-C6-C7-C8
32	m	103	BCR	C5-C6-C7-C8
32	m	103	BCR	C23-C24-C25-C26
33	A	406	SQD	C17-C18-C19-C20
33	a	405	SQD	C17-C18-C19-C20
30	c	503	CLA	O1D-CGD-O2D-CED
30	C	504	CLA	CBA-CGA-O2A-C1
30	M	101	CLA	CBA-CGA-O2A-C1
30	c	504	CLA	CBA-CGA-O2A-C1
30	m	101	CLA	CBA-CGA-O2A-C1
41	15	315	A86	C33-C34-O4-C38
41	15	316	A86	C33-C34-O4-C38
41	31	316	A86	C33-C34-O4-C38
41	33	316	A86	C33-C34-O4-C38
41	35	315	A86	C33-C34-O4-C38
41	35	316	A86	C33-C34-O4-C38
41	38	302	A86	C33-C34-O4-C38
36	c	519	LMG	C4-C5-C6-O5
36	B	619	LMG	C29-C30-C31-C32
36	b	618	LMG	C29-C30-C31-C32
42	32	302	LMU	C2-C3-C4-C5
36	Q	301	LMG	C10-C11-C12-C13
36	c	519	LMG	C10-C11-C12-C13
30	16	301	CLA	C5-C6-C7-C8
30	36	301	CLA	C5-C6-C7-C8
33	A	406	SQD	C14-C15-C16-C17
30	39	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	C	508	CLA	C11-C10-C8-C7
30	W	102	CLA	C12-C13-C15-C16
30	W	103	CLA	C6-C7-C8-C10
30	W	103	CLA	C11-C12-C13-C15
30	c	508	CLA	C11-C10-C8-C7
30	w	102	CLA	C12-C13-C15-C16
30	w	103	CLA	C6-C7-C8-C10
30	w	103	CLA	C11-C12-C13-C15
31	A	403	PHO	C2-C3-C5-C6
31	d	403	PHO	C2-C3-C5-C6
39	D	404	PL9	C28-C29-C31-C32
39	d	405	PL9	C28-C29-C31-C32
30	c	510	CLA	C3-C5-C6-C7
30	M	101	CLA	O1A-CGA-O2A-C1
30	m	101	CLA	O1A-CGA-O2A-C1
33	a	405	SQD	C14-C15-C16-C17
30	c	522	CLA	C8-C10-C11-C12
41	11	316	A86	C3-C4-C5-C6
41	12	304	A86	C3-C4-C5-C6
41	13	301	A86	C3-C4-C5-C6
41	13	316	A86	C3-C4-C5-C6
41	15	315	A86	C3-C4-C5-C6
41	15	316	A86	C3-C4-C5-C6
41	18	302	A86	C3-C4-C5-C6
41	19	310	A86	C11-C10-C9-C8
41	19	311	A86	C1-C2-C3-C4
41	20	210	A86	C1-C2-C3-C4
41	31	316	A86	C3-C4-C5-C6
41	32	304	A86	C3-C4-C5-C6
41	33	302	A86	C3-C4-C5-C6
41	33	316	A86	C3-C4-C5-C6
41	35	315	A86	C3-C4-C5-C6
41	35	316	A86	C3-C4-C5-C6
41	38	302	A86	C3-C4-C5-C6
41	39	310	A86	C11-C10-C9-C8
41	39	311	A86	C1-C2-C3-C4
41	40	210	A86	C1-C2-C3-C4
30	20	202	CLA	CBD-CGD-O2D-CED
30	40	202	CLA	CBD-CGD-O2D-CED
30	B	602	CLA	C16-C17-C18-C19
30	B	611	CLA	C16-C17-C18-C20
30	b	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	b	611	CLA	C16-C17-C18-C20
30	18	305	CLA	C16-C17-C18-C19
30	38	305	CLA	C16-C17-C18-C19
38	H	102	DGD	O6D-C5D-C6D-O5D
38	h	102	DGD	O6D-C5D-C6D-O5D
30	19	306	CLA	O1D-CGD-O2D-CED
30	B	602	CLA	CBA-CGA-O2A-C1
30	Z	102	CLA	CBA-CGA-O2A-C1
30	b	602	CLA	CBA-CGA-O2A-C1
30	c	524	CLA	CBA-CGA-O2A-C1
36	B	619	LMG	C29-C28-O8-C9
36	b	618	LMG	C29-C28-O8-C9
30	B	615	CLA	C2A-CAA-CBA-CGA
30	b	615	CLA	C2A-CAA-CBA-CGA
30	17	303	CLA	C2A-CAA-CBA-CGA
30	17	307	CLA	C2A-CAA-CBA-CGA
30	18	307	CLA	C2A-CAA-CBA-CGA
30	37	303	CLA	C2A-CAA-CBA-CGA
30	38	307	CLA	C2A-CAA-CBA-CGA
30	C	520	CLA	C8-C10-C11-C12
30	c	502	CLA	C10-C11-C12-C13
35	d	409	LHG	C33-C34-C35-C36
36	12	301	LMG	C32-C33-C34-C35
35	L	101	LHG	C33-C34-C35-C36
30	C	502	CLA	C10-C11-C12-C13
30	W	102	CLA	C5-C6-C7-C8
30	w	102	CLA	C5-C6-C7-C8
30	18	309	CLA	C10-C11-C12-C13
30	38	309	CLA	C10-C11-C12-C13
30	C	510	CLA	C3-C5-C6-C7
36	B	620	LMG	C11-C12-C13-C14
36	b	619	LMG	C11-C12-C13-C14
36	32	301	LMG	C32-C33-C34-C35
38	j	101	DGD	C6A-C7A-C8A-C9A
30	D	405	CLA	C5-C6-C7-C8
33	L	103	SQD	C12-C13-C14-C15
33	L	103	SQD	C17-C18-C19-C20
33	l	101	SQD	C17-C18-C19-C20
36	12	301	LMG	C14-C15-C16-C17
38	J	101	DGD	C6A-C7A-C8A-C9A
33	A	406	SQD	C7-C8-C9-C10
33	a	405	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
36	B	620	LMG	C11-C10-O7-C8
36	b	619	LMG	C11-C10-O7-C8
33	l	101	SQD	C12-C13-C14-C15
36	Q	301	LMG	C17-C18-C19-C20
36	c	519	LMG	C17-C18-C19-C20
38	C	516	DGD	C3B-C4B-C5B-C6B
38	c	517	DGD	C3B-C4B-C5B-C6B
30	M	101	CLA	C5-C6-C7-C8
30	b	614	CLA	C15-C16-C17-C18
30	c	507	CLA	C13-C15-C16-C17
30	d	406	CLA	C5-C6-C7-C8
30	m	101	CLA	C5-C6-C7-C8
30	21	305	CLA	CBD-CGD-O2D-CED
30	41	305	CLA	CBD-CGD-O2D-CED
35	A	408	LHG	C13-C14-C15-C16
35	a	407	LHG	C13-C14-C15-C16
36	Q	301	LMG	O9-C10-O7-C8
36	W	101	LMG	O9-C10-O7-C8
36	w	101	LMG	O9-C10-O7-C8
42	12	302	LMU	C4-C5-C6-C7
30	B	614	CLA	C15-C16-C17-C18
30	C	507	CLA	C13-C15-C16-C17
30	c	514	CLA	C15-C16-C17-C18
33	B	621	SQD	O47-C45-C46-O48
33	b	620	SQD	O47-C45-C46-O48
30	C	521	CLA	C16-C17-C18-C20
30	c	523	CLA	C16-C17-C18-C20
30	C	503	CLA	C13-C15-C16-C17
30	C	514	CLA	C15-C16-C17-C18
30	C	520	CLA	C10-C11-C12-C13
30	c	503	CLA	C13-C15-C16-C17
30	c	522	CLA	C10-C11-C12-C13
30	18	303	CLA	C8-C10-C11-C12
30	38	303	CLA	C8-C10-C11-C12
30	B	609	CLA	C2-C3-C5-C6
30	D	406	CLA	C2-C3-C5-C6
30	b	609	CLA	C2-C3-C5-C6
30	d	407	CLA	C2-C3-C5-C6
30	B	615	CLA	C6-C7-C8-C9
30	C	503	CLA	C11-C12-C13-C14
30	C	505	CLA	C6-C7-C8-C9
30	Z	102	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	W	102	CLA	C14-C13-C15-C16
30	W	103	CLA	C6-C7-C8-C9
30	b	610	CLA	C14-C13-C15-C16
30	b	615	CLA	C6-C7-C8-C9
30	c	503	CLA	C11-C12-C13-C14
30	c	505	CLA	C6-C7-C8-C9
30	c	524	CLA	C14-C13-C15-C16
30	w	102	CLA	C14-C13-C15-C16
30	w	103	CLA	C6-C7-C8-C9
30	11	307	CLA	C6-C7-C8-C9
30	12	311	CLA	C6-C7-C8-C9
30	13	308	CLA	C6-C7-C8-C9
30	14	308	CLA	C6-C7-C8-C9
30	19	303	CLA	C11-C12-C13-C14
30	20	204	CLA	C14-C13-C15-C16
30	20	209	CLA	C11-C10-C8-C9
30	21	307	CLA	C14-C13-C15-C16
30	31	307	CLA	C6-C7-C8-C9
30	32	311	CLA	C6-C7-C8-C9
30	33	309	CLA	C6-C7-C8-C9
30	34	308	CLA	C6-C7-C8-C9
30	39	303	CLA	C11-C12-C13-C14
30	40	209	CLA	C11-C10-C8-C9
30	41	307	CLA	C14-C13-C15-C16
30	C	507	CLA	C2A-CAA-CBA-CGA
30	M	101	CLA	C2A-CAA-CBA-CGA
30	c	507	CLA	C2A-CAA-CBA-CGA
30	m	101	CLA	C2A-CAA-CBA-CGA
30	15	302	CLA	C2A-CAA-CBA-CGA
30	31	306	CLA	C2A-CAA-CBA-CGA
30	32	310	CLA	C2A-CAA-CBA-CGA
30	33	308	CLA	C2A-CAA-CBA-CGA
30	34	307	CLA	C2A-CAA-CBA-CGA
30	35	302	CLA	C2A-CAA-CBA-CGA
35	L	101	LHG	C28-C29-C30-C31
35	d	409	LHG	C28-C29-C30-C31
36	W	101	LMG	C18-C19-C20-C21
36	w	101	LMG	C18-C19-C20-C21
41	19	309	A86	C-C1-C24-C25
41	39	309	A86	C-C1-C24-C25
41	19	309	A86	C2-C1-C24-C25
41	39	309	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
30	A	404	CLA	C1A-C2A-CAA-CBA
30	B	604	CLA	C1A-C2A-CAA-CBA
30	B	606	CLA	C1A-C2A-CAA-CBA
30	B	607	CLA	C1A-C2A-CAA-CBA
30	B	611	CLA	C1A-C2A-CAA-CBA
30	B	623	CLA	C1A-C2A-CAA-CBA
30	C	504	CLA	C1A-C2A-CAA-CBA
30	C	512	CLA	C1A-C2A-CAA-CBA
30	C	513	CLA	C1A-C2A-CAA-CBA
30	D	401	CLA	C1A-C2A-CAA-CBA
30	D	402	CLA	C1A-C2A-CAA-CBA
30	M	101	CLA	C1A-C2A-CAA-CBA
30	W	103	CLA	C1A-C2A-CAA-CBA
30	a	403	CLA	C1A-C2A-CAA-CBA
30	b	604	CLA	C1A-C2A-CAA-CBA
30	b	606	CLA	C1A-C2A-CAA-CBA
30	b	607	CLA	C1A-C2A-CAA-CBA
30	b	611	CLA	C1A-C2A-CAA-CBA
30	b	622	CLA	C1A-C2A-CAA-CBA
30	c	504	CLA	C1A-C2A-CAA-CBA
30	c	512	CLA	C1A-C2A-CAA-CBA
30	d	401	CLA	C1A-C2A-CAA-CBA
30	d	402	CLA	C1A-C2A-CAA-CBA
30	m	101	CLA	C1A-C2A-CAA-CBA
30	w	103	CLA	C1A-C2A-CAA-CBA
30	11	301	CLA	C1A-C2A-CAA-CBA
30	11	304	CLA	C1A-C2A-CAA-CBA
30	11	306	CLA	C1A-C2A-CAA-CBA
30	12	305	CLA	C1A-C2A-CAA-CBA
30	12	308	CLA	C1A-C2A-CAA-CBA
30	12	310	CLA	C1A-C2A-CAA-CBA
30	13	302	CLA	C1A-C2A-CAA-CBA
30	13	305	CLA	C1A-C2A-CAA-CBA
30	13	307	CLA	C1A-C2A-CAA-CBA
30	14	302	CLA	C1A-C2A-CAA-CBA
30	14	305	CLA	C1A-C2A-CAA-CBA
30	14	307	CLA	C1A-C2A-CAA-CBA
30	15	304	CLA	C1A-C2A-CAA-CBA
30	15	306	CLA	C1A-C2A-CAA-CBA
30	15	308	CLA	C1A-C2A-CAA-CBA
30	16	305	CLA	C1A-C2A-CAA-CBA
30	16	306	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	17	306	CLA	C1A-C2A-CAA-CBA
30	17	307	CLA	C1A-C2A-CAA-CBA
30	18	306	CLA	C1A-C2A-CAA-CBA
30	18	308	CLA	C1A-C2A-CAA-CBA
30	18	309	CLA	C1A-C2A-CAA-CBA
30	18	311	CLA	C1A-C2A-CAA-CBA
30	19	304	CLA	C1A-C2A-CAA-CBA
30	19	306	CLA	C1A-C2A-CAA-CBA
30	20	205	CLA	C1A-C2A-CAA-CBA
30	20	206	CLA	C1A-C2A-CAA-CBA
30	21	304	CLA	C1A-C2A-CAA-CBA
30	21	305	CLA	C1A-C2A-CAA-CBA
30	21	309	CLA	C1A-C2A-CAA-CBA
30	31	301	CLA	C1A-C2A-CAA-CBA
30	31	304	CLA	C1A-C2A-CAA-CBA
30	31	306	CLA	C1A-C2A-CAA-CBA
30	32	305	CLA	C1A-C2A-CAA-CBA
30	32	308	CLA	C1A-C2A-CAA-CBA
30	32	310	CLA	C1A-C2A-CAA-CBA
30	33	303	CLA	C1A-C2A-CAA-CBA
30	33	306	CLA	C1A-C2A-CAA-CBA
30	33	308	CLA	C1A-C2A-CAA-CBA
30	34	302	CLA	C1A-C2A-CAA-CBA
30	34	305	CLA	C1A-C2A-CAA-CBA
30	34	307	CLA	C1A-C2A-CAA-CBA
30	35	304	CLA	C1A-C2A-CAA-CBA
30	35	306	CLA	C1A-C2A-CAA-CBA
30	35	308	CLA	C1A-C2A-CAA-CBA
30	36	305	CLA	C1A-C2A-CAA-CBA
30	36	306	CLA	C1A-C2A-CAA-CBA
30	37	306	CLA	C1A-C2A-CAA-CBA
30	37	307	CLA	C1A-C2A-CAA-CBA
30	38	306	CLA	C1A-C2A-CAA-CBA
30	38	308	CLA	C1A-C2A-CAA-CBA
30	38	309	CLA	C1A-C2A-CAA-CBA
30	38	311	CLA	C1A-C2A-CAA-CBA
30	39	304	CLA	C1A-C2A-CAA-CBA
30	39	306	CLA	C1A-C2A-CAA-CBA
30	40	205	CLA	C1A-C2A-CAA-CBA
30	40	206	CLA	C1A-C2A-CAA-CBA
30	41	304	CLA	C1A-C2A-CAA-CBA
30	41	305	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	41	309	CLA	C1A-C2A-CAA-CBA
30	B	602	CLA	C16-C17-C18-C20
30	B	610	CLA	C16-C17-C18-C20
30	b	602	CLA	C16-C17-C18-C20
30	b	610	CLA	C16-C17-C18-C20
30	17	301	CLA	C16-C17-C18-C19
30	18	305	CLA	C16-C17-C18-C20
30	37	301	CLA	C16-C17-C18-C19
30	38	305	CLA	C16-C17-C18-C20
36	c	519	LMG	O9-C10-O7-C8
36	32	301	LMG	C15-C16-C17-C18
38	C	516	DGD	CBA-CCA-CDA-CEA
32	B	624	BCR	C13-C14-C15-C16
32	b	623	BCR	C13-C14-C15-C16
41	20	212	A86	C3-C4-C5-C6
41	20	213	A86	C11-C10-C9-C8
41	21	314	A86	C11-C10-C9-C8
41	40	212	A86	C3-C4-C5-C6
41	40	213	A86	C11-C10-C9-C8
41	41	314	A86	C11-C10-C9-C8
30	19	308	CLA	O1D-CGD-O2D-CED
30	39	308	CLA	O1D-CGD-O2D-CED
30	C	507	CLA	C8-C10-C11-C12
42	12	302	LMU	C1-C2-C3-C4
35	A	408	LHG	C3-O3-P-O6
35	B	622	LHG	C3-O3-P-O6
35	a	407	LHG	C3-O3-P-O6
35	b	621	LHG	C3-O3-P-O6
35	B	622	LHG	C33-C34-C35-C36
35	L	101	LHG	C32-C33-C34-C35
35	d	409	LHG	C32-C33-C34-C35
38	c	517	DGD	CBA-CCA-CDA-CEA
36	w	101	LMG	C17-C18-C19-C20
30	C	504	CLA	O1A-CGA-O2A-C1
30	Z	102	CLA	O1A-CGA-O2A-C1
30	C	505	CLA	C10-C11-C12-C13
30	c	505	CLA	C10-C11-C12-C13
30	31	307	CLA	C15-C16-C17-C18
35	B	622	LHG	O6-C4-C5-C6
35	b	621	LHG	O6-C4-C5-C6
35	b	621	LHG	C33-C34-C35-C36
36	W	101	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	c	507	CLA	C8-C10-C11-C12
36	b	619	LMG	C31-C32-C33-C34
36	D	408	LMG	O6-C5-C6-O5
36	d	410	LMG	O6-C5-C6-O5
36	B	620	LMG	C31-C32-C33-C34
42	32	302	LMU	C4-C5-C6-C7
30	B	601	CLA	C10-C11-C12-C13
30	32	311	CLA	C15-C16-C17-C18
38	J	101	DGD	O1B-C1B-O2G-C2G
38	j	101	DGD	O1B-C1B-O2G-C2G
36	w	101	LMG	C30-C31-C32-C33
30	b	601	CLA	C10-C11-C12-C13
30	20	209	CLA	C15-C16-C17-C18
30	34	308	CLA	C15-C16-C17-C18
30	40	209	CLA	C15-C16-C17-C18
36	W	101	LMG	C30-C31-C32-C33
30	B	602	CLA	O1A-CGA-O2A-C1
30	b	602	CLA	O1A-CGA-O2A-C1
30	c	504	CLA	O1A-CGA-O2A-C1
30	c	524	CLA	O1A-CGA-O2A-C1
30	33	309	CLA	C15-C16-C17-C18
30	B	610	CLA	C16-C17-C18-C19
30	b	610	CLA	C16-C17-C18-C19
35	A	408	LHG	C4-C5-C6-O8
35	A	408	LHG	C30-C31-C32-C33
35	a	407	LHG	C4-C5-C6-O8
35	a	407	LHG	C30-C31-C32-C33
36	B	619	LMG	C30-C31-C32-C33
36	D	408	LMG	O1-C7-C8-C9
36	W	101	LMG	O1-C7-C8-C9
36	W	101	LMG	C7-C8-C9-O8
36	b	618	LMG	C30-C31-C32-C33
36	d	410	LMG	O1-C7-C8-C9
36	w	101	LMG	O1-C7-C8-C9
36	w	101	LMG	C7-C8-C9-O8
30	C	511	CLA	C5-C6-C7-C8
30	M	101	CLA	C10-C11-C12-C13
30	c	511	CLA	C5-C6-C7-C8
30	m	101	CLA	C10-C11-C12-C13
36	B	620	LMG	C34-C35-C36-C37
36	b	619	LMG	C34-C35-C36-C37
38	H	102	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
38	C	517	DGD	C5D-C6D-O5D-C1E
38	c	518	DGD	C5D-C6D-O5D-C1E
30	B	604	CLA	C13-C15-C16-C17
30	Z	102	CLA	C13-C15-C16-C17
30	b	604	CLA	C13-C15-C16-C17
30	c	524	CLA	C13-C15-C16-C17
36	B	620	LMG	C13-C14-C15-C16
36	Q	301	LMG	C37-C38-C39-C40
36	b	619	LMG	C13-C14-C15-C16
30	11	307	CLA	CAA-CBA-CGA-O2A
30	12	311	CLA	CAA-CBA-CGA-O2A
30	13	308	CLA	CAA-CBA-CGA-O2A
30	14	308	CLA	CAA-CBA-CGA-O2A
30	31	307	CLA	CAA-CBA-CGA-O2A
30	32	311	CLA	CAA-CBA-CGA-O2A
30	33	309	CLA	CAA-CBA-CGA-O2A
30	34	308	CLA	CAA-CBA-CGA-O2A
38	h	102	DGD	C1A-C2A-C3A-C4A
36	c	519	LMG	C37-C38-C39-C40
35	l	102	LHG	C13-C14-C15-C16
38	H	102	DGD	CBA-CCA-CDA-CEA
35	L	101	LHG	O1-C1-C2-O2
35	d	409	LHG	O1-C1-C2-O2
41	20	211	A86	C24-C25-C26-C27
41	21	311	A86	C24-C25-C26-C27
41	40	211	A86	C24-C25-C26-C27
41	41	311	A86	C24-C25-C26-C27
35	L	102	LHG	C13-C14-C15-C16
38	h	102	DGD	CBA-CCA-CDA-CEA
42	32	302	LMU	C1-C2-C3-C4
35	B	622	LHG	C27-C28-C29-C30
35	b	621	LHG	C27-C28-C29-C30
38	h	102	DGD	CBB-CCB-CDB-CEB
30	C	509	CLA	C5-C6-C7-C8
38	C	516	DGD	O6E-C5E-C6E-O5E
38	c	517	DGD	O6E-C5E-C6E-O5E
30	B	609	CLA	C4-C3-C5-C6
30	b	609	CLA	C4-C3-C5-C6
31	A	403	PHO	C4-C3-C5-C6
31	d	403	PHO	C4-C3-C5-C6
38	H	102	DGD	CBB-CCB-CDB-CEB
30	C	502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	c	502	CLA	CBA-CGA-O2A-C1
33	l	101	SQD	C24-C23-O48-C46
30	c	509	CLA	C5-C6-C7-C8
30	11	307	CLA	C15-C16-C17-C18
30	12	311	CLA	C15-C16-C17-C18
30	13	308	CLA	C15-C16-C17-C18
30	14	308	CLA	C15-C16-C17-C18
31	A	403	PHO	C8-C10-C11-C12
31	d	403	PHO	C8-C10-C11-C12
30	18	303	CLA	C5-C6-C7-C8
30	38	303	CLA	C5-C6-C7-C8
31	D	403	PHO	C5-C6-C7-C8
31	d	404	PHO	C5-C6-C7-C8
30	11	306	CLA	O1D-CGD-O2D-CED
30	12	310	CLA	O1D-CGD-O2D-CED
30	13	307	CLA	O1D-CGD-O2D-CED
30	14	307	CLA	O1D-CGD-O2D-CED
36	W	101	LMG	C15-C16-C17-C18
36	w	101	LMG	C15-C16-C17-C18
38	J	101	DGD	CDA-CEA-CFA-CGA
30	31	303	CLA	CBA-CGA-O2A-C1
30	32	307	CLA	CBA-CGA-O2A-C1
30	33	305	CLA	CBA-CGA-O2A-C1
30	34	304	CLA	CBA-CGA-O2A-C1
33	L	103	SQD	C24-C23-O48-C46
35	L	102	LHG	O10-C23-O8-C6
35	l	102	LHG	O10-C23-O8-C6
30	C	519	CLA	C16-C17-C18-C19
38	j	101	DGD	CDA-CEA-CFA-CGA
30	B	611	CLA	C15-C16-C17-C18
30	b	611	CLA	C15-C16-C17-C18
30	c	513	CLA	O1D-CGD-O2D-CED
30	B	605	CLA	C5-C6-C7-C8
30	W	102	CLA	C15-C16-C17-C18
30	b	605	CLA	C5-C6-C7-C8
30	w	102	CLA	C15-C16-C17-C18
30	38	305	CLA	C10-C11-C12-C13
36	12	301	LMG	O1-C7-C8-O7
38	C	516	DGD	O2G-C2G-C3G-O3G
38	c	517	DGD	O2G-C2G-C3G-O3G
41	21	313	A86	C33-C34-O4-C38
41	41	313	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
35	L	101	LHG	C27-C28-C29-C30
35	d	409	LHG	C27-C28-C29-C30
30	18	305	CLA	C10-C11-C12-C13
30	z	101	CLA	C16-C17-C18-C19
30	C	513	CLA	O1D-CGD-O2D-CED
30	C	506	CLA	C4-C3-C5-C6
30	c	506	CLA	C4-C3-C5-C6
30	B	601	CLA	C11-C10-C8-C7
30	B	610	CLA	C12-C13-C15-C16
30	B	612	CLA	C6-C7-C8-C10
30	B	623	CLA	C11-C10-C8-C7
30	C	503	CLA	C11-C12-C13-C15
30	C	505	CLA	C11-C12-C13-C15
30	C	506	CLA	C2-C3-C5-C6
30	C	513	CLA	C11-C10-C8-C7
30	C	519	CLA	C11-C12-C13-C15
30	C	520	CLA	C11-C10-C8-C7
30	D	402	CLA	C12-C13-C15-C16
30	M	101	CLA	C6-C7-C8-C10
30	b	601	CLA	C11-C10-C8-C7
30	b	610	CLA	C12-C13-C15-C16
30	b	612	CLA	C6-C7-C8-C10
30	b	622	CLA	C11-C10-C8-C7
30	c	503	CLA	C11-C12-C13-C15
30	c	505	CLA	C11-C12-C13-C15
30	c	506	CLA	C2-C3-C5-C6
30	c	513	CLA	C11-C10-C8-C7
30	c	522	CLA	C11-C10-C8-C7
30	d	402	CLA	C12-C13-C15-C16
30	m	101	CLA	C6-C7-C8-C10
30	z	101	CLA	C11-C12-C13-C15
30	11	301	CLA	C11-C10-C8-C7
30	12	305	CLA	C11-C10-C8-C7
30	13	302	CLA	C11-C10-C8-C7
30	14	302	CLA	C11-C10-C8-C7
30	16	302	CLA	C11-C10-C8-C7
30	17	308	CLA	C6-C7-C8-C10
30	18	301	CLA	C12-C13-C15-C16
30	18	303	CLA	C12-C13-C15-C16
30	18	305	CLA	C6-C7-C8-C10
30	19	303	CLA	C11-C12-C13-C15
30	20	204	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	20	209	CLA	C11-C10-C8-C7
30	21	303	CLA	C11-C10-C8-C7
30	21	303	CLA	C11-C12-C13-C15
30	21	307	CLA	C12-C13-C15-C16
30	31	301	CLA	C11-C10-C8-C7
30	32	305	CLA	C11-C10-C8-C7
30	33	303	CLA	C11-C10-C8-C7
30	34	302	CLA	C11-C10-C8-C7
30	36	302	CLA	C11-C10-C8-C7
30	37	308	CLA	C6-C7-C8-C10
30	38	301	CLA	C12-C13-C15-C16
30	38	303	CLA	C12-C13-C15-C16
30	38	305	CLA	C6-C7-C8-C10
30	39	303	CLA	C11-C12-C13-C15
30	40	204	CLA	C12-C13-C15-C16
30	40	209	CLA	C11-C10-C8-C7
30	41	303	CLA	C11-C10-C8-C7
30	41	303	CLA	C11-C12-C13-C15
30	41	307	CLA	C12-C13-C15-C16
30	16	301	CLA	C3-C5-C6-C7
30	36	301	CLA	C3-C5-C6-C7
36	B	620	LMG	C21-C22-C23-C24
36	b	619	LMG	C21-C22-C23-C24
30	B	605	CLA	C11-C12-C13-C14
30	B	606	CLA	C11-C10-C8-C9
30	B	607	CLA	C14-C13-C15-C16
30	B	610	CLA	C14-C13-C15-C16
30	B	623	CLA	C6-C7-C8-C9
30	B	623	CLA	C11-C10-C8-C9
30	C	505	CLA	C11-C12-C13-C14
30	C	506	CLA	C14-C13-C15-C16
30	C	507	CLA	C11-C12-C13-C14
30	C	508	CLA	C11-C10-C8-C9
30	C	513	CLA	C11-C10-C8-C9
30	C	519	CLA	C6-C7-C8-C9
30	Z	102	CLA	C6-C7-C8-C9
30	Z	102	CLA	C11-C12-C13-C14
30	W	103	CLA	C11-C12-C13-C14
30	W	103	CLA	C14-C13-C15-C16
30	b	605	CLA	C11-C12-C13-C14
30	b	606	CLA	C11-C10-C8-C9
30	b	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	b	622	CLA	C6-C7-C8-C9
30	b	622	CLA	C11-C10-C8-C9
30	c	505	CLA	C11-C12-C13-C14
30	c	506	CLA	C14-C13-C15-C16
30	c	508	CLA	C11-C10-C8-C9
30	c	513	CLA	C11-C10-C8-C9
30	c	524	CLA	C6-C7-C8-C9
30	c	524	CLA	C11-C12-C13-C14
30	z	101	CLA	C6-C7-C8-C9
30	w	103	CLA	C11-C12-C13-C14
30	w	103	CLA	C14-C13-C15-C16
30	11	301	CLA	C11-C10-C8-C9
30	12	305	CLA	C11-C10-C8-C9
30	13	302	CLA	C11-C10-C8-C9
30	14	302	CLA	C11-C10-C8-C9
30	16	304	CLA	C6-C7-C8-C9
30	17	301	CLA	C14-C13-C15-C16
30	17	308	CLA	C6-C7-C8-C9
30	18	301	CLA	C14-C13-C15-C16
30	18	303	CLA	C14-C13-C15-C16
30	18	305	CLA	C6-C7-C8-C9
30	18	310	CLA	C14-C13-C15-C16
30	19	301	CLA	C11-C10-C8-C9
30	19	303	CLA	C14-C13-C15-C16
30	21	303	CLA	C11-C10-C8-C9
30	31	301	CLA	C11-C10-C8-C9
30	32	305	CLA	C11-C10-C8-C9
30	33	303	CLA	C11-C10-C8-C9
30	34	302	CLA	C11-C10-C8-C9
30	36	304	CLA	C6-C7-C8-C9
30	37	301	CLA	C14-C13-C15-C16
30	37	308	CLA	C6-C7-C8-C9
30	38	301	CLA	C14-C13-C15-C16
30	38	303	CLA	C14-C13-C15-C16
30	38	305	CLA	C6-C7-C8-C9
30	38	310	CLA	C14-C13-C15-C16
30	39	301	CLA	C11-C10-C8-C9
30	39	303	CLA	C14-C13-C15-C16
30	40	204	CLA	C14-C13-C15-C16
30	41	303	CLA	C11-C10-C8-C9
30	11	303	CLA	CBA-CGA-O2A-C1
30	11	315	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	12	303	CLA	CBA-CGA-O2A-C1
30	12	307	CLA	CBA-CGA-O2A-C1
30	12	312	CLA	CBA-CGA-O2A-C1
30	13	304	CLA	CBA-CGA-O2A-C1
30	14	301	CLA	CBA-CGA-O2A-C1
30	14	304	CLA	CBA-CGA-O2A-C1
35	A	408	LHG	C32-C33-C34-C35
35	a	407	LHG	C32-C33-C34-C35
38	h	102	DGD	C5A-C6A-C7A-C8A
32	B	618	BCR	C7-C8-C9-C34
32	b	617	BCR	C7-C8-C9-C34
41	11	316	A86	C7-C6-C8-C9
41	12	304	A86	C7-C6-C8-C9
41	13	301	A86	C7-C6-C8-C9
41	13	316	A86	C7-C6-C8-C9
41	15	315	A86	C7-C6-C8-C9
41	15	316	A86	C7-C6-C8-C9
41	18	302	A86	C7-C6-C8-C9
41	20	201	A86	C-C1-C24-C25
41	20	212	A86	C7-C6-C8-C9
41	21	310	A86	C-C1-C24-C25
41	31	316	A86	C7-C6-C8-C9
41	32	304	A86	C7-C6-C8-C9
41	33	302	A86	C7-C6-C8-C9
41	33	316	A86	C7-C6-C8-C9
41	35	315	A86	C7-C6-C8-C9
41	35	316	A86	C7-C6-C8-C9
41	38	302	A86	C7-C6-C8-C9
41	40	201	A86	C-C1-C24-C25
41	40	212	A86	C7-C6-C8-C9
41	41	310	A86	C-C1-C24-C25
36	m	102	LMG	C16-C17-C18-C19
38	H	102	DGD	C5A-C6A-C7A-C8A
32	A	405	BCR	C11-C12-C13-C14
32	H	101	BCR	C21-C22-C23-C24
32	a	404	BCR	C11-C12-C13-C14
32	h	101	BCR	C21-C22-C23-C24
41	11	314	A86	C2-C1-C24-C25
41	12	319	A86	C2-C1-C24-C25
41	13	315	A86	C2-C1-C24-C25
41	13	317	A86	C2-C1-C24-C25
41	15	314	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
41	16	313	A86	C2-C1-C24-C25
41	17	316	A86	C2-C1-C24-C25
41	20	212	A86	C5-C6-C8-C9
41	21	310	A86	C2-C1-C24-C25
41	31	314	A86	C2-C1-C24-C25
41	32	318	A86	C2-C1-C24-C25
41	32	319	A86	C2-C1-C24-C25
41	33	317	A86	C2-C1-C24-C25
41	35	314	A86	C2-C1-C24-C25
41	36	313	A86	C2-C1-C24-C25
41	37	316	A86	C2-C1-C24-C25
41	40	212	A86	C5-C6-C8-C9
41	41	310	A86	C2-C1-C24-C25
36	M	102	LMG	C16-C17-C18-C19
30	B	608	CLA	C13-C15-C16-C17
30	b	608	CLA	C13-C15-C16-C17
38	C	517	DGD	C5A-C6A-C7A-C8A
38	H	102	DGD	CCB-CDB-CEB-CFB
38	c	518	DGD	C5A-C6A-C7A-C8A
30	17	301	CLA	CBA-CGA-O2A-C1
30	37	301	CLA	CBA-CGA-O2A-C1
36	M	102	LMG	C29-C28-O8-C9
36	m	102	LMG	C29-C28-O8-C9
38	h	102	DGD	CCB-CDB-CEB-CFB
30	C	519	CLA	C16-C17-C18-C20
30	z	101	CLA	C16-C17-C18-C20
30	c	513	CLA	C13-C15-C16-C17
35	L	101	LHG	O6-C4-C5-C6
35	d	409	LHG	O6-C4-C5-C6
35	B	622	LHG	C32-C33-C34-C35
35	L	102	LHG	C30-C31-C32-C33
35	b	621	LHG	C32-C33-C34-C35
35	l	102	LHG	C30-C31-C32-C33
36	D	408	LMG	C20-C21-C22-C23
38	C	516	DGD	C5A-C6A-C7A-C8A
38	c	517	DGD	C5A-C6A-C7A-C8A
38	c	518	DGD	C4A-C5A-C6A-C7A
30	40	203	CLA	O1D-CGD-O2D-CED
36	B	619	LMG	C13-C14-C15-C16
36	b	618	LMG	C13-C14-C15-C16
36	d	410	LMG	C20-C21-C22-C23
38	C	517	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
30	B	606	CLA	C13-C15-C16-C17
30	C	513	CLA	C13-C15-C16-C17
30	b	606	CLA	C13-C15-C16-C17
30	20	203	CLA	O1D-CGD-O2D-CED
36	B	619	LMG	C36-C37-C38-C39
36	Q	301	LMG	C29-C30-C31-C32
30	B	611	CLA	CBA-CGA-O2A-C1
30	b	611	CLA	CBA-CGA-O2A-C1
36	b	618	LMG	C36-C37-C38-C39
30	31	306	CLA	O1D-CGD-O2D-CED
30	B	601	CLA	C3A-C2A-CAA-CBA
30	C	513	CLA	C3A-C2A-CAA-CBA
30	b	601	CLA	C3A-C2A-CAA-CBA
30	b	622	CLA	C3A-C2A-CAA-CBA
30	c	513	CLA	C3A-C2A-CAA-CBA
30	15	305	CLA	C3A-C2A-CAA-CBA
30	21	301	CLA	C3A-C2A-CAA-CBA
30	35	305	CLA	C3A-C2A-CAA-CBA
30	41	301	CLA	C3A-C2A-CAA-CBA
40	e	101	HEM	C2A-CAA-CBA-CGA
30	17	305	CLA	C10-C11-C12-C13
36	c	519	LMG	C29-C30-C31-C32
30	38	301	CLA	O1D-CGD-O2D-CED
41	11	310	A86	O-C13-C14-C15
41	11	312	A86	O-C13-C14-C15
41	12	315	A86	O-C13-C14-C15
41	12	317	A86	O-C13-C14-C15
41	13	311	A86	O-C13-C14-C15
41	13	313	A86	O-C13-C14-C15
41	14	311	A86	O-C13-C14-C15
41	14	313	A86	O-C13-C14-C15
41	15	310	A86	O-C13-C14-C15
41	15	312	A86	O-C13-C14-C15
41	16	312	A86	O-C13-C14-C15
41	17	302	A86	O-C13-C14-C15
41	17	313	A86	O-C13-C14-C15
41	18	313	A86	O-C13-C14-C15
41	19	309	A86	O-C13-C14-C15
41	20	213	A86	O-C13-C14-C15
41	21	310	A86	O-C13-C14-C15
41	21	314	A86	O-C13-C14-C15
41	31	310	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
41	31	312	A86	O-C13-C14-C15
41	32	314	A86	O-C13-C14-C15
41	32	316	A86	O-C13-C14-C15
41	33	312	A86	O-C13-C14-C15
41	33	314	A86	O-C13-C14-C15
41	34	311	A86	O-C13-C14-C15
41	34	313	A86	O-C13-C14-C15
41	35	310	A86	O-C13-C14-C15
41	35	312	A86	O-C13-C14-C15
41	36	312	A86	O-C13-C14-C15
41	37	313	A86	O-C13-C14-C15
41	38	313	A86	O-C13-C14-C15
41	39	309	A86	O-C13-C14-C15
41	40	213	A86	O-C13-C14-C15
41	41	310	A86	O-C13-C14-C15
41	41	314	A86	O-C13-C14-C15
35	A	408	LHG	C12-C13-C14-C15
35	a	407	LHG	C12-C13-C14-C15
30	37	305	CLA	C10-C11-C12-C13
30	31	315	CLA	CBA-CGA-O2A-C1
30	32	303	CLA	CBA-CGA-O2A-C1
30	33	301	CLA	CBA-CGA-O2A-C1
30	34	301	CLA	CBA-CGA-O2A-C1
33	l	101	SQD	C25-C26-C27-C28
30	17	308	CLA	C13-C15-C16-C17
30	37	308	CLA	C13-C15-C16-C17
30	18	301	CLA	O1D-CGD-O2D-CED
30	34	307	CLA	O1D-CGD-O2D-CED
33	B	621	SQD	C44-C45-C46-O48
33	L	103	SQD	C44-C45-C46-O48
33	b	620	SQD	C44-C45-C46-O48
33	l	101	SQD	C44-C45-C46-O48
36	Q	301	LMG	O1-C7-C8-C9
36	c	519	LMG	O1-C7-C8-C9
38	C	516	DGD	C1G-C2G-C3G-O3G
38	c	517	DGD	C1G-C2G-C3G-O3G
30	38	307	CLA	CBD-CGD-O2D-CED
33	L	103	SQD	C25-C26-C27-C28
33	a	405	SQD	C28-C29-C30-C31
35	L	102	LHG	C9-C10-C11-C12
35	l	102	LHG	C9-C10-C11-C12
36	w	101	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
39	D	407	PL9	C32-C33-C34-C36
39	d	408	PL9	C32-C33-C34-C36
30	32	307	CLA	O1A-CGA-O2A-C1
30	34	304	CLA	O1A-CGA-O2A-C1
33	A	406	SQD	C28-C29-C30-C31
36	D	408	LMG	C34-C35-C36-C37
36	W	101	LMG	C32-C33-C34-C35
36	d	410	LMG	C34-C35-C36-C37
30	33	308	CLA	O1D-CGD-O2D-CED
30	31	303	CLA	O1A-CGA-O2A-C1
30	33	305	CLA	O1A-CGA-O2A-C1
30	B	609	CLA	C5-C6-C7-C8
30	c	505	CLA	O1D-CGD-O2D-CED
30	32	310	CLA	O1D-CGD-O2D-CED
30	W	102	CLA	O1D-CGD-O2D-CED
30	b	609	CLA	C5-C6-C7-C8
36	Q	301	LMG	C28-C29-C30-C31
36	c	519	LMG	C28-C29-C30-C31
30	C	502	CLA	O1A-CGA-O2A-C1
30	c	502	CLA	O1A-CGA-O2A-C1
30	11	303	CLA	O1A-CGA-O2A-C1
30	12	307	CLA	O1A-CGA-O2A-C1
30	13	304	CLA	O1A-CGA-O2A-C1
30	14	304	CLA	O1A-CGA-O2A-C1
30	C	505	CLA	O1D-CGD-O2D-CED
30	w	102	CLA	O1D-CGD-O2D-CED
35	B	622	LHG	O6-C4-C5-O7
35	L	101	LHG	O6-C4-C5-O7
35	b	621	LHG	O6-C4-C5-O7
35	d	409	LHG	O6-C4-C5-O7
30	18	307	CLA	CBD-CGD-O2D-CED
38	h	102	DGD	C6A-C7A-C8A-C9A
35	l	102	LHG	C29-C30-C31-C32
36	b	619	LMG	C19-C20-C21-C22
38	H	102	DGD	C6A-C7A-C8A-C9A
30	41	305	CLA	O1D-CGD-O2D-CED
36	B	620	LMG	C19-C20-C21-C22
36	W	101	LMG	C22-C23-C24-C25
36	w	101	LMG	C22-C23-C24-C25
30	12	303	CLA	O1A-CGA-O2A-C1
30	12	312	CLA	O1A-CGA-O2A-C1
30	14	301	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
35	L	102	LHG	C29-C30-C31-C32
33	L	103	SQD	O47-C45-C46-O48
33	l	101	SQD	O47-C45-C46-O48
35	A	408	LHG	O7-C5-C6-O8
35	a	407	LHG	O7-C5-C6-O8
36	D	408	LMG	O1-C7-C8-O7
36	d	410	LMG	O1-C7-C8-O7
30	B	605	CLA	CBD-CGD-O2D-CED
30	C	514	CLA	CBA-CGA-O2A-C1
30	c	514	CLA	CBA-CGA-O2A-C1
30	21	305	CLA	O1D-CGD-O2D-CED
41	17	302	A86	C11-C10-C9-C8
41	17	315	A86	C11-C10-C9-C8
41	17	315	A86	C24-C25-C26-C27
41	19	310	A86	C3-C4-C5-C6
41	37	302	A86	C11-C10-C9-C8
41	37	315	A86	C11-C10-C9-C8
41	37	315	A86	C24-C25-C26-C27
41	39	310	A86	C3-C4-C5-C6
36	Q	301	LMG	C11-C10-O7-C8
41	11	313	A86	C10-C11-C13-C14
41	12	318	A86	C10-C11-C13-C14
41	13	314	A86	C10-C11-C13-C14
41	14	314	A86	C10-C11-C13-C14
41	15	313	A86	C10-C11-C13-C14
41	17	302	A86	C10-C11-C13-C14
41	17	314	A86	C10-C11-C13-C14
41	18	315	A86	C10-C11-C13-C14
41	31	313	A86	C10-C11-C13-C14
41	32	317	A86	C10-C11-C13-C14
41	33	315	A86	C10-C11-C13-C14
41	34	314	A86	C10-C11-C13-C14
41	35	313	A86	C10-C11-C13-C14
41	37	302	A86	C10-C11-C13-C14
41	37	314	A86	C10-C11-C13-C14
41	38	315	A86	C10-C11-C13-C14
30	A	402	CLA	C2-C1-O2A-CGA
30	B	615	CLA	C2-C1-O2A-CGA
30	a	402	CLA	C2-C1-O2A-CGA
30	b	615	CLA	C2-C1-O2A-CGA
30	18	303	CLA	C2-C1-O2A-CGA
30	21	301	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
30	38	303	CLA	C2-C1-O2A-CGA
30	41	301	CLA	C2-C1-O2A-CGA
30	11	315	CLA	O1A-CGA-O2A-C1
30	17	301	CLA	O1A-CGA-O2A-C1
30	B	613	CLA	C8-C10-C11-C12
30	b	613	CLA	C8-C10-C11-C12
30	A	404	CLA	C11-C10-C8-C9
30	B	605	CLA	C6-C7-C8-C9
30	C	514	CLA	C14-C13-C15-C16
30	C	521	CLA	C11-C10-C8-C9
30	D	402	CLA	C11-C10-C8-C9
30	D	402	CLA	C14-C13-C15-C16
30	a	403	CLA	C11-C10-C8-C9
30	b	605	CLA	C6-C7-C8-C9
30	c	507	CLA	C11-C12-C13-C14
30	c	514	CLA	C14-C13-C15-C16
30	c	523	CLA	C11-C10-C8-C9
30	d	402	CLA	C11-C10-C8-C9
30	d	402	CLA	C14-C13-C15-C16
30	11	303	CLA	C11-C12-C13-C14
30	11	315	CLA	C14-C13-C15-C16
30	12	303	CLA	C14-C13-C15-C16
30	12	307	CLA	C11-C12-C13-C14
30	12	312	CLA	C14-C13-C15-C16
30	13	304	CLA	C11-C12-C13-C14
30	14	301	CLA	C14-C13-C15-C16
30	14	304	CLA	C11-C12-C13-C14
30	18	303	CLA	C11-C10-C8-C9
30	18	309	CLA	C11-C10-C8-C9
30	20	202	CLA	C11-C10-C8-C9
30	21	303	CLA	C11-C12-C13-C14
30	31	315	CLA	C14-C13-C15-C16
30	32	303	CLA	C14-C13-C15-C16
30	33	301	CLA	C14-C13-C15-C16
30	34	301	CLA	C14-C13-C15-C16
30	38	303	CLA	C11-C10-C8-C9
30	38	309	CLA	C11-C10-C8-C9
30	40	202	CLA	C11-C10-C8-C9
30	41	303	CLA	C11-C12-C13-C14
35	L	102	LHG	C10-C11-C12-C13
30	b	605	CLA	CBD-CGD-O2D-CED
35	l	102	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	b	618	LMG	C38-C39-C40-C41
30	37	301	CLA	O1A-CGA-O2A-C1
35	L	101	LHG	C17-C18-C19-C20
36	B	619	LMG	C38-C39-C40-C41
36	D	408	LMG	C39-C40-C41-C42
36	Q	301	LMG	C30-C31-C32-C33
30	11	302	CLA	C2A-CAA-CBA-CGA
30	12	306	CLA	C2A-CAA-CBA-CGA
30	13	303	CLA	C2A-CAA-CBA-CGA
30	14	303	CLA	C2A-CAA-CBA-CGA
30	31	302	CLA	C2A-CAA-CBA-CGA
30	32	306	CLA	C2A-CAA-CBA-CGA
30	32	308	CLA	C2A-CAA-CBA-CGA
30	33	304	CLA	C2A-CAA-CBA-CGA
30	33	306	CLA	C2A-CAA-CBA-CGA
30	34	303	CLA	C2A-CAA-CBA-CGA
30	34	305	CLA	C2A-CAA-CBA-CGA
30	D	402	CLA	C16-C17-C18-C19
30	d	402	CLA	C16-C17-C18-C19
30	21	306	CLA	C16-C17-C18-C19
30	41	306	CLA	C16-C17-C18-C19
32	A	405	BCR	C23-C24-C25-C26
32	A	405	BCR	C23-C24-C25-C30
32	A	409	BCR	C23-C24-C25-C26
32	A	409	BCR	C23-C24-C25-C30
32	B	617	BCR	C23-C24-C25-C26
32	B	618	BCR	C23-C24-C25-C26
32	F	101	BCR	C23-C24-C25-C26
32	F	101	BCR	C23-C24-C25-C30
32	H	101	BCR	C23-C24-C25-C26
32	Y	101	BCR	C1-C6-C7-C8
32	Y	101	BCR	C23-C24-C25-C26
32	Y	101	BCR	C23-C24-C25-C30
32	a	404	BCR	C23-C24-C25-C26
32	a	404	BCR	C23-C24-C25-C30
32	a	408	BCR	C23-C24-C25-C26
32	a	408	BCR	C23-C24-C25-C30
32	b	616	BCR	C23-C24-C25-C26
32	b	617	BCR	C23-C24-C25-C26
32	c	520	BCR	C1-C6-C7-C8
32	c	520	BCR	C23-C24-C25-C26
32	c	520	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
32	f	101	BCR	C23-C24-C25-C26
32	f	101	BCR	C23-C24-C25-C30
32	h	101	BCR	C23-C24-C25-C26
30	33	305	CLA	C10-C11-C12-C13
30	34	304	CLA	C10-C11-C12-C13
35	d	409	LHG	C17-C18-C19-C20
36	d	410	LMG	C39-C40-C41-C42
38	h	102	DGD	C3B-C4B-C5B-C6B
38	C	517	DGD	C4E-C5E-C6E-O5E
38	c	518	DGD	C4E-C5E-C6E-O5E
36	B	620	LMG	C17-C18-C19-C20
36	b	619	LMG	C17-C18-C19-C20
36	c	519	LMG	C30-C31-C32-C33
38	H	102	DGD	C3B-C4B-C5B-C6B
30	21	303	CLA	O1D-CGD-O2D-CED
30	41	303	CLA	O1D-CGD-O2D-CED
41	20	201	A86	C2-C1-C24-C25
41	20	201	A86	C33-C34-O4-C38
41	40	201	A86	C2-C1-C24-C25
30	31	303	CLA	C10-C11-C12-C13
30	32	307	CLA	C10-C11-C12-C13
38	c	517	DGD	C6B-C7B-C8B-C9B
35	A	408	LHG	C8-C7-O7-C5
35	a	407	LHG	C8-C7-O7-C5
36	c	519	LMG	C11-C10-O7-C8
38	C	516	DGD	C6B-C7B-C8B-C9B
38	C	516	DGD	C9A-CAA-CBA-CCA
30	B	613	CLA	CBD-CGD-O2D-CED
30	17	303	CLA	C8-C10-C11-C12
30	37	303	CLA	C8-C10-C11-C12
36	12	301	LMG	C13-C14-C15-C16
36	c	519	LMG	C33-C34-C35-C36
38	c	517	DGD	C9A-CAA-CBA-CCA
35	L	102	LHG	O6-C4-C5-C6
35	l	102	LHG	O6-C4-C5-C6
36	Q	301	LMG	C33-C34-C35-C36
36	32	301	LMG	C11-C12-C13-C14
30	B	605	CLA	C11-C12-C13-C15
30	B	606	CLA	C11-C10-C8-C7
30	B	607	CLA	C12-C13-C15-C16
30	B	612	CLA	C11-C10-C8-C7
30	B	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	B	623	CLA	C6-C7-C8-C10
30	C	506	CLA	C12-C13-C15-C16
30	C	507	CLA	C11-C12-C13-C15
30	C	508	CLA	C12-C13-C15-C16
30	C	510	CLA	C12-C13-C15-C16
30	C	514	CLA	C12-C13-C15-C16
30	C	519	CLA	C6-C7-C8-C10
30	C	521	CLA	C11-C10-C8-C7
30	D	402	CLA	C11-C10-C8-C7
30	D	405	CLA	C11-C12-C13-C15
30	Z	102	CLA	C6-C7-C8-C10
30	b	605	CLA	C11-C12-C13-C15
30	b	606	CLA	C11-C10-C8-C7
30	b	607	CLA	C12-C13-C15-C16
30	b	612	CLA	C11-C10-C8-C7
30	b	614	CLA	C11-C10-C8-C7
30	b	622	CLA	C6-C7-C8-C10
30	c	506	CLA	C12-C13-C15-C16
30	c	507	CLA	C11-C12-C13-C15
30	c	508	CLA	C12-C13-C15-C16
30	c	510	CLA	C12-C13-C15-C16
30	c	514	CLA	C12-C13-C15-C16
30	c	523	CLA	C11-C10-C8-C7
30	c	524	CLA	C6-C7-C8-C10
30	d	402	CLA	C11-C10-C8-C7
30	d	406	CLA	C11-C12-C13-C15
30	z	101	CLA	C6-C7-C8-C10
30	11	303	CLA	C11-C12-C13-C15
30	11	307	CLA	C12-C13-C15-C16
30	11	315	CLA	C12-C13-C15-C16
30	12	303	CLA	C12-C13-C15-C16
30	12	307	CLA	C11-C12-C13-C15
30	12	311	CLA	C12-C13-C15-C16
30	12	312	CLA	C12-C13-C15-C16
30	13	304	CLA	C11-C12-C13-C15
30	13	308	CLA	C12-C13-C15-C16
30	14	301	CLA	C12-C13-C15-C16
30	14	304	CLA	C11-C12-C13-C15
30	14	308	CLA	C12-C13-C15-C16
30	15	301	CLA	C11-C10-C8-C7
30	16	301	CLA	C12-C13-C15-C16
30	16	304	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	17	301	CLA	C12-C13-C15-C16
30	18	303	CLA	C11-C10-C8-C7
30	18	309	CLA	C11-C10-C8-C7
30	18	310	CLA	C12-C13-C15-C16
30	19	301	CLA	C11-C10-C8-C7
30	19	303	CLA	C12-C13-C15-C16
30	20	202	CLA	C11-C10-C8-C7
30	20	202	CLA	C12-C13-C15-C16
30	21	301	CLA	C11-C10-C8-C7
30	31	307	CLA	C12-C13-C15-C16
30	31	315	CLA	C12-C13-C15-C16
30	32	303	CLA	C12-C13-C15-C16
30	32	311	CLA	C12-C13-C15-C16
30	33	301	CLA	C12-C13-C15-C16
30	34	301	CLA	C12-C13-C15-C16
30	35	301	CLA	C11-C10-C8-C7
30	36	301	CLA	C12-C13-C15-C16
30	36	304	CLA	C6-C7-C8-C10
30	37	301	CLA	C12-C13-C15-C16
30	38	303	CLA	C11-C10-C8-C7
30	38	309	CLA	C11-C10-C8-C7
30	38	310	CLA	C12-C13-C15-C16
30	39	301	CLA	C11-C10-C8-C7
30	39	303	CLA	C12-C13-C15-C16
30	40	202	CLA	C11-C10-C8-C7
30	40	202	CLA	C12-C13-C15-C16
30	41	301	CLA	C11-C10-C8-C7
36	12	301	LMG	C11-C12-C13-C14
41	11	312	A86	C3-C4-C5-C6
41	11	314	A86	C1-C2-C3-C4
41	12	317	A86	C3-C4-C5-C6
41	12	319	A86	C1-C2-C3-C4
41	13	313	A86	C3-C4-C5-C6
41	13	315	A86	C1-C2-C3-C4
41	13	317	A86	C1-C2-C3-C4
41	14	313	A86	C3-C4-C5-C6
41	15	312	A86	C3-C4-C5-C6
41	15	314	A86	C1-C2-C3-C4
41	16	312	A86	C3-C4-C5-C6
41	16	313	A86	C1-C2-C3-C4
41	17	313	A86	C3-C4-C5-C6
41	17	316	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
41	20	212	A86	C11-C10-C9-C8
41	20	213	A86	C3-C4-C5-C6
41	21	314	A86	C3-C4-C5-C6
41	31	312	A86	C3-C4-C5-C6
41	31	314	A86	C1-C2-C3-C4
41	32	316	A86	C3-C4-C5-C6
41	32	318	A86	C1-C2-C3-C4
41	32	319	A86	C1-C2-C3-C4
41	33	314	A86	C3-C4-C5-C6
41	33	317	A86	C1-C2-C3-C4
41	34	313	A86	C3-C4-C5-C6
41	35	312	A86	C3-C4-C5-C6
41	35	314	A86	C1-C2-C3-C4
41	36	312	A86	C3-C4-C5-C6
41	36	313	A86	C1-C2-C3-C4
41	37	313	A86	C3-C4-C5-C6
41	37	316	A86	C1-C2-C3-C4
41	40	212	A86	C11-C10-C9-C8
41	40	213	A86	C3-C4-C5-C6
41	41	314	A86	C3-C4-C5-C6
30	b	613	CLA	CBD-CGD-O2D-CED
30	17	308	CLA	C16-C17-C18-C20
30	37	308	CLA	C16-C17-C18-C20
41	40	201	A86	C33-C34-O4-C38
30	18	301	CLA	C5-C6-C7-C8
30	38	301	CLA	C5-C6-C7-C8
30	D	405	CLA	C2A-CAA-CBA-CGA
30	d	406	CLA	C2A-CAA-CBA-CGA
30	31	304	CLA	C2A-CAA-CBA-CGA
32	C	515	BCR	C35-C13-C14-C15
32	c	516	BCR	C35-C13-C14-C15
38	J	101	DGD	C4A-C5A-C6A-C7A
38	C	517	DGD	C1B-C2B-C3B-C4B
38	c	518	DGD	C1B-C2B-C3B-C4B
35	B	622	LHG	C34-C35-C36-C37
35	b	621	LHG	C34-C35-C36-C37
38	j	101	DGD	C4A-C5A-C6A-C7A
30	A	402	CLA	C13-C15-C16-C17
30	B	604	CLA	CBA-CGA-O2A-C1
30	C	503	CLA	CBA-CGA-O2A-C1
30	b	604	CLA	CBA-CGA-O2A-C1
30	c	503	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
40	E	101	HEM	C2A-CAA-CBA-CGA
30	D	401	CLA	C10-C11-C12-C13
30	a	402	CLA	C13-C15-C16-C17
30	d	401	CLA	C10-C11-C12-C13
30	B	601	CLA	CAD-CBD-CGD-O2D
30	B	613	CLA	CAD-CBD-CGD-O2D
30	C	513	CLA	CAD-CBD-CGD-O2D
30	C	514	CLA	CAD-CBD-CGD-O2D
30	W	102	CLA	CAD-CBD-CGD-O2D
30	W	103	CLA	CAD-CBD-CGD-O2D
30	b	601	CLA	CAD-CBD-CGD-O2D
30	b	613	CLA	CAD-CBD-CGD-O2D
30	c	513	CLA	CAD-CBD-CGD-O2D
30	c	514	CLA	CAD-CBD-CGD-O2D
30	w	102	CLA	CAD-CBD-CGD-O2D
30	w	103	CLA	CAD-CBD-CGD-O2D
30	11	306	CLA	CAD-CBD-CGD-O2D
30	12	310	CLA	CAD-CBD-CGD-O2D
30	13	307	CLA	CAD-CBD-CGD-O2D
30	14	307	CLA	CAD-CBD-CGD-O2D
30	17	307	CLA	CAD-CBD-CGD-O2D
30	18	304	CLA	CAD-CBD-CGD-O2D
30	18	308	CLA	CAD-CBD-CGD-O2D
30	19	305	CLA	CAD-CBD-CGD-O2D
30	21	306	CLA	CAD-CBD-CGD-O2D
30	31	306	CLA	CAD-CBD-CGD-O2D
30	32	310	CLA	CAD-CBD-CGD-O2D
30	33	308	CLA	CAD-CBD-CGD-O2D
30	34	307	CLA	CAD-CBD-CGD-O2D
30	37	307	CLA	CAD-CBD-CGD-O2D
30	38	304	CLA	CAD-CBD-CGD-O2D
30	38	308	CLA	CAD-CBD-CGD-O2D
30	39	305	CLA	CAD-CBD-CGD-O2D
30	41	306	CLA	CAD-CBD-CGD-O2D
31	A	403	PHO	CAD-CBD-CGD-O2D
31	d	403	PHO	CAD-CBD-CGD-O2D
41	21	312	A86	C28-C27-C29-C30
41	41	312	A86	C28-C27-C29-C30
30	C	509	CLA	C13-C15-C16-C17
30	D	402	CLA	C13-C15-C16-C17
30	d	402	CLA	C13-C15-C16-C17
32	B	617	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	B	618	BCR	C22-C23-C24-C25
32	b	616	BCR	C6-C7-C8-C9
32	b	617	BCR	C22-C23-C24-C25
30	C	504	CLA	C4-C3-C5-C6
30	c	504	CLA	C4-C3-C5-C6
38	J	101	DGD	O6D-C1D-O3G-C3G
38	j	101	DGD	O6D-C1D-O3G-C3G
30	c	509	CLA	C13-C15-C16-C17
36	B	620	LMG	O1-C7-C8-C9
36	b	619	LMG	O1-C7-C8-C9
36	32	301	LMG	O1-C7-C8-C9
41	11	316	A86	C12-C11-C13-O
41	12	304	A86	C12-C11-C13-O
41	13	301	A86	C12-C11-C13-O
41	13	316	A86	C12-C11-C13-O
41	15	315	A86	C12-C11-C13-O
41	15	316	A86	C12-C11-C13-O
41	16	310	A86	C12-C11-C13-O
41	17	311	A86	C12-C11-C13-O
41	18	302	A86	C12-C11-C13-O
41	19	310	A86	C12-C11-C13-O
41	31	316	A86	C12-C11-C13-O
41	32	304	A86	C12-C11-C13-O
41	33	302	A86	C12-C11-C13-O
41	33	316	A86	C12-C11-C13-O
41	35	315	A86	C12-C11-C13-O
41	35	316	A86	C12-C11-C13-O
41	36	310	A86	C12-C11-C13-O
41	37	311	A86	C12-C11-C13-O
41	38	302	A86	C12-C11-C13-O
41	39	310	A86	C12-C11-C13-O
30	31	315	CLA	O1A-CGA-O2A-C1
30	32	303	CLA	O1A-CGA-O2A-C1
30	33	301	CLA	O1A-CGA-O2A-C1
30	34	301	CLA	O1A-CGA-O2A-C1
38	c	518	DGD	O1A-C1A-O1G-C1G
30	18	303	CLA	C2A-CAA-CBA-CGA
30	38	303	CLA	C2A-CAA-CBA-CGA
35	L	102	LHG	C33-C34-C35-C36
35	l	102	LHG	C33-C34-C35-C36
30	C	507	CLA	C16-C17-C18-C19
30	D	402	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	c	507	CLA	C16-C17-C18-C19
30	d	402	CLA	C16-C17-C18-C20
30	B	609	CLA	CHA-CBD-CGD-O1D
30	B	609	CLA	CHA-CBD-CGD-O2D
30	B	610	CLA	CHA-CBD-CGD-O1D
30	B	612	CLA	CHA-CBD-CGD-O1D
30	B	612	CLA	CHA-CBD-CGD-O2D
30	B	615	CLA	CHA-CBD-CGD-O1D
30	C	503	CLA	CHA-CBD-CGD-O1D
30	C	503	CLA	CHA-CBD-CGD-O2D
30	C	507	CLA	CHA-CBD-CGD-O1D
30	C	508	CLA	CHA-CBD-CGD-O1D
30	C	509	CLA	CHA-CBD-CGD-O1D
30	C	509	CLA	CHA-CBD-CGD-O2D
30	C	510	CLA	CHA-CBD-CGD-O1D
30	C	510	CLA	CHA-CBD-CGD-O2D
30	C	512	CLA	CHA-CBD-CGD-O2D
30	b	609	CLA	CHA-CBD-CGD-O1D
30	b	609	CLA	CHA-CBD-CGD-O2D
30	b	610	CLA	CHA-CBD-CGD-O1D
30	b	612	CLA	CHA-CBD-CGD-O1D
30	b	612	CLA	CHA-CBD-CGD-O2D
30	b	615	CLA	CHA-CBD-CGD-O1D
30	c	503	CLA	CHA-CBD-CGD-O1D
30	c	503	CLA	CHA-CBD-CGD-O2D
30	c	507	CLA	CHA-CBD-CGD-O1D
30	c	508	CLA	CHA-CBD-CGD-O1D
30	c	509	CLA	CHA-CBD-CGD-O1D
30	c	509	CLA	CHA-CBD-CGD-O2D
30	c	510	CLA	CHA-CBD-CGD-O1D
30	c	510	CLA	CHA-CBD-CGD-O2D
30	c	512	CLA	CHA-CBD-CGD-O2D
30	11	303	CLA	CHA-CBD-CGD-O1D
30	11	303	CLA	CHA-CBD-CGD-O2D
30	11	305	CLA	CHA-CBD-CGD-O2D
30	11	308	CLA	CHA-CBD-CGD-O1D
30	11	308	CLA	CHA-CBD-CGD-O2D
30	12	307	CLA	CHA-CBD-CGD-O1D
30	12	307	CLA	CHA-CBD-CGD-O2D
30	12	309	CLA	CHA-CBD-CGD-O2D
30	12	313	CLA	CHA-CBD-CGD-O1D
30	12	313	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	13	304	CLA	CHA-CBD-CGD-O1D
30	13	304	CLA	CHA-CBD-CGD-O2D
30	13	306	CLA	CHA-CBD-CGD-O2D
30	13	309	CLA	CHA-CBD-CGD-O1D
30	13	309	CLA	CHA-CBD-CGD-O2D
30	14	304	CLA	CHA-CBD-CGD-O1D
30	14	304	CLA	CHA-CBD-CGD-O2D
30	14	306	CLA	CHA-CBD-CGD-O2D
30	14	309	CLA	CHA-CBD-CGD-O1D
30	14	309	CLA	CHA-CBD-CGD-O2D
30	15	305	CLA	CHA-CBD-CGD-O1D
30	15	308	CLA	CHA-CBD-CGD-O1D
30	15	308	CLA	CHA-CBD-CGD-O2D
30	16	308	CLA	CHA-CBD-CGD-O1D
30	16	308	CLA	CHA-CBD-CGD-O2D
30	17	309	CLA	CHA-CBD-CGD-O1D
30	17	310	CLA	CHA-CBD-CGD-O1D
30	18	309	CLA	CHA-CBD-CGD-O1D
30	19	303	CLA	CHA-CBD-CGD-O1D
30	19	303	CLA	CHA-CBD-CGD-O2D
30	21	303	CLA	CHA-CBD-CGD-O1D
30	31	303	CLA	CHA-CBD-CGD-O1D
30	31	303	CLA	CHA-CBD-CGD-O2D
30	31	305	CLA	CHA-CBD-CGD-O2D
30	31	307	CLA	CHA-CBD-CGD-O1D
30	31	308	CLA	CHA-CBD-CGD-O1D
30	31	308	CLA	CHA-CBD-CGD-O2D
30	32	307	CLA	CHA-CBD-CGD-O1D
30	32	307	CLA	CHA-CBD-CGD-O2D
30	32	309	CLA	CHA-CBD-CGD-O2D
30	32	311	CLA	CHA-CBD-CGD-O1D
30	32	312	CLA	CHA-CBD-CGD-O1D
30	32	312	CLA	CHA-CBD-CGD-O2D
30	33	305	CLA	CHA-CBD-CGD-O1D
30	33	305	CLA	CHA-CBD-CGD-O2D
30	33	307	CLA	CHA-CBD-CGD-O2D
30	33	309	CLA	CHA-CBD-CGD-O1D
30	33	310	CLA	CHA-CBD-CGD-O1D
30	33	310	CLA	CHA-CBD-CGD-O2D
30	34	304	CLA	CHA-CBD-CGD-O1D
30	34	304	CLA	CHA-CBD-CGD-O2D
30	34	306	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	34	308	CLA	CHA-CBD-CGD-O1D
30	34	309	CLA	CHA-CBD-CGD-O1D
30	34	309	CLA	CHA-CBD-CGD-O2D
30	35	305	CLA	CHA-CBD-CGD-O1D
30	35	308	CLA	CHA-CBD-CGD-O1D
30	35	308	CLA	CHA-CBD-CGD-O2D
30	36	308	CLA	CHA-CBD-CGD-O1D
30	36	308	CLA	CHA-CBD-CGD-O2D
30	37	309	CLA	CHA-CBD-CGD-O1D
30	37	310	CLA	CHA-CBD-CGD-O1D
30	38	309	CLA	CHA-CBD-CGD-O1D
30	39	303	CLA	CHA-CBD-CGD-O1D
30	39	303	CLA	CHA-CBD-CGD-O2D
30	41	303	CLA	CHA-CBD-CGD-O1D
30	c	510	CLA	C5-C6-C7-C8
30	B	611	CLA	O1A-CGA-O2A-C1
30	b	611	CLA	O1A-CGA-O2A-C1
38	C	517	DGD	O1A-C1A-O1G-C1G
32	A	409	BCR	C11-C10-C9-C8
32	a	408	BCR	C11-C10-C9-C8
35	L	102	LHG	C27-C28-C29-C30
33	A	406	SQD	O6-C44-C45-O47
33	a	405	SQD	O6-C44-C45-O47
36	B	620	LMG	O1-C7-C8-O7
36	Q	301	LMG	O1-C7-C8-O7
36	W	101	LMG	O7-C8-C9-O8
36	b	619	LMG	O1-C7-C8-O7
36	c	519	LMG	O1-C7-C8-O7
36	w	101	LMG	O7-C8-C9-O8
36	32	301	LMG	O1-C7-C8-O7
30	18	301	CLA	CBA-CGA-O2A-C1
30	38	301	CLA	CBA-CGA-O2A-C1
35	l	102	LHG	C27-C28-C29-C30
36	B	619	LMG	C12-C13-C14-C15
36	b	618	LMG	C12-C13-C14-C15
30	C	510	CLA	C5-C6-C7-C8
30	11	301	CLA	C5-C6-C7-C8
30	14	302	CLA	C5-C6-C7-C8
30	C	514	CLA	O1A-CGA-O2A-C1
30	c	514	CLA	O1A-CGA-O2A-C1
31	D	403	PHO	C16-C17-C18-C20
41	11	313	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
41	11	316	A86	C10-C11-C13-O
41	11	316	A86	C13-C14-C15-O1
41	12	304	A86	C10-C11-C13-O
41	12	304	A86	C13-C14-C15-O1
41	12	318	A86	C10-C11-C13-O
41	13	301	A86	C10-C11-C13-O
41	13	301	A86	C13-C14-C15-O1
41	13	314	A86	C10-C11-C13-O
41	13	316	A86	C10-C11-C13-O
41	13	316	A86	C13-C14-C15-O1
41	14	314	A86	C10-C11-C13-O
41	15	313	A86	C10-C11-C13-O
41	15	315	A86	C10-C11-C13-O
41	15	315	A86	C13-C14-C15-O1
41	15	316	A86	C10-C11-C13-O
41	15	316	A86	C13-C14-C15-O1
41	16	310	A86	C10-C11-C13-O
41	17	302	A86	C13-C14-C15-O1
41	17	314	A86	C10-C11-C13-O
41	17	315	A86	C13-C14-C15-O1
41	18	302	A86	C10-C11-C13-O
41	18	302	A86	C13-C14-C15-O1
41	18	315	A86	C10-C11-C13-O
41	19	311	A86	C13-C14-C15-O1
41	20	201	A86	C13-C14-C15-O1
41	31	313	A86	C10-C11-C13-O
41	31	316	A86	C10-C11-C13-O
41	31	316	A86	C13-C14-C15-O1
41	32	304	A86	C10-C11-C13-O
41	32	304	A86	C13-C14-C15-O1
41	32	317	A86	C10-C11-C13-O
41	33	302	A86	C10-C11-C13-O
41	33	302	A86	C13-C14-C15-O1
41	33	315	A86	C10-C11-C13-O
41	33	316	A86	C10-C11-C13-O
41	33	316	A86	C13-C14-C15-O1
41	34	314	A86	C10-C11-C13-O
41	35	313	A86	C10-C11-C13-O
41	35	315	A86	C10-C11-C13-O
41	35	315	A86	C13-C14-C15-O1
41	35	316	A86	C10-C11-C13-O
41	35	316	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
41	36	310	A86	C10-C11-C13-O
41	37	302	A86	C13-C14-C15-O1
41	37	314	A86	C10-C11-C13-O
41	37	315	A86	C13-C14-C15-O1
41	38	302	A86	C10-C11-C13-O
41	38	302	A86	C13-C14-C15-O1
41	38	315	A86	C10-C11-C13-O
41	39	310	A86	C13-C14-C15-O1
41	39	311	A86	C13-C14-C15-O1
41	40	201	A86	C13-C14-C15-O1
30	20	202	CLA	O1D-CGD-O2D-CED
30	40	202	CLA	O1D-CGD-O2D-CED
30	D	401	CLA	C4-C3-C5-C6
30	d	401	CLA	C4-C3-C5-C6
36	W	101	LMG	C16-C17-C18-C19
36	w	101	LMG	C16-C17-C18-C19
30	12	305	CLA	C5-C6-C7-C8
30	13	302	CLA	C5-C6-C7-C8
30	B	614	CLA	C11-C10-C8-C9
30	C	504	CLA	C11-C12-C13-C14
30	C	510	CLA	C14-C13-C15-C16
30	b	614	CLA	C11-C10-C8-C9
30	c	504	CLA	C11-C12-C13-C14
30	c	510	CLA	C14-C13-C15-C16
30	15	301	CLA	C11-C10-C8-C9
30	20	202	CLA	C14-C13-C15-C16
30	21	301	CLA	C11-C12-C13-C14
30	21	303	CLA	C6-C7-C8-C9
30	31	303	CLA	C11-C12-C13-C14
30	32	307	CLA	C11-C12-C13-C14
30	33	305	CLA	C11-C12-C13-C14
30	34	304	CLA	C11-C12-C13-C14
30	35	301	CLA	C11-C10-C8-C9
30	40	202	CLA	C14-C13-C15-C16
30	41	301	CLA	C11-C12-C13-C14
30	41	303	CLA	C6-C7-C8-C9
30	C	503	CLA	O1A-CGA-O2A-C1
32	B	617	BCR	C11-C12-C13-C35
32	b	616	BCR	C11-C12-C13-C35
41	11	314	A86	C-C1-C24-C25
41	12	319	A86	C-C1-C24-C25
41	13	315	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
41	13	317	A86	C-C1-C24-C25
41	15	314	A86	C-C1-C24-C25
41	16	313	A86	C-C1-C24-C25
41	17	315	A86	C-C1-C24-C25
41	17	316	A86	C-C1-C24-C25
41	31	314	A86	C-C1-C24-C25
41	32	318	A86	C-C1-C24-C25
41	32	319	A86	C-C1-C24-C25
41	33	317	A86	C-C1-C24-C25
41	35	314	A86	C-C1-C24-C25
41	36	313	A86	C-C1-C24-C25
41	37	315	A86	C-C1-C24-C25
41	37	316	A86	C-C1-C24-C25
41	20	201	A86	C35-C34-O4-C38
41	40	201	A86	C35-C34-O4-C38
41	11	316	A86	C5-C6-C8-C9
41	12	304	A86	C5-C6-C8-C9
41	13	301	A86	C5-C6-C8-C9
41	13	316	A86	C5-C6-C8-C9
41	15	315	A86	C5-C6-C8-C9
41	15	316	A86	C5-C6-C8-C9
41	17	315	A86	C2-C1-C24-C25
41	18	302	A86	C5-C6-C8-C9
41	31	316	A86	C5-C6-C8-C9
41	32	304	A86	C5-C6-C8-C9
41	33	302	A86	C5-C6-C8-C9
41	33	316	A86	C5-C6-C8-C9
41	35	315	A86	C5-C6-C8-C9
41	35	316	A86	C5-C6-C8-C9
41	37	315	A86	C2-C1-C24-C25
41	38	302	A86	C5-C6-C8-C9
30	B	613	CLA	O1D-CGD-O2D-CED
30	C	509	CLA	C1A-C2A-CAA-CBA
30	c	509	CLA	C1A-C2A-CAA-CBA
30	C	507	CLA	C16-C17-C18-C20
30	c	507	CLA	C16-C17-C18-C20
30	21	306	CLA	C16-C17-C18-C20
30	41	306	CLA	C16-C17-C18-C20
31	d	404	PHO	C16-C17-C18-C20
30	31	315	CLA	C13-C15-C16-C17
30	32	303	CLA	C13-C15-C16-C17
30	33	301	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	34	301	CLA	C13-C15-C16-C17
30	D	401	CLA	C2-C1-O2A-CGA
30	W	103	CLA	C2-C1-O2A-CGA
30	d	401	CLA	C2-C1-O2A-CGA
30	w	103	CLA	C2-C1-O2A-CGA
35	b	621	LHG	C28-C29-C30-C31
36	b	618	LMG	C19-C20-C21-C22
38	c	518	DGD	C6B-C7B-C8B-C9B
38	c	518	DGD	CBB-CCB-CDB-CEB
41	21	313	A86	C1-C2-C3-C4
41	41	313	A86	C1-C2-C3-C4
30	b	613	CLA	O1D-CGD-O2D-CED
30	c	503	CLA	O1A-CGA-O2A-C1
30	12	307	CLA	C10-C11-C12-C13
30	14	304	CLA	C10-C11-C12-C13
35	B	622	LHG	C28-C29-C30-C31
36	B	619	LMG	C19-C20-C21-C22
38	C	517	DGD	C6B-C7B-C8B-C9B
38	C	517	DGD	CBB-CCB-CDB-CEB
30	11	303	CLA	C10-C11-C12-C13
30	13	304	CLA	C10-C11-C12-C13
35	A	408	LHG	C3-O3-P-O4
35	A	408	LHG	C4-O6-P-O4
35	B	622	LHG	C3-O3-P-O5
35	L	101	LHG	C4-O6-P-O5
35	L	102	LHG	C3-O3-P-O5
35	a	407	LHG	C3-O3-P-O4
35	a	407	LHG	C4-O6-P-O4
35	b	621	LHG	C3-O3-P-O5
35	d	409	LHG	C4-O6-P-O5
35	l	102	LHG	C3-O3-P-O5
30	C	519	CLA	CBD-CGD-O2D-CED
30	z	101	CLA	CBD-CGD-O2D-CED
36	B	619	LMG	C18-C19-C20-C21
36	b	618	LMG	C18-C19-C20-C21
36	12	301	LMG	C30-C31-C32-C33
30	b	604	CLA	O1A-CGA-O2A-C1
30	D	405	CLA	C13-C15-C16-C17
30	c	508	CLA	C5-C6-C7-C8
30	d	406	CLA	C13-C15-C16-C17
30	C	508	CLA	C5-C6-C7-C8
30	B	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	D	401	CLA	C16-C17-C18-C19
30	d	401	CLA	C16-C17-C18-C19
30	21	301	CLA	C16-C17-C18-C19
30	41	301	CLA	C16-C17-C18-C19
30	B	604	CLA	CAD-CBD-CGD-O1D
30	B	609	CLA	CAD-CBD-CGD-O1D
30	B	612	CLA	CAD-CBD-CGD-O1D
30	C	503	CLA	CAD-CBD-CGD-O1D
30	C	505	CLA	CAD-CBD-CGD-O1D
30	C	506	CLA	CAD-CBD-CGD-O1D
30	C	507	CLA	CAD-CBD-CGD-O1D
30	C	508	CLA	CAD-CBD-CGD-O1D
30	C	521	CLA	CAD-CBD-CGD-O1D
30	b	604	CLA	CAD-CBD-CGD-O1D
30	b	609	CLA	CAD-CBD-CGD-O1D
30	b	612	CLA	CAD-CBD-CGD-O1D
30	c	503	CLA	CAD-CBD-CGD-O1D
30	c	505	CLA	CAD-CBD-CGD-O1D
30	c	506	CLA	CAD-CBD-CGD-O1D
30	c	507	CLA	CAD-CBD-CGD-O1D
30	c	508	CLA	CAD-CBD-CGD-O1D
30	c	523	CLA	CAD-CBD-CGD-O1D
30	11	303	CLA	CAD-CBD-CGD-O1D
30	11	305	CLA	CAD-CBD-CGD-O1D
30	12	307	CLA	CAD-CBD-CGD-O1D
30	12	309	CLA	CAD-CBD-CGD-O1D
30	13	304	CLA	CAD-CBD-CGD-O1D
30	13	306	CLA	CAD-CBD-CGD-O1D
30	14	304	CLA	CAD-CBD-CGD-O1D
30	14	306	CLA	CAD-CBD-CGD-O1D
30	15	302	CLA	CAD-CBD-CGD-O1D
30	15	303	CLA	CAD-CBD-CGD-O1D
30	16	307	CLA	CAD-CBD-CGD-O1D
30	17	304	CLA	CAD-CBD-CGD-O1D
30	17	305	CLA	CAD-CBD-CGD-O1D
30	18	305	CLA	CAD-CBD-CGD-O1D
30	19	303	CLA	CAD-CBD-CGD-O1D
30	21	303	CLA	CAD-CBD-CGD-O1D
30	31	303	CLA	CAD-CBD-CGD-O1D
30	31	305	CLA	CAD-CBD-CGD-O1D
30	31	307	CLA	CAD-CBD-CGD-O1D
30	32	307	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	32	309	CLA	CAD-CBD-CGD-O1D
30	32	311	CLA	CAD-CBD-CGD-O1D
30	33	305	CLA	CAD-CBD-CGD-O1D
30	33	307	CLA	CAD-CBD-CGD-O1D
30	33	309	CLA	CAD-CBD-CGD-O1D
30	34	304	CLA	CAD-CBD-CGD-O1D
30	34	306	CLA	CAD-CBD-CGD-O1D
30	34	308	CLA	CAD-CBD-CGD-O1D
30	35	302	CLA	CAD-CBD-CGD-O1D
30	35	303	CLA	CAD-CBD-CGD-O1D
30	36	307	CLA	CAD-CBD-CGD-O1D
30	37	304	CLA	CAD-CBD-CGD-O1D
30	37	305	CLA	CAD-CBD-CGD-O1D
30	38	305	CLA	CAD-CBD-CGD-O1D
30	39	303	CLA	CAD-CBD-CGD-O1D
30	41	303	CLA	CAD-CBD-CGD-O1D
41	17	311	A86	C26-C27-C29-C30
41	37	311	A86	C26-C27-C29-C30
38	C	516	DGD	C4D-C5D-C6D-O5D
30	21	303	CLA	C10-C11-C12-C13
30	41	303	CLA	C10-C11-C12-C13
30	19	308	CLA	C4C-C3C-CAC-CBC
30	39	308	CLA	C4C-C3C-CAC-CBC
30	18	301	CLA	O1A-CGA-O2A-C1
30	38	301	CLA	O1A-CGA-O2A-C1
38	H	102	DGD	CCA-CDA-CEA-CFA
38	h	102	DGD	CCA-CDA-CEA-CFA
36	b	619	LMG	C22-C23-C24-C25
38	c	517	DGD	C4D-C5D-C6D-O5D
36	B	620	LMG	C22-C23-C24-C25
39	d	405	PL9	C30-C29-C31-C32
30	B	601	CLA	C12-C13-C15-C16
30	C	504	CLA	C11-C12-C13-C15
30	C	506	CLA	C11-C12-C13-C15
30	C	509	CLA	C6-C7-C8-C10
30	C	519	CLA	C12-C13-C15-C16
30	C	520	CLA	C12-C13-C15-C16
30	b	601	CLA	C12-C13-C15-C16
30	c	504	CLA	C11-C12-C13-C15
30	c	506	CLA	C11-C12-C13-C15
30	c	509	CLA	C6-C7-C8-C10
30	c	522	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	z	101	CLA	C12-C13-C15-C16
30	11	309	CLA	C3A-C2A-CAA-CBA
30	12	314	CLA	C3A-C2A-CAA-CBA
30	13	310	CLA	C3A-C2A-CAA-CBA
30	14	310	CLA	C3A-C2A-CAA-CBA
30	15	303	CLA	C11-C12-C13-C15
30	16	302	CLA	C6-C7-C8-C10
30	18	305	CLA	C11-C12-C13-C15
30	21	301	CLA	C11-C12-C13-C15
30	21	303	CLA	C6-C7-C8-C10
30	31	303	CLA	C11-C12-C13-C15
30	32	307	CLA	C11-C12-C13-C15
30	33	305	CLA	C11-C12-C13-C15
30	33	309	CLA	C12-C13-C15-C16
30	34	304	CLA	C11-C12-C13-C15
30	34	308	CLA	C12-C13-C15-C16
30	35	303	CLA	C11-C12-C13-C15
30	36	302	CLA	C6-C7-C8-C10
30	38	305	CLA	C11-C12-C13-C15
30	41	301	CLA	C11-C12-C13-C15
30	41	303	CLA	C6-C7-C8-C10
31	A	403	PHO	C11-C10-C8-C7
31	d	403	PHO	C11-C10-C8-C7
35	L	101	LHG	C23-C24-C25-C26
35	L	102	LHG	O6-C4-C5-O7
35	d	409	LHG	C23-C24-C25-C26
35	l	102	LHG	O6-C4-C5-O7
36	32	301	LMG	C16-C17-C18-C19
32	C	518	BCR	C19-C20-C21-C22
32	c	521	BCR	C19-C20-C21-C22
41	11	316	A86	C24-C25-C26-C27
41	12	304	A86	C24-C25-C26-C27
41	13	301	A86	C24-C25-C26-C27
41	13	316	A86	C24-C25-C26-C27
41	15	315	A86	C24-C25-C26-C27
41	15	316	A86	C24-C25-C26-C27
41	18	302	A86	C24-C25-C26-C27
41	31	316	A86	C24-C25-C26-C27
41	32	304	A86	C24-C25-C26-C27
41	33	302	A86	C24-C25-C26-C27
41	33	316	A86	C24-C25-C26-C27
41	35	315	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
41	35	316	A86	C24-C25-C26-C27
41	38	302	A86	C24-C25-C26-C27
38	C	516	DGD	O6D-C5D-C6D-O5D
38	c	517	DGD	O6D-C5D-C6D-O5D
35	l	102	LHG	C35-C36-C37-C38
30	15	307	CLA	C13-C15-C16-C17
30	35	307	CLA	C13-C15-C16-C17
35	L	102	LHG	C35-C36-C37-C38
38	C	517	DGD	C7B-C8B-C9B-CAB
38	c	518	DGD	C7B-C8B-C9B-CAB
30	21	307	CLA	C15-C16-C17-C18
30	41	307	CLA	C15-C16-C17-C18
30	C	514	CLA	C16-C17-C18-C19
38	C	517	DGD	C1A-C2A-C3A-C4A
38	c	518	DGD	C1A-C2A-C3A-C4A
36	w	101	LMG	C38-C39-C40-C41
38	C	516	DGD	C2D-C1D-O3G-C3G
38	c	517	DGD	C2D-C1D-O3G-C3G
36	B	619	LMG	C16-C17-C18-C19
36	b	618	LMG	C16-C17-C18-C19
30	16	301	CLA	CBA-CGA-O2A-C1
30	32	305	CLA	C5-C6-C7-C8
36	W	101	LMG	C38-C39-C40-C41
38	h	102	DGD	C5B-C6B-C7B-C8B
30	c	514	CLA	C16-C17-C18-C19
30	17	308	CLA	C16-C17-C18-C19
30	37	308	CLA	C16-C17-C18-C19
30	18	303	CLA	C10-C11-C12-C13
30	19	301	CLA	C13-C15-C16-C17
30	21	306	CLA	C5-C6-C7-C8
30	31	301	CLA	C5-C6-C7-C8
30	33	303	CLA	C5-C6-C7-C8
30	34	302	CLA	C5-C6-C7-C8
30	38	303	CLA	C10-C11-C12-C13
30	39	301	CLA	C13-C15-C16-C17
30	41	306	CLA	C5-C6-C7-C8
31	A	403	PHO	C5-C6-C7-C8
30	16	301	CLA	O1A-CGA-O2A-C1
31	d	403	PHO	C5-C6-C7-C8
39	D	404	PL9	C30-C29-C31-C32
30	36	301	CLA	CBA-CGA-O2A-C1
38	H	102	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
30	B	612	CLA	C11-C10-C8-C9
30	B	623	CLA	C11-C12-C13-C14
30	C	502	CLA	C14-C13-C15-C16
30	C	508	CLA	C14-C13-C15-C16
30	C	519	CLA	C14-C13-C15-C16
30	D	405	CLA	C11-C12-C13-C14
30	b	612	CLA	C11-C10-C8-C9
30	b	622	CLA	C11-C12-C13-C14
30	c	502	CLA	C14-C13-C15-C16
30	c	508	CLA	C14-C13-C15-C16
30	d	406	CLA	C11-C12-C13-C14
30	z	101	CLA	C14-C13-C15-C16
30	11	307	CLA	C14-C13-C15-C16
30	12	311	CLA	C14-C13-C15-C16
30	13	308	CLA	C14-C13-C15-C16
30	14	308	CLA	C14-C13-C15-C16
30	16	301	CLA	C14-C13-C15-C16
30	21	301	CLA	C11-C10-C8-C9
30	31	307	CLA	C14-C13-C15-C16
30	32	311	CLA	C14-C13-C15-C16
30	33	309	CLA	C14-C13-C15-C16
30	34	308	CLA	C14-C13-C15-C16
30	36	301	CLA	C14-C13-C15-C16
30	41	301	CLA	C11-C10-C8-C9
30	11	315	CLA	O1D-CGD-O2D-CED
30	36	301	CLA	O1A-CGA-O2A-C1
35	l	102	LHG	C12-C13-C14-C15
38	J	101	DGD	CDB-CEB-CFB-CGB
38	j	101	DGD	CDB-CEB-CFB-CGB
30	11	304	CLA	C2A-CAA-CBA-CGA
30	12	308	CLA	C2A-CAA-CBA-CGA
30	13	305	CLA	C2A-CAA-CBA-CGA
30	14	305	CLA	C2A-CAA-CBA-CGA
35	L	102	LHG	C12-C13-C14-C15
36	w	101	LMG	C36-C37-C38-C39
41	19	310	A86	C-C1-C24-C25
41	39	310	A86	C-C1-C24-C25
30	41	303	CLA	C3-C5-C6-C7
30	C	513	CLA	C10-C11-C12-C13
36	w	101	LMG	C21-C22-C23-C24
36	W	101	LMG	C21-C22-C23-C24
36	W	101	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
30	19	308	CLA	C2C-C3C-CAC-CBC
30	c	513	CLA	C10-C11-C12-C13
30	39	308	CLA	C2C-C3C-CAC-CBC
30	21	303	CLA	C3-C5-C6-C7
30	B	608	CLA	CBD-CGD-O2D-CED
30	C	520	CLA	O1A-CGA-O2A-C1
30	D	401	CLA	C2-C3-C5-C6
30	d	401	CLA	C2-C3-C5-C6
30	B	615	CLA	C5-C6-C7-C8
30	17	301	CLA	C8-C10-C11-C12
35	b	621	LHG	C29-C30-C31-C32
30	b	615	CLA	C5-C6-C7-C8
30	21	307	CLA	C13-C15-C16-C17
30	41	307	CLA	C13-C15-C16-C17
30	12	303	CLA	O1D-CGD-O2D-CED
30	c	522	CLA	O1A-CGA-O2A-C1
30	12	312	CLA	O1D-CGD-O2D-CED
38	H	102	DGD	O2G-C1B-C2B-C3B
38	h	102	DGD	O2G-C1B-C2B-C3B
33	l	101	SQD	C24-C25-C26-C27
30	B	603	CLA	C2A-CAA-CBA-CGA
30	C	506	CLA	C2A-CAA-CBA-CGA
30	b	603	CLA	C2A-CAA-CBA-CGA
30	c	506	CLA	C2A-CAA-CBA-CGA
33	L	103	SQD	C24-C25-C26-C27
35	B	622	LHG	C29-C30-C31-C32
38	H	102	DGD	C4A-C5A-C6A-C7A
38	h	102	DGD	C4A-C5A-C6A-C7A
36	b	619	LMG	O10-C28-O8-C9
30	14	301	CLA	O1D-CGD-O2D-CED
30	37	301	CLA	C8-C10-C11-C12
38	C	516	DGD	C8A-C9A-CAA-CBA
36	B	620	LMG	O10-C28-O8-C9
36	32	301	LMG	C13-C14-C15-C16
30	b	608	CLA	CBD-CGD-O2D-CED
41	11	313	A86	C12-C11-C13-C14
41	12	318	A86	C12-C11-C13-C14
41	13	314	A86	C12-C11-C13-C14
41	14	314	A86	C12-C11-C13-C14
41	15	313	A86	C12-C11-C13-C14
41	17	302	A86	C12-C11-C13-C14
41	17	314	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
41	18	315	A86	C12-C11-C13-C14
41	21	313	A86	C12-C11-C13-C14
41	31	313	A86	C12-C11-C13-C14
41	32	317	A86	C12-C11-C13-C14
41	33	315	A86	C12-C11-C13-C14
41	34	314	A86	C12-C11-C13-C14
41	35	313	A86	C12-C11-C13-C14
41	37	302	A86	C12-C11-C13-C14
41	37	314	A86	C12-C11-C13-C14
41	38	315	A86	C12-C11-C13-C14
41	41	313	A86	C12-C11-C13-C14
38	c	517	DGD	C8A-C9A-CAA-CBA
30	C	520	CLA	CBA-CGA-O2A-C1
30	c	522	CLA	CBA-CGA-O2A-C1
30	C	519	CLA	C5-C6-C7-C8
30	11	315	CLA	C13-C15-C16-C17
30	12	303	CLA	C13-C15-C16-C17
30	B	605	CLA	O1D-CGD-O2D-CED
30	C	519	CLA	O1D-CGD-O2D-CED
30	b	605	CLA	O1D-CGD-O2D-CED
32	H	101	BCR	C23-C24-C25-C30
32	h	101	BCR	C23-C24-C25-C30
30	z	101	CLA	O1D-CGD-O2D-CED
30	z	101	CLA	C5-C6-C7-C8
30	12	312	CLA	C13-C15-C16-C17
30	14	301	CLA	C13-C15-C16-C17
30	16	303	CLA	C2A-CAA-CBA-CGA
30	36	303	CLA	C2A-CAA-CBA-CGA
36	B	620	LMG	C32-C33-C34-C35
35	L	102	LHG	C4-O6-P-O3
35	l	102	LHG	C4-O6-P-O3
36	b	619	LMG	C32-C33-C34-C35
36	12	301	LMG	C7-C8-C9-O8
30	38	307	CLA	O1D-CGD-O2D-CED
30	39	303	CLA	CBD-CGD-O2D-CED
30	C	511	CLA	C11-C12-C13-C15
30	c	511	CLA	C11-C12-C13-C15
30	17	305	CLA	C11-C10-C8-C7
30	17	305	CLA	C11-C12-C13-C15
30	37	305	CLA	C11-C10-C8-C7
30	37	305	CLA	C11-C12-C13-C15
30	20	209	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	40	209	CLA	CAA-CBA-CGA-O2A
35	d	409	LHG	C10-C11-C12-C13
30	C	509	CLA	C6-C7-C8-C9
30	c	509	CLA	C6-C7-C8-C9
30	15	303	CLA	C11-C12-C13-C14
30	16	302	CLA	C11-C10-C8-C9
30	18	305	CLA	C11-C12-C13-C14
30	35	303	CLA	C11-C12-C13-C14
30	36	302	CLA	C11-C10-C8-C9
30	38	305	CLA	C11-C12-C13-C14
30	18	301	CLA	C13-C15-C16-C17
30	38	301	CLA	C13-C15-C16-C17
32	C	518	BCR	C9-C10-C11-C12
32	c	521	BCR	C9-C10-C11-C12
30	B	603	CLA	C16-C17-C18-C20
30	b	603	CLA	C16-C17-C18-C20
30	21	301	CLA	C16-C17-C18-C20
30	41	301	CLA	C16-C17-C18-C20
36	B	619	LMG	C20-C21-C22-C23
36	b	618	LMG	C20-C21-C22-C23
38	C	517	DGD	C5B-C6B-C7B-C8B
38	c	518	DGD	C5B-C6B-C7B-C8B
35	L	101	LHG	C10-C11-C12-C13
30	B	606	CLA	C8-C10-C11-C12
30	b	606	CLA	C8-C10-C11-C12
35	L	101	LHG	C30-C31-C32-C33
30	31	307	CLA	CAA-CBA-CGA-O1A
30	32	311	CLA	CAA-CBA-CGA-O1A
30	33	309	CLA	CAA-CBA-CGA-O1A
30	34	308	CLA	CAA-CBA-CGA-O1A
30	19	303	CLA	CBD-CGD-O2D-CED
30	B	614	CLA	C13-C15-C16-C17
30	19	303	CLA	C3-C5-C6-C7
30	39	303	CLA	C3-C5-C6-C7
30	18	307	CLA	O1D-CGD-O2D-CED
35	d	409	LHG	C30-C31-C32-C33
30	b	614	CLA	C13-C15-C16-C17
30	C	509	CLA	CBA-CGA-O2A-C1
33	L	103	SQD	C11-C12-C13-C14
30	20	209	CLA	C8-C10-C11-C12
30	11	315	CLA	C3-C5-C6-C7
30	12	303	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	12	301	LMG	C15-C16-C17-C18
30	40	209	CLA	C8-C10-C11-C12
33	l	101	SQD	C11-C12-C13-C14
30	D	401	CLA	C16-C17-C18-C20
30	c	509	CLA	CBA-CGA-O2A-C1
35	A	408	LHG	C24-C23-O8-C6
35	a	407	LHG	C24-C23-O8-C6
36	Q	301	LMG	C29-C28-O8-C9
36	c	519	LMG	C29-C28-O8-C9
38	H	102	DGD	C2B-C3B-C4B-C5B
38	c	517	DGD	C8B-C9B-CAB-CBB
30	b	605	CLA	C8-C10-C11-C12
30	15	306	CLA	CAA-CBA-CGA-O2A
30	35	306	CLA	CAA-CBA-CGA-O2A
35	a	407	LHG	C31-C32-C33-C34
30	B	601	CLA	CAA-CBA-CGA-O2A
30	b	601	CLA	CAA-CBA-CGA-O2A
38	C	516	DGD	C8B-C9B-CAB-CBB
38	h	102	DGD	C2B-C3B-C4B-C5B
30	C	509	CLA	C10-C11-C12-C13
30	c	509	CLA	C10-C11-C12-C13
30	31	315	CLA	C8-C10-C11-C12
33	B	621	SQD	O10-C23-O48-C46
33	b	620	SQD	O10-C23-O48-C46
30	19	303	CLA	CBA-CGA-O2A-C1
30	39	303	CLA	CBA-CGA-O2A-C1
30	d	401	CLA	C16-C17-C18-C20
30	13	308	CLA	CAA-CBA-CGA-O1A
30	14	308	CLA	CAA-CBA-CGA-O1A
30	32	303	CLA	C8-C10-C11-C12
41	21	312	A86	C11-C10-C9-C8
41	41	312	A86	C11-C10-C9-C8
30	12	312	CLA	C3-C5-C6-C7
30	14	301	CLA	C3-C5-C6-C7
30	19	303	CLA	O1A-CGA-O2A-C1
30	39	303	CLA	O1A-CGA-O2A-C1
35	A	408	LHG	C31-C32-C33-C34
38	j	101	DGD	C3A-C4A-C5A-C6A
30	B	605	CLA	C8-C10-C11-C12
30	33	301	CLA	C8-C10-C11-C12
30	34	301	CLA	C8-C10-C11-C12
38	J	101	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
33	b	620	SQD	C12-C13-C14-C15
30	B	623	CLA	O1A-CGA-O2A-C1
30	Z	102	CLA	C3-C5-C6-C7
30	c	524	CLA	C3-C5-C6-C7
30	12	311	CLA	CAA-CBA-CGA-O1A
30	17	303	CLA	C4-C3-C5-C6
30	37	303	CLA	C4-C3-C5-C6
30	11	304	CLA	CAA-CBA-CGA-O2A
30	12	308	CLA	CAA-CBA-CGA-O2A
30	13	305	CLA	CAA-CBA-CGA-O2A
30	14	305	CLA	CAA-CBA-CGA-O2A
30	C	514	CLA	C10-C11-C12-C13
30	b	612	CLA	C5-C6-C7-C8
30	c	514	CLA	C10-C11-C12-C13
30	b	622	CLA	O1A-CGA-O2A-C1
33	B	621	SQD	C12-C13-C14-C15
30	B	612	CLA	C5-C6-C7-C8
30	12	312	CLA	C8-C10-C11-C12
30	11	307	CLA	CAA-CBA-CGA-O1A
30	11	304	CLA	CAA-CBA-CGA-O1A
30	12	308	CLA	CAA-CBA-CGA-O1A
30	13	305	CLA	CAA-CBA-CGA-O1A
30	14	305	CLA	CAA-CBA-CGA-O1A
30	17	306	CLA	CAA-CBA-CGA-O1A
30	32	308	CLA	CAA-CBA-CGA-O2A
30	34	305	CLA	CAA-CBA-CGA-O2A
30	37	306	CLA	CAA-CBA-CGA-O1A
40	E	101	HEM	CAD-CBD-CGD-O1D
30	A	404	CLA	C2-C1-O2A-CGA
30	B	610	CLA	C2-C1-O2A-CGA
30	C	506	CLA	C2-C1-O2A-CGA
30	C	511	CLA	C2-C1-O2A-CGA
30	a	403	CLA	C2-C1-O2A-CGA
30	b	610	CLA	C2-C1-O2A-CGA
30	c	506	CLA	C2-C1-O2A-CGA
30	c	511	CLA	C2-C1-O2A-CGA
30	11	315	CLA	C8-C10-C11-C12
31	A	403	PHO	C13-C15-C16-C17
31	d	403	PHO	C13-C15-C16-C17
30	12	303	CLA	C8-C10-C11-C12
30	14	301	CLA	C8-C10-C11-C12
30	21	304	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	31	304	CLA	CAA-CBA-CGA-O2A
30	31	308	CLA	CAA-CBA-CGA-O1A
30	32	312	CLA	CAA-CBA-CGA-O1A
30	33	306	CLA	CAA-CBA-CGA-O2A
30	33	310	CLA	CAA-CBA-CGA-O1A
30	34	309	CLA	CAA-CBA-CGA-O1A
30	41	304	CLA	CAA-CBA-CGA-O2A
40	e	101	HEM	CAD-CBD-CGD-O1D
30	C	511	CLA	C2A-CAA-CBA-CGA
30	c	511	CLA	C2A-CAA-CBA-CGA
36	12	301	LMG	O7-C8-C9-O8
30	39	303	CLA	O1D-CGD-O2D-CED
36	W	101	LMG	C34-C35-C36-C37
38	C	517	DGD	C8B-C9B-CAB-CBB
38	c	518	DGD	C8B-C9B-CAB-CBB
36	w	101	LMG	C34-C35-C36-C37
30	C	507	CLA	C3A-C2A-CAA-CBA
30	c	507	CLA	C3A-C2A-CAA-CBA
30	16	309	CLA	C3A-C2A-CAA-CBA
30	19	303	CLA	C3A-C2A-CAA-CBA
30	20	204	CLA	C3A-C2A-CAA-CBA
30	21	303	CLA	C3A-C2A-CAA-CBA
30	31	309	CLA	C3A-C2A-CAA-CBA
30	32	313	CLA	C3A-C2A-CAA-CBA
30	33	311	CLA	C3A-C2A-CAA-CBA
30	34	310	CLA	C3A-C2A-CAA-CBA
30	36	309	CLA	C3A-C2A-CAA-CBA
30	39	303	CLA	C3A-C2A-CAA-CBA
30	40	204	CLA	C3A-C2A-CAA-CBA
30	41	303	CLA	C3A-C2A-CAA-CBA
30	16	305	CLA	CAA-CBA-CGA-O2A
30	36	305	CLA	CAA-CBA-CGA-O2A
41	16	310	A86	O-C13-C14-C15
41	17	311	A86	O-C13-C14-C15
41	20	210	A86	O-C13-C14-C15
41	20	212	A86	O-C13-C14-C15
41	36	310	A86	O-C13-C14-C15
41	37	302	A86	O-C13-C14-C15
41	37	311	A86	O-C13-C14-C15
41	40	210	A86	O-C13-C14-C15
41	40	212	A86	O-C13-C14-C15
38	C	516	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
30	32	308	CLA	CAA-CBA-CGA-O1A
30	C	521	CLA	C4-C3-C5-C6
30	c	523	CLA	C4-C3-C5-C6
38	c	517	DGD	C2A-C3A-C4A-C5A
30	12	303	CLA	CBD-CGD-O2D-CED
39	D	404	PL9	C4-C3-C7-C8
39	d	405	PL9	C4-C3-C7-C8
30	B	605	CLA	C11-C10-C8-C9
30	b	605	CLA	C11-C10-C8-C9
30	15	307	CLA	C14-C13-C15-C16
30	17	308	CLA	C11-C10-C8-C9
30	18	303	CLA	C11-C12-C13-C14
30	35	307	CLA	C14-C13-C15-C16
30	37	308	CLA	C11-C10-C8-C9
30	38	303	CLA	C11-C12-C13-C14
30	19	303	CLA	O1D-CGD-O2D-CED
30	21	302	CLA	CAA-CBA-CGA-O1A
30	31	304	CLA	CAA-CBA-CGA-O1A
30	33	306	CLA	CAA-CBA-CGA-O1A
30	34	305	CLA	CAA-CBA-CGA-O1A
30	41	302	CLA	CAA-CBA-CGA-O1A
36	12	301	LMG	O1-C7-C8-C9
41	19	310	A86	C25-C26-C27-C28
41	39	310	A86	C25-C26-C27-C28
35	L	101	LHG	C35-C36-C37-C38
30	11	308	CLA	CAA-CBA-CGA-O1A
30	12	313	CLA	CAA-CBA-CGA-O1A
30	14	309	CLA	CAA-CBA-CGA-O1A
30	19	304	CLA	CAA-CBA-CGA-O1A
30	21	304	CLA	CAA-CBA-CGA-O1A
30	39	304	CLA	CAA-CBA-CGA-O1A
30	41	304	CLA	CAA-CBA-CGA-O1A
35	d	409	LHG	C35-C36-C37-C38
38	J	101	DGD	O1A-C1A-O1G-C1G
30	B	603	CLA	C16-C17-C18-C19
30	b	603	CLA	C16-C17-C18-C19
36	B	620	LMG	O6-C1-O1-C7
36	Q	301	LMG	O6-C1-O1-C7
36	b	619	LMG	O6-C1-O1-C7
36	c	519	LMG	O6-C1-O1-C7
30	17	306	CLA	CAA-CBA-CGA-O2A
30	18	306	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	18	311	CLA	CAA-CBA-CGA-O1A
30	37	306	CLA	CAA-CBA-CGA-O2A
30	38	306	CLA	CAA-CBA-CGA-O1A
30	38	311	CLA	CAA-CBA-CGA-O1A
38	j	101	DGD	C3B-C4B-C5B-C6B
30	13	309	CLA	CAA-CBA-CGA-O1A
30	16	306	CLA	CAA-CBA-CGA-O2A
30	20	208	CLA	CAA-CBA-CGA-O1A
30	36	306	CLA	CAA-CBA-CGA-O2A
30	40	208	CLA	CAA-CBA-CGA-O1A
30	B	603	CLA	C1A-C2A-CAA-CBA
30	C	519	CLA	C1A-C2A-CAA-CBA
30	b	603	CLA	C1A-C2A-CAA-CBA
30	z	101	CLA	C1A-C2A-CAA-CBA
30	11	302	CLA	C1A-C2A-CAA-CBA
30	12	306	CLA	C1A-C2A-CAA-CBA
30	13	303	CLA	C1A-C2A-CAA-CBA
30	14	303	CLA	C1A-C2A-CAA-CBA
30	15	305	CLA	C1A-C2A-CAA-CBA
30	21	307	CLA	C1A-C2A-CAA-CBA
30	31	302	CLA	C1A-C2A-CAA-CBA
30	32	306	CLA	C1A-C2A-CAA-CBA
30	33	304	CLA	C1A-C2A-CAA-CBA
30	34	303	CLA	C1A-C2A-CAA-CBA
30	35	305	CLA	C1A-C2A-CAA-CBA
30	41	307	CLA	C1A-C2A-CAA-CBA
30	C	510	CLA	C6-C7-C8-C10
30	W	102	CLA	C11-C12-C13-C15
30	c	510	CLA	C6-C7-C8-C10
30	w	102	CLA	C11-C12-C13-C15
30	C	509	CLA	O1A-CGA-O2A-C1
30	c	509	CLA	O1A-CGA-O2A-C1
38	j	101	DGD	O1A-C1A-O1G-C1G
30	15	304	CLA	CAA-CBA-CGA-O2A
30	18	311	CLA	CAA-CBA-CGA-O2A
30	19	304	CLA	CAA-CBA-CGA-O2A
30	35	304	CLA	CAA-CBA-CGA-O2A
30	38	311	CLA	CAA-CBA-CGA-O2A
30	39	304	CLA	CAA-CBA-CGA-O2A
38	J	101	DGD	C3B-C4B-C5B-C6B
32	Z	101	BCR	C19-C20-C21-C22
32	c	515	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
36	d	410	LMG	C15-C16-C17-C18
30	18	306	CLA	CAA-CBA-CGA-O2A
30	20	205	CLA	CAA-CBA-CGA-O1A
30	20	205	CLA	CAA-CBA-CGA-O2A
30	20	208	CLA	CAA-CBA-CGA-O2A
30	38	306	CLA	CAA-CBA-CGA-O2A
30	40	205	CLA	CAA-CBA-CGA-O2A
30	40	208	CLA	CAA-CBA-CGA-O2A
36	D	408	LMG	C15-C16-C17-C18
30	34	301	CLA	O1D-CGD-O2D-CED
30	C	519	CLA	C2A-CAA-CBA-CGA
30	z	101	CLA	C2A-CAA-CBA-CGA
30	20	202	CLA	C10-C11-C12-C13
30	40	202	CLA	C10-C11-C12-C13
36	D	408	LMG	C28-C29-C30-C31
30	16	305	CLA	CAA-CBA-CGA-O1A
30	16	306	CLA	CAA-CBA-CGA-O1A
30	19	302	CLA	CAA-CBA-CGA-O2A
30	36	306	CLA	CAA-CBA-CGA-O1A
30	39	302	CLA	CAA-CBA-CGA-O2A
30	40	205	CLA	CAA-CBA-CGA-O1A
36	B	619	LMG	C11-C12-C13-C14
36	b	618	LMG	C11-C12-C13-C14
30	16	302	CLA	C15-C16-C17-C18
30	41	306	CLA	C10-C11-C12-C13
35	d	409	LHG	C9-C10-C11-C12
35	L	101	LHG	C9-C10-C11-C12
30	21	306	CLA	C10-C11-C12-C13
30	36	302	CLA	C15-C16-C17-C18
30	31	308	CLA	CAA-CBA-CGA-O2A
30	36	305	CLA	CAA-CBA-CGA-O1A
40	E	101	HEM	CAD-CBD-CGD-O2D
40	e	101	HEM	CAA-CBA-CGA-O1A
40	e	101	HEM	CAD-CBD-CGD-O2D
35	b	621	LHG	C14-C15-C16-C17
30	w	102	CLA	C4-C3-C5-C6
35	B	622	LHG	C14-C15-C16-C17
36	d	410	LMG	C28-C29-C30-C31
30	C	521	CLA	C2-C3-C5-C6
39	D	404	PL9	C12-C11-C9-C8
39	d	405	PL9	C12-C11-C9-C8
30	15	304	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	18	304	CLA	CAA-CBA-CGA-O2A
30	19	307	CLA	CAA-CBA-CGA-O2A
30	32	312	CLA	CAA-CBA-CGA-O2A
30	33	310	CLA	CAA-CBA-CGA-O2A
30	34	309	CLA	CAA-CBA-CGA-O2A
30	35	304	CLA	CAA-CBA-CGA-O1A
30	38	304	CLA	CAA-CBA-CGA-O2A
30	39	307	CLA	CAA-CBA-CGA-O2A
40	E	101	HEM	CAA-CBA-CGA-O1A
30	32	303	CLA	O1D-CGD-O2D-CED
30	11	315	CLA	CBD-CGD-O2D-CED
30	12	312	CLA	CBD-CGD-O2D-CED
33	l	101	SQD	C9-C10-C11-C12
30	31	315	CLA	O1D-CGD-O2D-CED
41	11	310	A86	C13-C14-C15-C16
41	11	313	A86	C13-C14-C15-C16
41	12	315	A86	C13-C14-C15-C16
41	12	318	A86	C13-C14-C15-C16
41	13	311	A86	C13-C14-C15-C16
41	13	314	A86	C13-C14-C15-C16
41	14	311	A86	C13-C14-C15-C16
41	14	314	A86	C13-C14-C15-C16
41	15	310	A86	C13-C14-C15-C16
41	15	313	A86	C13-C14-C15-C16
41	17	314	A86	C13-C14-C15-C16
41	18	313	A86	C13-C14-C15-C16
41	18	315	A86	C13-C14-C15-C16
41	19	310	A86	C25-C26-C27-C29
41	21	310	A86	C13-C14-C15-C16
41	31	310	A86	C13-C14-C15-C16
41	31	313	A86	C13-C14-C15-C16
41	32	314	A86	C13-C14-C15-C16
41	32	317	A86	C13-C14-C15-C16
41	33	312	A86	C13-C14-C15-C16
41	33	315	A86	C13-C14-C15-C16
41	34	311	A86	C13-C14-C15-C16
41	34	314	A86	C13-C14-C15-C16
41	35	310	A86	C13-C14-C15-C16
41	35	313	A86	C13-C14-C15-C16
41	37	314	A86	C13-C14-C15-C16
41	38	313	A86	C13-C14-C15-C16
41	38	315	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
41	39	310	A86	C25-C26-C27-C29
41	41	310	A86	C13-C14-C15-C16
30	16	309	CLA	CAA-CBA-CGA-O2A
30	21	302	CLA	CAA-CBA-CGA-O2A
30	31	306	CLA	CAA-CBA-CGA-O2A
30	32	310	CLA	CAA-CBA-CGA-O2A
30	33	308	CLA	CAA-CBA-CGA-O2A
30	34	307	CLA	CAA-CBA-CGA-O2A
30	35	306	CLA	CAA-CBA-CGA-O1A
30	36	309	CLA	CAA-CBA-CGA-O2A
33	L	103	SQD	C9-C10-C11-C12
36	12	301	LMG	C31-C32-C33-C34
30	B	601	CLA	CBA-CGA-O2A-C1
30	b	601	CLA	CBA-CGA-O2A-C1
30	16	302	CLA	C8-C10-C11-C12
30	36	302	CLA	C8-C10-C11-C12
30	15	305	CLA	CAA-CBA-CGA-O2A
30	19	307	CLA	CAA-CBA-CGA-O1A
30	39	307	CLA	CAA-CBA-CGA-O1A
30	41	302	CLA	CAA-CBA-CGA-O2A
36	Q	301	LMG	C35-C36-C37-C38
30	C	514	CLA	C16-C17-C18-C20
30	c	514	CLA	C16-C17-C18-C20
36	c	519	LMG	C35-C36-C37-C38
36	B	620	LMG	C36-C37-C38-C39
36	b	619	LMG	C36-C37-C38-C39
38	H	102	DGD	C9B-CAB-CBB-CCB
38	h	102	DGD	C9B-CAB-CBB-CCB
31	D	403	PHO	O1D-CGD-O2D-CED
39	D	407	PL9	C39-C41-C42-C43
39	d	408	PL9	C39-C41-C42-C43
41	12	304	A86	C10-C11-C13-C14
41	13	316	A86	C10-C11-C13-C14
41	15	316	A86	C10-C11-C13-C14
41	16	310	A86	C10-C11-C13-C14
41	31	316	A86	C10-C11-C13-C14
41	32	304	A86	C10-C11-C13-C14
41	33	316	A86	C10-C11-C13-C14
41	35	316	A86	C10-C11-C13-C14
41	36	310	A86	C10-C11-C13-C14
30	15	306	CLA	CAA-CBA-CGA-O1A
30	17	307	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	20	206	CLA	CAA-CBA-CGA-O2A
30	20	207	CLA	CAA-CBA-CGA-O2A
30	35	305	CLA	CAA-CBA-CGA-O2A
30	37	307	CLA	CAA-CBA-CGA-O2A
30	40	207	CLA	CAA-CBA-CGA-O2A
30	33	301	CLA	O1D-CGD-O2D-CED
30	W	102	CLA	C4-C3-C5-C6
30	21	306	CLA	C2-C1-O2A-CGA
30	41	306	CLA	C2-C1-O2A-CGA
30	c	523	CLA	C2-C3-C5-C6
30	B	601	CLA	O1A-CGA-O2A-C1
30	b	601	CLA	O1A-CGA-O2A-C1
30	18	304	CLA	CAA-CBA-CGA-O1A
30	38	304	CLA	CAA-CBA-CGA-O1A
30	39	302	CLA	CAA-CBA-CGA-O1A
30	40	206	CLA	CAA-CBA-CGA-O2A
30	40	207	CLA	CAA-CBA-CGA-O1A
30	c	522	CLA	C14-C13-C15-C16
30	18	309	CLA	C14-C13-C15-C16
30	38	309	CLA	C14-C13-C15-C16
30	14	301	CLA	CBD-CGD-O2D-CED
33	L	103	SQD	C19-C20-C21-C22
30	19	302	CLA	CAA-CBA-CGA-O1A
30	20	206	CLA	CAA-CBA-CGA-O1A
30	20	207	CLA	CAA-CBA-CGA-O1A
30	40	206	CLA	CAA-CBA-CGA-O1A
33	l	101	SQD	C19-C20-C21-C22
30	18	301	CLA	C8-C10-C11-C12
30	38	301	CLA	C8-C10-C11-C12
31	D	403	PHO	CAA-CBA-CGA-O2A
30	20	204	CLA	C16-C17-C18-C19
30	40	204	CLA	C16-C17-C18-C19
40	E	101	HEM	CAA-CBA-CGA-O2A
40	e	101	HEM	CAA-CBA-CGA-O2A
36	B	619	LMG	C34-C35-C36-C37
36	b	618	LMG	C34-C35-C36-C37
30	a	403	CLA	O1A-CGA-O2A-C1
32	B	617	BCR	C23-C24-C25-C30
32	B	618	BCR	C23-C24-C25-C30
32	B	624	BCR	C23-C24-C25-C26
32	B	624	BCR	C23-C24-C25-C30
32	C	515	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
32	C	515	BCR	C23-C24-C25-C30
32	b	616	BCR	C23-C24-C25-C30
32	b	617	BCR	C23-C24-C25-C30
32	b	623	BCR	C23-C24-C25-C26
32	b	623	BCR	C23-C24-C25-C30
32	c	516	BCR	C23-C24-C25-C26
32	c	516	BCR	C23-C24-C25-C30
31	d	404	PHO	CAA-CBA-CGA-O2A
38	C	517	DGD	CCB-CDB-CEB-CFB
38	H	102	DGD	C1G-C2G-C3G-O3G
38	c	518	DGD	CCB-CDB-CEB-CFB
38	h	102	DGD	C1G-C2G-C3G-O3G
30	b	608	CLA	O1D-CGD-O2D-CED
30	20	203	CLA	CAA-CBA-CGA-O2A
30	A	404	CLA	O1A-CGA-O2A-C1
30	a	403	CLA	CBA-CGA-O2A-C1
39	D	407	PL9	C15-C14-C16-C17
39	d	408	PL9	C15-C14-C16-C17
32	A	409	BCR	C17-C18-C19-C20
32	a	408	BCR	C17-C18-C19-C20
30	16	309	CLA	CAA-CBA-CGA-O1A
30	36	309	CLA	CAA-CBA-CGA-O1A
30	40	203	CLA	CAA-CBA-CGA-O2A
36	c	519	LMG	C16-C17-C18-C19
36	Q	301	LMG	C16-C17-C18-C19
30	11	308	CLA	CAA-CBA-CGA-O2A
30	31	315	CLA	C3-C5-C6-C7
30	33	301	CLA	C3-C5-C6-C7
30	34	301	CLA	C3-C5-C6-C7
30	17	307	CLA	C4C-C3C-CAC-CBC
30	37	307	CLA	C4C-C3C-CAC-CBC
30	B	608	CLA	O1D-CGD-O2D-CED
30	12	313	CLA	CAA-CBA-CGA-O2A
30	13	309	CLA	CAA-CBA-CGA-O2A
30	14	309	CLA	CAA-CBA-CGA-O2A
30	B	605	CLA	C2A-CAA-CBA-CGA
30	b	605	CLA	C2A-CAA-CBA-CGA
30	11	305	CLA	C2A-CAA-CBA-CGA
30	12	309	CLA	C2A-CAA-CBA-CGA
30	13	306	CLA	C2A-CAA-CBA-CGA
30	14	306	CLA	C2A-CAA-CBA-CGA
30	21	306	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	21	307	CLA	C2A-CAA-CBA-CGA
30	31	305	CLA	C2A-CAA-CBA-CGA
30	32	309	CLA	C2A-CAA-CBA-CGA
30	33	307	CLA	C2A-CAA-CBA-CGA
30	34	306	CLA	C2A-CAA-CBA-CGA
30	41	306	CLA	C2A-CAA-CBA-CGA
30	41	307	CLA	C2A-CAA-CBA-CGA
30	B	623	CLA	CBA-CGA-O2A-C1
30	32	303	CLA	C3-C5-C6-C7
30	15	305	CLA	CAA-CBA-CGA-O1A
30	35	305	CLA	CAA-CBA-CGA-O1A
31	d	404	PHO	O1D-CGD-O2D-CED
30	31	306	CLA	CAA-CBA-CGA-O1A
30	32	310	CLA	CAA-CBA-CGA-O1A
30	34	307	CLA	CAA-CBA-CGA-O1A
30	39	306	CLA	CAA-CBA-CGA-O2A
30	A	404	CLA	CBA-CGA-O2A-C1
36	32	301	LMG	C2-C1-O1-C7
30	19	306	CLA	CAA-CBA-CGA-O2A
30	21	305	CLA	CAA-CBA-CGA-O1A
30	41	305	CLA	CAA-CBA-CGA-O1A
30	19	305	CLA	CAA-CBA-CGA-O1A
30	21	305	CLA	CAA-CBA-CGA-O2A
30	33	308	CLA	CAA-CBA-CGA-O1A
30	39	305	CLA	CAA-CBA-CGA-O1A
30	41	305	CLA	CAA-CBA-CGA-O2A
30	B	611	CLA	C2A-CAA-CBA-CGA
30	b	611	CLA	C2A-CAA-CBA-CGA
38	H	102	DGD	C4B-C5B-C6B-C7B
30	17	307	CLA	CAA-CBA-CGA-O1A
30	20	203	CLA	CAA-CBA-CGA-O1A
30	37	307	CLA	CAA-CBA-CGA-O1A
30	40	203	CLA	CAA-CBA-CGA-O1A
32	Y	101	BCR	C16-C17-C18-C36
32	c	520	BCR	C16-C17-C18-C36
38	h	102	DGD	C4B-C5B-C6B-C7B
30	C	521	CLA	CAA-CBA-CGA-O2A
30	c	523	CLA	CAA-CBA-CGA-O2A
30	15	307	CLA	CAA-CBA-CGA-O2A
30	20	202	CLA	CAA-CBA-CGA-O2A
30	40	202	CLA	CAA-CBA-CGA-O2A
30	B	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	Z	102	CLA	C4-C3-C5-C6
30	b	604	CLA	C4-C3-C5-C6
30	c	524	CLA	C4-C3-C5-C6
30	C	505	CLA	C5-C6-C7-C8
30	c	505	CLA	C5-C6-C7-C8
30	11	306	CLA	CAA-CBA-CGA-O2A
30	14	307	CLA	CAA-CBA-CGA-O2A
30	C	504	CLA	C2-C3-C5-C6
30	W	102	CLA	C2-C3-C5-C6
30	c	504	CLA	C2-C3-C5-C6
30	w	102	CLA	C2-C3-C5-C6
30	17	305	CLA	C16-C17-C18-C19
30	37	305	CLA	C16-C17-C18-C19
30	35	307	CLA	CAA-CBA-CGA-O2A
38	J	101	DGD	O1G-C1A-C2A-C3A
38	j	101	DGD	O1G-C1A-C2A-C3A
30	B	601	CLA	C14-C13-C15-C16
30	B	602	CLA	C6-C7-C8-C9
30	B	615	CLA	C14-C13-C15-C16
30	C	519	CLA	C11-C10-C8-C9
30	C	520	CLA	C14-C13-C15-C16
30	b	601	CLA	C14-C13-C15-C16
30	b	602	CLA	C6-C7-C8-C9
30	b	615	CLA	C14-C13-C15-C16
30	z	101	CLA	C11-C10-C8-C9
30	17	305	CLA	C11-C12-C13-C14
30	37	305	CLA	C11-C12-C13-C14
36	w	101	LMG	C39-C40-C41-C42
30	12	310	CLA	CAA-CBA-CGA-O2A
30	13	307	CLA	CAA-CBA-CGA-O2A
36	W	101	LMG	C39-C40-C41-C42
30	15	303	CLA	C3A-C2A-CAA-CBA
30	35	303	CLA	C3A-C2A-CAA-CBA
35	B	622	LHG	C10-C11-C12-C13
30	21	307	CLA	O1A-CGA-O2A-C1
36	w	101	LMG	O10-C28-O8-C9
30	C	502	CLA	CAA-CBA-CGA-O2A
35	a	407	LHG	C16-C17-C18-C19
30	18	308	CLA	CAA-CBA-CGA-O2A
30	C	502	CLA	CAD-CBD-CGD-O2D
30	C	504	CLA	CAD-CBD-CGD-O2D
30	C	519	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	c	502	CLA	CAD-CBD-CGD-O2D
30	c	504	CLA	CAD-CBD-CGD-O2D
30	z	101	CLA	CAD-CBD-CGD-O2D
30	11	302	CLA	CAD-CBD-CGD-O2D
30	11	307	CLA	CAD-CBD-CGD-O2D
30	12	306	CLA	CAD-CBD-CGD-O2D
30	12	311	CLA	CAD-CBD-CGD-O2D
30	13	303	CLA	CAD-CBD-CGD-O2D
30	13	308	CLA	CAD-CBD-CGD-O2D
30	14	303	CLA	CAD-CBD-CGD-O2D
30	14	308	CLA	CAD-CBD-CGD-O2D
30	15	305	CLA	CAD-CBD-CGD-O2D
30	15	306	CLA	CAD-CBD-CGD-O2D
30	16	303	CLA	CAD-CBD-CGD-O2D
30	16	309	CLA	CAD-CBD-CGD-O2D
30	17	306	CLA	CAD-CBD-CGD-O2D
30	17	308	CLA	CAD-CBD-CGD-O2D
30	19	307	CLA	CAD-CBD-CGD-O2D
30	20	209	CLA	CAD-CBD-CGD-O2D
30	21	304	CLA	CAD-CBD-CGD-O2D
30	21	305	CLA	CAD-CBD-CGD-O2D
30	31	302	CLA	CAD-CBD-CGD-O2D
30	32	306	CLA	CAD-CBD-CGD-O2D
30	33	304	CLA	CAD-CBD-CGD-O2D
30	34	303	CLA	CAD-CBD-CGD-O2D
30	35	305	CLA	CAD-CBD-CGD-O2D
30	35	306	CLA	CAD-CBD-CGD-O2D
30	36	303	CLA	CAD-CBD-CGD-O2D
30	36	309	CLA	CAD-CBD-CGD-O2D
30	37	306	CLA	CAD-CBD-CGD-O2D
30	37	308	CLA	CAD-CBD-CGD-O2D
30	39	307	CLA	CAD-CBD-CGD-O2D
30	40	209	CLA	CAD-CBD-CGD-O2D
30	41	304	CLA	CAD-CBD-CGD-O2D
30	41	305	CLA	CAD-CBD-CGD-O2D
41	20	211	A86	C28-C27-C29-C30
41	21	311	A86	C28-C27-C29-C30
41	40	211	A86	C28-C27-C29-C30
41	41	311	A86	C28-C27-C29-C30
30	17	305	CLA	C16-C17-C18-C20
30	37	305	CLA	C16-C17-C18-C20
33	b	620	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
38	C	517	DGD	O1B-C1B-O2G-C2G
38	c	518	DGD	O1B-C1B-O2G-C2G
30	41	307	CLA	O1A-CGA-O2A-C1
35	A	408	LHG	C16-C17-C18-C19
35	b	621	LHG	C10-C11-C12-C13
30	B	605	CLA	C13-C15-C16-C17
30	b	605	CLA	C13-C15-C16-C17
30	c	513	CLA	C15-C16-C17-C18
30	18	308	CLA	CAA-CBA-CGA-O1A
30	38	308	CLA	CAA-CBA-CGA-O1A
30	38	308	CLA	CAA-CBA-CGA-O2A
30	A	404	CLA	CAA-CBA-CGA-O2A
30	W	103	CLA	CAA-CBA-CGA-O2A
30	a	403	CLA	CAA-CBA-CGA-O2A
30	c	502	CLA	CAA-CBA-CGA-O2A
30	C	513	CLA	C15-C16-C17-C18
30	b	622	CLA	CBA-CGA-O2A-C1
33	B	621	SQD	C24-C25-C26-C27
30	C	509	CLA	C3-C5-C6-C7
30	17	310	CLA	CAA-CBA-CGA-O2A
30	Z	102	CLA	C2-C3-C5-C6
30	c	524	CLA	C2-C3-C5-C6
39	D	407	PL9	C28-C29-C31-C32
39	d	408	PL9	C28-C29-C31-C32
30	w	103	CLA	CAA-CBA-CGA-O2A
36	W	101	LMG	O10-C28-O8-C9
41	11	314	A86	C5-C6-C8-C9
41	12	319	A86	C5-C6-C8-C9
41	13	315	A86	C5-C6-C8-C9
41	13	317	A86	C5-C6-C8-C9
41	15	314	A86	C5-C6-C8-C9
41	16	313	A86	C5-C6-C8-C9
41	17	316	A86	C5-C6-C8-C9
41	31	314	A86	C5-C6-C8-C9
41	32	318	A86	C5-C6-C8-C9
41	32	319	A86	C5-C6-C8-C9
41	33	317	A86	C5-C6-C8-C9
41	35	314	A86	C5-C6-C8-C9
41	36	313	A86	C5-C6-C8-C9
41	37	316	A86	C5-C6-C8-C9
39	D	407	PL9	C29-C31-C32-C33
39	d	408	PL9	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
41	21	313	A86	C12-C11-C13-O
41	41	313	A86	C12-C11-C13-O
30	12	310	CLA	CAA-CBA-CGA-O1A
30	13	307	CLA	CAA-CBA-CGA-O1A
30	15	302	CLA	CAA-CBA-CGA-O1A
30	17	310	CLA	CAA-CBA-CGA-O1A
30	21	309	CLA	CAA-CBA-CGA-O1A
30	35	302	CLA	CAA-CBA-CGA-O1A
30	37	310	CLA	CAA-CBA-CGA-O1A
30	37	310	CLA	CAA-CBA-CGA-O2A
30	41	309	CLA	CAA-CBA-CGA-O1A
30	21	307	CLA	CBA-CGA-O2A-C1
31	D	403	PHO	CBD-CGD-O2D-CED
30	18	310	CLA	C13-C15-C16-C17
30	11	306	CLA	CAA-CBA-CGA-O1A
30	14	307	CLA	CAA-CBA-CGA-O1A
30	15	308	CLA	CAA-CBA-CGA-O2A
30	16	307	CLA	CAA-CBA-CGA-O2A
30	35	308	CLA	CAA-CBA-CGA-O1A
30	35	308	CLA	CAA-CBA-CGA-O2A
30	36	307	CLA	CAA-CBA-CGA-O2A
31	d	404	PHO	CBD-CGD-O2D-CED
30	38	310	CLA	C13-C15-C16-C17
30	C	504	CLA	O2A-C1-C2-C3
30	C	510	CLA	O2A-C1-C2-C3
30	c	504	CLA	O2A-C1-C2-C3
30	c	510	CLA	O2A-C1-C2-C3
31	A	403	PHO	O2A-C1-C2-C3
31	d	403	PHO	O2A-C1-C2-C3
30	41	307	CLA	CBA-CGA-O2A-C1
30	17	301	CLA	C13-C15-C16-C17
30	37	301	CLA	C13-C15-C16-C17
30	16	302	CLA	CAA-CBA-CGA-O2A
30	36	302	CLA	CAA-CBA-CGA-O2A
30	c	509	CLA	C3-C5-C6-C7
30	15	308	CLA	CAA-CBA-CGA-O1A
30	16	307	CLA	CAA-CBA-CGA-O1A
30	18	307	CLA	CAA-CBA-CGA-O1A
30	18	307	CLA	CAA-CBA-CGA-O2A
30	19	306	CLA	CAA-CBA-CGA-O1A
30	36	307	CLA	CAA-CBA-CGA-O1A
30	38	307	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	38	307	CLA	CAA-CBA-CGA-O2A
30	39	306	CLA	CAA-CBA-CGA-O1A
30	14	302	CLA	C8-C10-C11-C12
30	B	607	CLA	CHA-CBD-CGD-O1D
30	C	507	CLA	CHA-CBD-CGD-O2D
30	C	508	CLA	CHA-CBD-CGD-O2D
30	C	513	CLA	CHA-CBD-CGD-O2D
30	b	607	CLA	CHA-CBD-CGD-O1D
30	c	507	CLA	CHA-CBD-CGD-O2D
30	c	508	CLA	CHA-CBD-CGD-O2D
30	c	513	CLA	CHA-CBD-CGD-O2D
30	16	302	CLA	CHA-CBD-CGD-O1D
30	16	302	CLA	CHA-CBD-CGD-O2D
30	16	305	CLA	CHA-CBD-CGD-O2D
30	16	307	CLA	CHA-CBD-CGD-O1D
30	17	310	CLA	CHA-CBD-CGD-O2D
30	18	306	CLA	CHA-CBD-CGD-O1D
30	18	306	CLA	CHA-CBD-CGD-O2D
30	18	309	CLA	CHA-CBD-CGD-O2D
30	18	310	CLA	CHA-CBD-CGD-O1D
30	18	310	CLA	CHA-CBD-CGD-O2D
30	19	304	CLA	CHA-CBD-CGD-O1D
30	19	304	CLA	CHA-CBD-CGD-O2D
30	19	306	CLA	CHA-CBD-CGD-O1D
30	19	306	CLA	CHA-CBD-CGD-O2D
30	20	205	CLA	CHA-CBD-CGD-O1D
30	20	205	CLA	CHA-CBD-CGD-O2D
30	20	206	CLA	CHA-CBD-CGD-O1D
30	20	206	CLA	CHA-CBD-CGD-O2D
30	20	207	CLA	CHA-CBD-CGD-O1D
30	20	208	CLA	CHA-CBD-CGD-O1D
30	20	208	CLA	CHA-CBD-CGD-O2D
30	21	303	CLA	CHA-CBD-CGD-O2D
30	21	308	CLA	CHA-CBD-CGD-O1D
30	21	308	CLA	CHA-CBD-CGD-O2D
30	21	309	CLA	CHA-CBD-CGD-O1D
30	21	309	CLA	CHA-CBD-CGD-O2D
30	36	302	CLA	CHA-CBD-CGD-O1D
30	36	302	CLA	CHA-CBD-CGD-O2D
30	36	305	CLA	CHA-CBD-CGD-O2D
30	36	307	CLA	CHA-CBD-CGD-O1D
30	37	310	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	38	306	CLA	CHA-CBD-CGD-O1D
30	38	306	CLA	CHA-CBD-CGD-O2D
30	38	309	CLA	CHA-CBD-CGD-O2D
30	38	310	CLA	CHA-CBD-CGD-O1D
30	38	310	CLA	CHA-CBD-CGD-O2D
30	39	304	CLA	CHA-CBD-CGD-O1D
30	39	304	CLA	CHA-CBD-CGD-O2D
30	39	306	CLA	CHA-CBD-CGD-O1D
30	39	306	CLA	CHA-CBD-CGD-O2D
30	40	205	CLA	CHA-CBD-CGD-O1D
30	40	205	CLA	CHA-CBD-CGD-O2D
30	40	206	CLA	CHA-CBD-CGD-O1D
30	40	206	CLA	CHA-CBD-CGD-O2D
30	40	207	CLA	CHA-CBD-CGD-O1D
30	40	208	CLA	CHA-CBD-CGD-O1D
30	40	208	CLA	CHA-CBD-CGD-O2D
30	41	303	CLA	CHA-CBD-CGD-O2D
30	41	308	CLA	CHA-CBD-CGD-O1D
30	41	308	CLA	CHA-CBD-CGD-O2D
30	41	309	CLA	CHA-CBD-CGD-O1D
30	41	309	CLA	CHA-CBD-CGD-O2D
32	B	616	BCR	C19-C20-C21-C22
32	m	103	BCR	C19-C20-C21-C22
30	d	402	CLA	C4C-C3C-CAC-CBC
39	D	404	PL9	C32-C33-C34-C36
39	d	405	PL9	C32-C33-C34-C36
30	D	402	CLA	C4C-C3C-CAC-CBC
30	41	305	CLA	C4C-C3C-CAC-CBC
32	F	101	BCR	C11-C10-C9-C8
32	f	101	BCR	C11-C10-C9-C8
30	21	305	CLA	C4C-C3C-CAC-CBC
36	D	408	LMG	C16-C17-C18-C19
30	21	307	CLA	C16-C17-C18-C20
30	41	307	CLA	C16-C17-C18-C20
30	16	304	CLA	CAA-CBA-CGA-O2A
30	17	301	CLA	CAA-CBA-CGA-O2A
30	36	304	CLA	CAA-CBA-CGA-O2A
30	37	301	CLA	CAA-CBA-CGA-O2A
38	C	517	DGD	O1G-C1G-C2G-O2G
38	c	518	DGD	O1G-C1G-C2G-O2G
36	d	410	LMG	C16-C17-C18-C19
30	11	301	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	16	307	CLA	C2A-CAA-CBA-CGA
30	36	307	CLA	C2A-CAA-CBA-CGA
30	41	309	CLA	CAA-CBA-CGA-O2A
31	D	403	PHO	CHA-CBD-CGD-O1D
31	d	404	PHO	CHA-CBD-CGD-O1D
41	17	311	A86	C10-C11-C13-O
41	21	313	A86	C10-C11-C13-O
41	37	311	A86	C10-C11-C13-O
41	41	313	A86	C10-C11-C13-O
30	40	206	CLA	C4C-C3C-CAC-CBC
30	B	605	CLA	CBA-CGA-O2A-C1
30	b	605	CLA	CBA-CGA-O2A-C1
35	d	409	LHG	C11-C12-C13-C14
35	L	101	LHG	C11-C12-C13-C14
30	d	401	CLA	CBD-CGD-O2D-CED
30	15	302	CLA	CAA-CBA-CGA-O2A
30	21	309	CLA	CAA-CBA-CGA-O2A
30	35	302	CLA	CAA-CBA-CGA-O2A
30	20	206	CLA	C4C-C3C-CAC-CBC
30	A	404	CLA	C11-C10-C8-C7
30	B	604	CLA	C11-C10-C8-C7
30	B	623	CLA	C11-C12-C13-C15
30	C	520	CLA	C6-C7-C8-C10
30	a	403	CLA	C11-C10-C8-C7
30	b	604	CLA	C11-C10-C8-C7
30	b	622	CLA	C11-C12-C13-C15
30	c	522	CLA	C6-C7-C8-C10
30	20	202	CLA	C16-C17-C18-C19
30	40	202	CLA	C16-C17-C18-C19
30	13	302	CLA	C8-C10-C11-C12
30	19	305	CLA	CAA-CBA-CGA-O2A
35	l	102	LHG	C11-C10-C9-C8
38	h	102	DGD	CDB-CEB-CFB-CGB
30	17	305	CLA	C11-C10-C8-C9
30	37	305	CLA	C11-C10-C8-C9
30	12	305	CLA	C8-C10-C11-C12
30	21	305	CLA	C2C-C3C-CAC-CBC
38	H	102	DGD	CDB-CEB-CFB-CGB
30	11	309	CLA	CAA-CBA-CGA-O1A
30	12	314	CLA	CAA-CBA-CGA-O1A
30	39	305	CLA	CAA-CBA-CGA-O2A
30	W	103	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
33	A	406	SQD	C5-C6-S-O8
33	a	405	SQD	C5-C6-S-O8
30	D	401	CLA	CBD-CGD-O2D-CED
30	41	305	CLA	C2C-C3C-CAC-CBC
30	w	103	CLA	CAA-CBA-CGA-O1A
35	L	102	LHG	C11-C10-C9-C8
30	14	310	CLA	CAA-CBA-CGA-O1A
41	12	317	A86	C-C1-C24-C25
41	32	316	A86	C-C1-C24-C25
41	34	313	A86	C-C1-C24-C25
41	35	312	A86	C-C1-C24-C25
30	C	506	CLA	C10-C11-C12-C13
30	21	303	CLA	C15-C16-C17-C18
30	B	608	CLA	C4-C3-C5-C6
30	b	608	CLA	C4-C3-C5-C6
33	A	406	SQD	C30-C31-C32-C33
30	c	506	CLA	C10-C11-C12-C13
30	13	310	CLA	CAA-CBA-CGA-O1A
30	C	521	CLA	CAA-CBA-CGA-O1A
30	c	523	CLA	CAA-CBA-CGA-O1A
33	A	406	SQD	C35-C36-C37-C38
33	a	405	SQD	C30-C31-C32-C33
33	a	405	SQD	C35-C36-C37-C38
30	c	522	CLA	C15-C16-C17-C18
30	41	303	CLA	C15-C16-C17-C18
35	B	622	LHG	C11-C12-C13-C14
30	19	303	CLA	C1A-C2A-CAA-CBA
30	20	203	CLA	C1A-C2A-CAA-CBA
30	21	308	CLA	C1A-C2A-CAA-CBA
30	39	303	CLA	C1A-C2A-CAA-CBA
30	40	203	CLA	C1A-C2A-CAA-CBA
30	41	308	CLA	C1A-C2A-CAA-CBA
35	b	621	LHG	C11-C12-C13-C14
36	B	619	LMG	C37-C38-C39-C40
36	b	618	LMG	C37-C38-C39-C40
30	15	307	CLA	CAA-CBA-CGA-O1A
30	40	202	CLA	CAA-CBA-CGA-O1A
36	c	519	LMG	C39-C40-C41-C42
30	C	520	CLA	C15-C16-C17-C18
30	20	202	CLA	CAA-CBA-CGA-O1A
30	35	307	CLA	CAA-CBA-CGA-O1A
36	Q	301	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	20	204	CLA	CAA-CBA-CGA-O2A
30	40	204	CLA	CAA-CBA-CGA-O2A
35	a	407	LHG	C18-C19-C20-C21
31	D	403	PHO	C8-C10-C11-C12
36	32	301	LMG	C31-C32-C33-C34
31	d	404	PHO	C8-C10-C11-C12
30	C	502	CLA	CAA-CBA-CGA-O1A
30	c	502	CLA	CAA-CBA-CGA-O1A
30	16	302	CLA	CAA-CBA-CGA-O1A
30	B	605	CLA	C10-C11-C12-C13
30	b	605	CLA	C10-C11-C12-C13
35	A	408	LHG	C18-C19-C20-C21
35	L	102	LHG	C17-C18-C19-C20
30	a	403	CLA	CAA-CBA-CGA-O1A
30	36	302	CLA	CAA-CBA-CGA-O1A
35	d	409	LHG	C34-C35-C36-C37
30	A	404	CLA	CAA-CBA-CGA-O1A
35	l	102	LHG	C17-C18-C19-C20
38	C	517	DGD	CCA-CDA-CEA-CFA
30	21	308	CLA	CAA-CBA-CGA-O2A
30	41	308	CLA	CAA-CBA-CGA-O2A
35	d	409	LHG	C16-C17-C18-C19
38	c	518	DGD	CCA-CDA-CEA-CFA
30	11	302	CLA	O1D-CGD-O2D-CED
30	b	607	CLA	C8-C10-C11-C12
30	37	305	CLA	C5-C6-C7-C8
35	L	101	LHG	C16-C17-C18-C19
38	j	101	DGD	CCA-CDA-CEA-CFA
30	13	303	CLA	O1D-CGD-O2D-CED
36	Q	301	LMG	C34-C35-C36-C37
39	d	408	PL9	C12-C11-C9-C10
35	L	101	LHG	C34-C35-C36-C37
36	12	301	LMG	C16-C17-C18-C19
30	17	305	CLA	C5-C6-C7-C8
30	19	308	CLA	CAA-CBA-CGA-O2A
30	39	308	CLA	CAA-CBA-CGA-O2A
30	B	607	CLA	CAD-CBD-CGD-O1D
30	b	607	CLA	CAD-CBD-CGD-O1D
30	11	307	CLA	CAD-CBD-CGD-O1D
30	12	311	CLA	CAD-CBD-CGD-O1D
30	13	308	CLA	CAD-CBD-CGD-O1D
30	14	308	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	18	307	CLA	CAD-CBD-CGD-O1D
30	18	309	CLA	CAD-CBD-CGD-O1D
30	19	301	CLA	CAD-CBD-CGD-O1D
30	21	302	CLA	CAD-CBD-CGD-O1D
30	38	307	CLA	CAD-CBD-CGD-O1D
30	38	309	CLA	CAD-CBD-CGD-O1D
30	39	301	CLA	CAD-CBD-CGD-O1D
30	41	302	CLA	CAD-CBD-CGD-O1D
41	20	211	A86	C26-C27-C29-C30
41	21	311	A86	C26-C27-C29-C30
41	40	211	A86	C26-C27-C29-C30
41	41	311	A86	C26-C27-C29-C30
30	c	508	CLA	CAA-CBA-CGA-O2A
30	B	607	CLA	C8-C10-C11-C12
30	B	607	CLA	C10-C11-C12-C13
30	b	607	CLA	C10-C11-C12-C13
36	c	519	LMG	C34-C35-C36-C37
38	J	101	DGD	CCA-CDA-CEA-CFA
30	B	605	CLA	O1A-CGA-O2A-C1
30	b	605	CLA	O1A-CGA-O2A-C1
30	16	304	CLA	C16-C17-C18-C19
30	C	506	CLA	CAA-CBA-CGA-O2A
30	C	508	CLA	CAA-CBA-CGA-O2A
30	c	506	CLA	CAA-CBA-CGA-O2A
30	21	303	CLA	CAA-CBA-CGA-O2A
30	32	305	CLA	C8-C10-C11-C12
30	33	303	CLA	C8-C10-C11-C12
30	39	308	CLA	CAA-CBA-CGA-O1A
36	M	102	LMG	C8-C9-O8-C28
36	m	102	LMG	C8-C9-O8-C28
30	21	306	CLA	C13-C15-C16-C17
30	C	514	CLA	CAA-CBA-CGA-O2A
30	C	519	CLA	CAA-CBA-CGA-O2A
30	Z	102	CLA	CAA-CBA-CGA-O2A
30	c	511	CLA	CAA-CBA-CGA-O2A
30	c	514	CLA	CAA-CBA-CGA-O2A
30	c	524	CLA	CAA-CBA-CGA-O2A
30	z	101	CLA	CAA-CBA-CGA-O2A
30	15	303	CLA	CAA-CBA-CGA-O2A
30	17	305	CLA	CAA-CBA-CGA-O2A
30	18	309	CLA	CAA-CBA-CGA-O2A
30	35	303	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	38	309	CLA	CAA-CBA-CGA-O2A
30	31	301	CLA	C8-C10-C11-C12
30	34	302	CLA	C8-C10-C11-C12
30	41	306	CLA	C13-C15-C16-C17
30	31	309	CLA	CAA-CBA-CGA-O1A
30	34	310	CLA	CAA-CBA-CGA-O1A
30	C	504	CLA	C3-C5-C6-C7
30	c	504	CLA	C3-C5-C6-C7
30	16	304	CLA	CAA-CBA-CGA-O1A
30	36	304	CLA	CAA-CBA-CGA-O1A
30	33	306	CLA	C2C-C3C-CAC-CBC
39	D	407	PL9	C12-C11-C9-C10
30	40	204	CLA	C8-C10-C11-C12
41	33	314	A86	C-C1-C24-C25
41	37	313	A86	C-C1-C24-C25
30	B	604	CLA	C11-C12-C13-C15
30	B	610	CLA	C11-C10-C8-C7
30	B	610	CLA	C11-C12-C13-C15
30	C	502	CLA	C12-C13-C15-C16
30	b	604	CLA	C11-C12-C13-C15
30	b	610	CLA	C11-C10-C8-C7
30	b	610	CLA	C11-C12-C13-C15
30	c	502	CLA	C12-C13-C15-C16
30	11	302	CLA	C3A-C2A-CAA-CBA
30	12	306	CLA	C3A-C2A-CAA-CBA
30	13	303	CLA	C3A-C2A-CAA-CBA
30	14	303	CLA	C3A-C2A-CAA-CBA
30	15	301	CLA	C12-C13-C15-C16
30	17	303	CLA	C2-C3-C5-C6
30	18	305	CLA	C11-C10-C8-C7
30	31	302	CLA	C3A-C2A-CAA-CBA
30	32	306	CLA	C3A-C2A-CAA-CBA
30	33	304	CLA	C3A-C2A-CAA-CBA
30	34	303	CLA	C3A-C2A-CAA-CBA
30	35	301	CLA	C12-C13-C15-C16
30	37	303	CLA	C2-C3-C5-C6
30	38	305	CLA	C11-C10-C8-C7
30	17	301	CLA	CAA-CBA-CGA-O1A
30	37	301	CLA	CAA-CBA-CGA-O1A
36	D	408	LMG	O9-C10-C11-C12
36	d	410	LMG	O9-C10-C11-C12
38	C	516	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
30	12	314	CLA	CAA-CBA-CGA-O2A
30	13	310	CLA	CAA-CBA-CGA-O2A
30	14	310	CLA	CAA-CBA-CGA-O2A
30	15	309	CLA	CAA-CBA-CGA-O2A
30	18	312	CLA	CAA-CBA-CGA-O2A
30	19	308	CLA	CAA-CBA-CGA-O1A
30	32	313	CLA	CAA-CBA-CGA-O1A
30	33	311	CLA	CAA-CBA-CGA-O1A
30	35	309	CLA	CAA-CBA-CGA-O2A
30	38	312	CLA	CAA-CBA-CGA-O2A
30	14	303	CLA	O1D-CGD-O2D-CED
30	C	511	CLA	CAA-CBA-CGA-O2A
30	11	303	CLA	CAA-CBA-CGA-O2A
30	12	307	CLA	CAA-CBA-CGA-O2A
30	13	304	CLA	CAA-CBA-CGA-O2A
30	14	304	CLA	CAA-CBA-CGA-O2A
30	18	305	CLA	CAA-CBA-CGA-O2A
30	21	306	CLA	CAA-CBA-CGA-O2A
30	31	301	CLA	CAA-CBA-CGA-O2A
30	31	303	CLA	CAA-CBA-CGA-O2A
30	32	305	CLA	CAA-CBA-CGA-O2A
30	32	307	CLA	CAA-CBA-CGA-O2A
30	33	303	CLA	CAA-CBA-CGA-O2A
30	33	305	CLA	CAA-CBA-CGA-O2A
30	34	302	CLA	CAA-CBA-CGA-O2A
30	34	304	CLA	CAA-CBA-CGA-O2A
30	37	305	CLA	CAA-CBA-CGA-O2A
30	38	305	CLA	CAA-CBA-CGA-O2A
30	41	303	CLA	CAA-CBA-CGA-O2A
30	41	306	CLA	CAA-CBA-CGA-O2A
30	20	204	CLA	C8-C10-C11-C12
30	37	303	CLA	C4C-C3C-CAC-CBC
32	B	618	BCR	C17-C18-C19-C20
32	C	515	BCR	C17-C18-C19-C20
32	b	617	BCR	C17-C18-C19-C20
32	c	516	BCR	C17-C18-C19-C20
41	11	310	A86	C2-C1-C24-C25
41	12	315	A86	C2-C1-C24-C25
41	13	311	A86	C2-C1-C24-C25
41	14	311	A86	C2-C1-C24-C25
41	15	310	A86	C2-C1-C24-C25
41	18	313	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
41	19	310	A86	C2-C1-C24-C25
41	31	310	A86	C2-C1-C24-C25
41	32	314	A86	C2-C1-C24-C25
41	33	312	A86	C2-C1-C24-C25
41	34	311	A86	C2-C1-C24-C25
41	35	310	A86	C2-C1-C24-C25
41	38	313	A86	C2-C1-C24-C25
41	39	310	A86	C2-C1-C24-C25
30	C	506	CLA	CAA-CBA-CGA-O1A
30	c	506	CLA	CAA-CBA-CGA-O1A
30	18	305	CLA	CAA-CBA-CGA-O1A
30	20	204	CLA	CAA-CBA-CGA-O1A
30	38	305	CLA	CAA-CBA-CGA-O1A
30	40	204	CLA	CAA-CBA-CGA-O1A
38	c	517	DGD	O1B-C1B-C2B-C3B
30	21	308	CLA	CAA-CBA-CGA-O1A
30	41	308	CLA	CAA-CBA-CGA-O1A
32	Y	101	BCR	C19-C20-C21-C22
32	c	520	BCR	C19-C20-C21-C22
36	B	620	LMG	C20-C21-C22-C23
30	20	202	CLA	C16-C17-C18-C20
30	40	202	CLA	C16-C17-C18-C20
41	11	316	A86	O-C13-C14-C15
41	12	304	A86	O-C13-C14-C15
41	13	301	A86	O-C13-C14-C15
41	13	316	A86	O-C13-C14-C15
41	15	315	A86	O-C13-C14-C15
41	15	316	A86	O-C13-C14-C15
41	17	315	A86	O-C13-C14-C15
41	18	302	A86	O-C13-C14-C15
41	31	316	A86	O-C13-C14-C15
41	32	304	A86	O-C13-C14-C15
41	33	302	A86	O-C13-C14-C15
41	33	316	A86	O-C13-C14-C15
41	35	315	A86	O-C13-C14-C15
41	35	316	A86	O-C13-C14-C15
41	37	315	A86	O-C13-C14-C15
41	38	302	A86	O-C13-C14-C15
30	19	303	CLA	CAA-CBA-CGA-O2A
30	39	303	CLA	CAA-CBA-CGA-O2A
38	C	517	DGD	O6D-C1D-O3G-C3G
38	c	518	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
30	b	602	CLA	C13-C15-C16-C17
30	18	309	CLA	C13-C15-C16-C17
30	38	309	CLA	C13-C15-C16-C17
36	b	619	LMG	C20-C21-C22-C23
30	C	508	CLA	CAA-CBA-CGA-O1A
30	C	511	CLA	CAA-CBA-CGA-O1A
30	c	508	CLA	CAA-CBA-CGA-O1A
30	c	511	CLA	CAA-CBA-CGA-O1A
33	A	406	SQD	O49-C7-C8-C9
39	D	407	PL9	C44-C46-C47-C48
39	d	408	PL9	C44-C46-C47-C48
30	11	309	CLA	CAA-CBA-CGA-O2A
30	17	303	CLA	C4C-C3C-CAC-CBC
38	h	102	DGD	C8A-C9A-CAA-CBA
30	B	602	CLA	C13-C15-C16-C17
39	D	407	PL9	C31-C32-C33-C34
39	d	408	PL9	C31-C32-C33-C34
30	31	304	CLA	C2C-C3C-CAC-CBC
38	H	102	DGD	C8A-C9A-CAA-CBA
30	z	101	CLA	CAA-CBA-CGA-O1A
30	21	306	CLA	CAA-CBA-CGA-O1A
30	41	306	CLA	CAA-CBA-CGA-O1A
33	a	405	SQD	O49-C7-C8-C9
30	21	301	CLA	C2A-CAA-CBA-CGA
30	41	301	CLA	C2A-CAA-CBA-CGA
30	36	304	CLA	C16-C17-C18-C19
30	18	312	CLA	CAA-CBA-CGA-O1A
30	35	309	CLA	CAA-CBA-CGA-O1A
30	17	307	CLA	C2C-C3C-CAC-CBC
30	32	308	CLA	C2C-C3C-CAC-CBC
30	C	519	CLA	CAA-CBA-CGA-O1A
30	Z	102	CLA	CAA-CBA-CGA-O1A
30	15	309	CLA	CAA-CBA-CGA-O1A
30	38	312	CLA	CAA-CBA-CGA-O1A

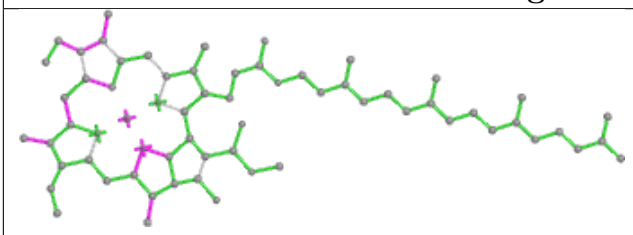
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	17	302	A86	C31-C32-C33-C34-C35-C36
41	37	302	A86	C31-C32-C33-C34-C35-C36

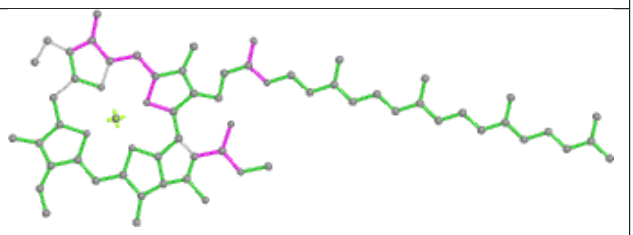
No monomer is involved in short contacts.

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

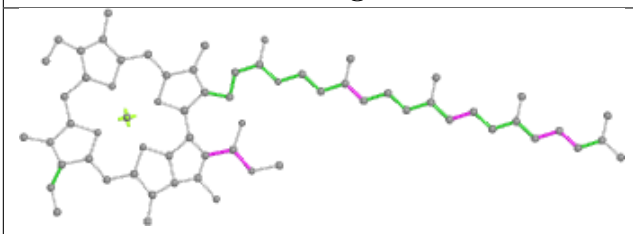
Ligand CLA b 608



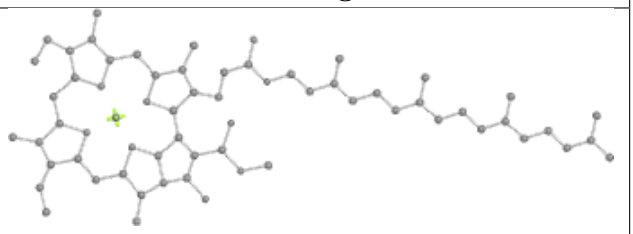
Bond lengths



Bond angles

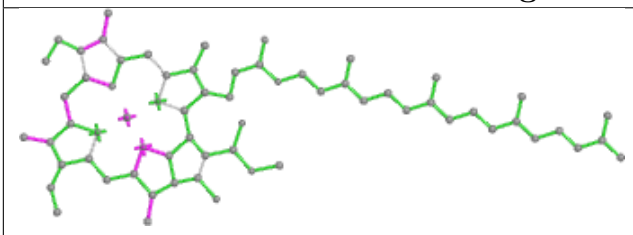


Torsions

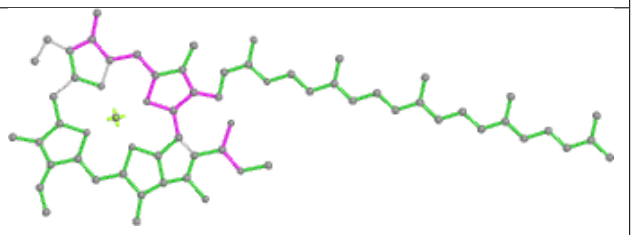


Rings

Ligand CLA 32 303



Bond lengths



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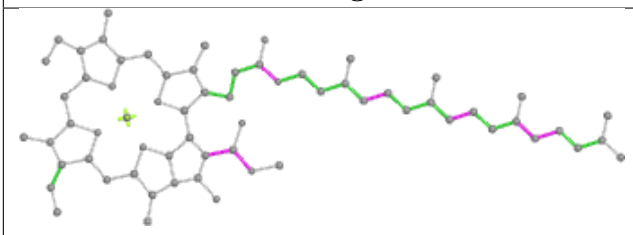

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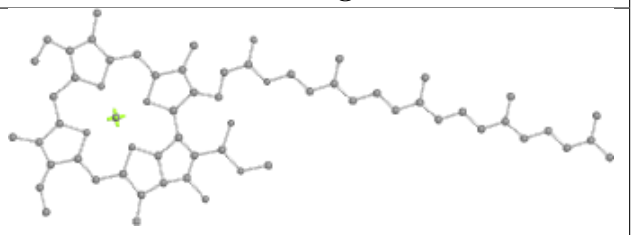
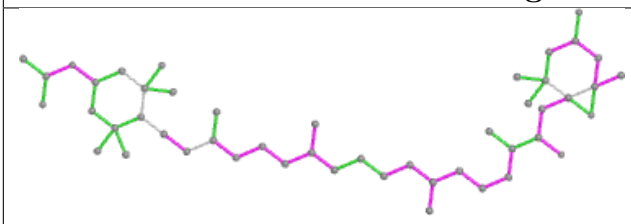
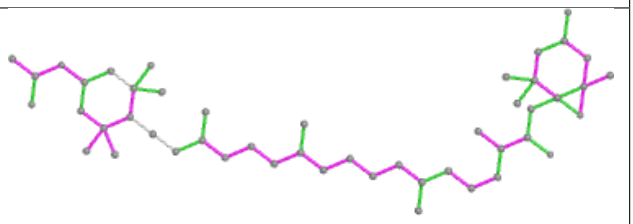


Rings

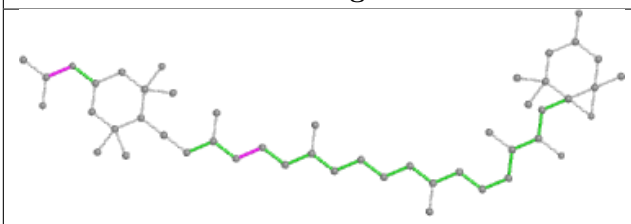
Ligand A86 11 311



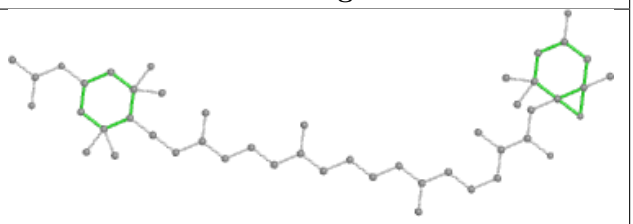
Bond lengths



Bond angles

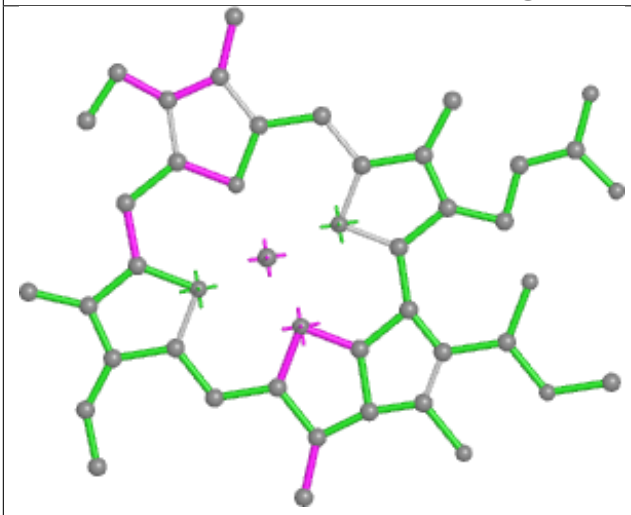


Torsions

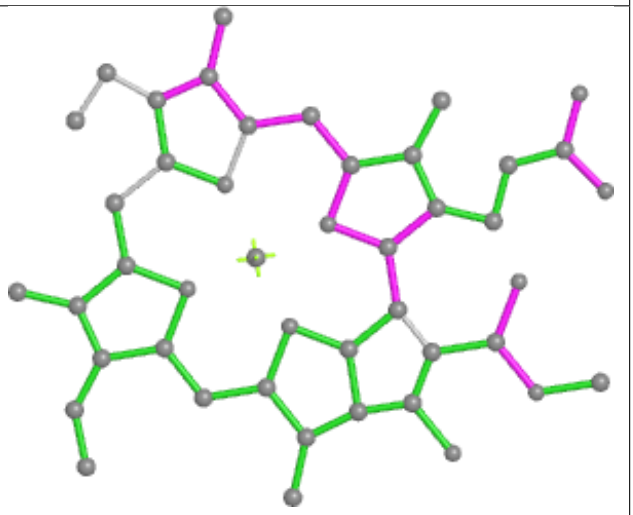


Rings

Ligand CLA 34 307



Bond lengths



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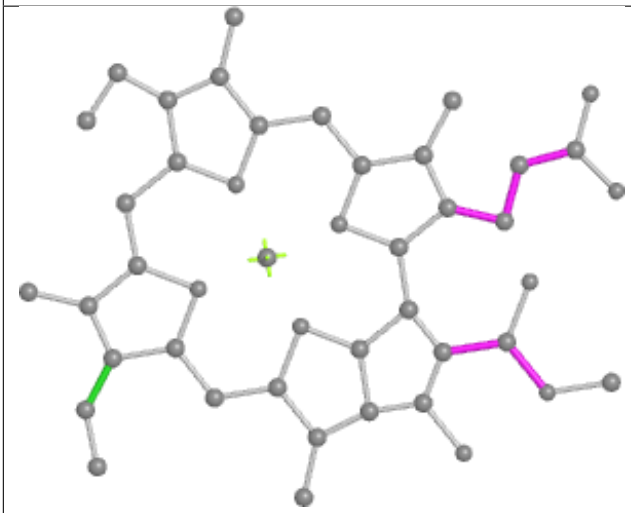
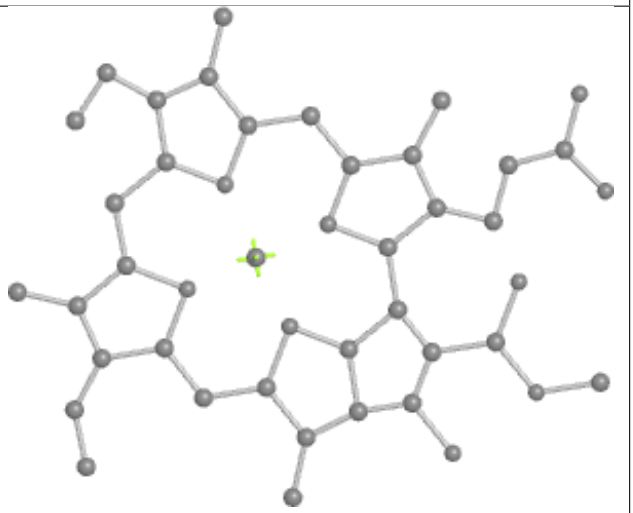
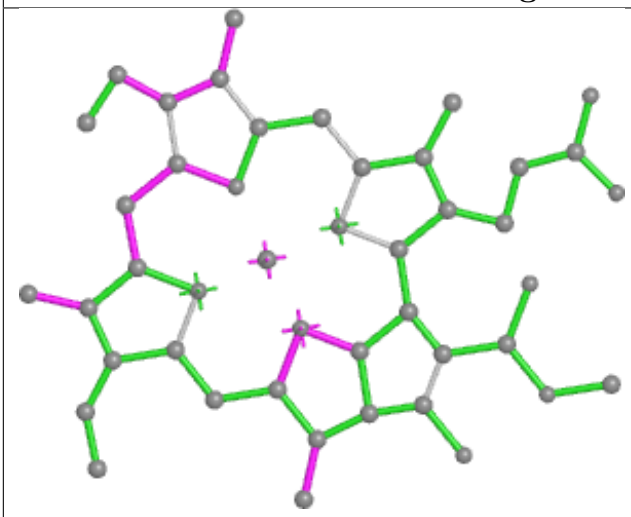


Torsions



Rings

Ligand CLA 34 309



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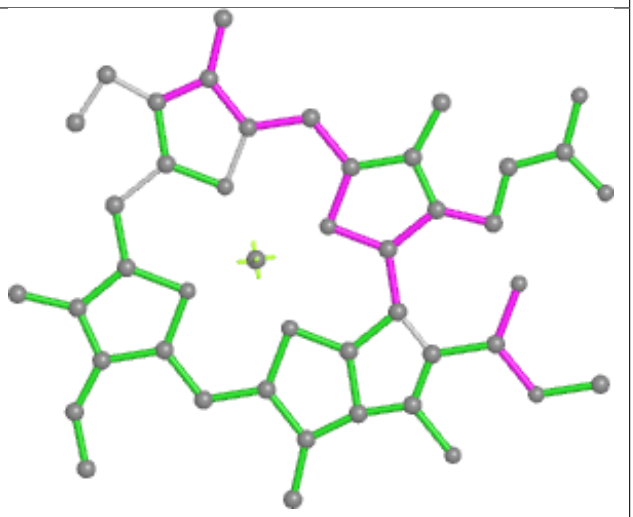

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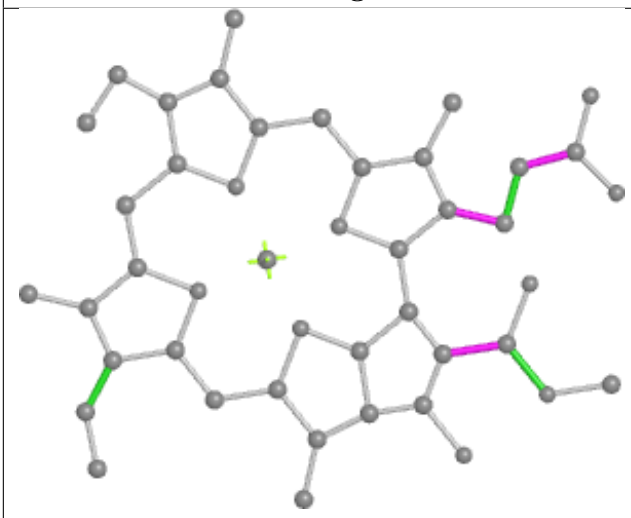

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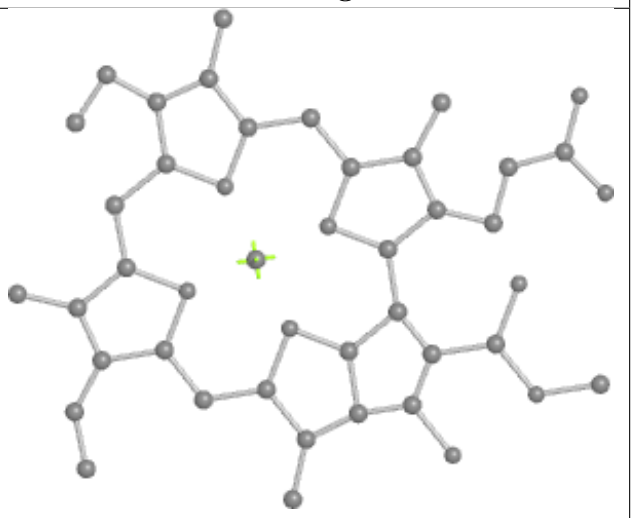
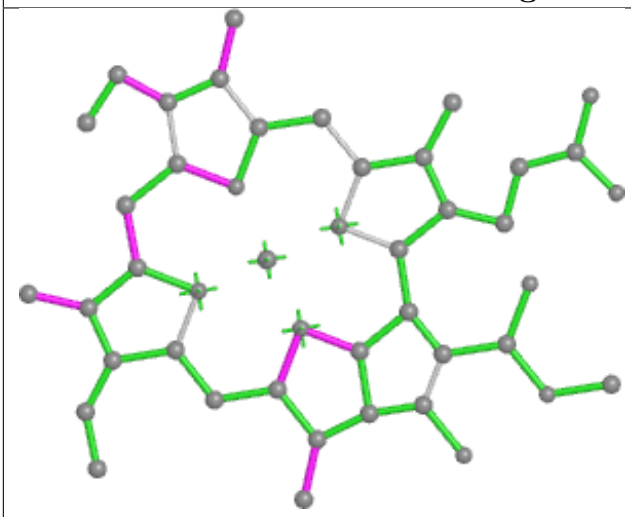


Rings

Ligand CLA 32 309



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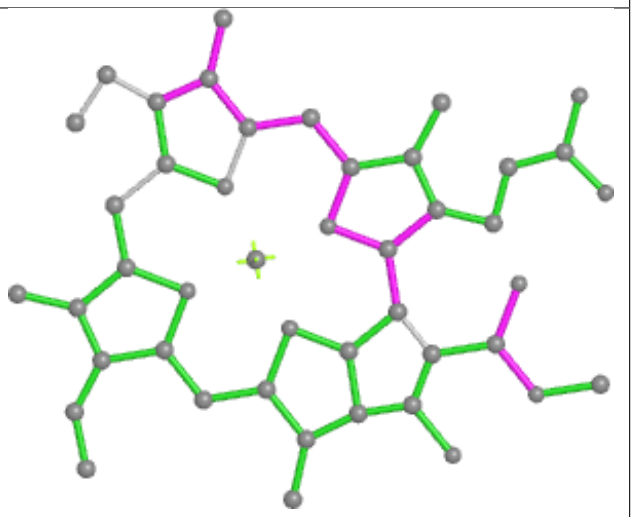

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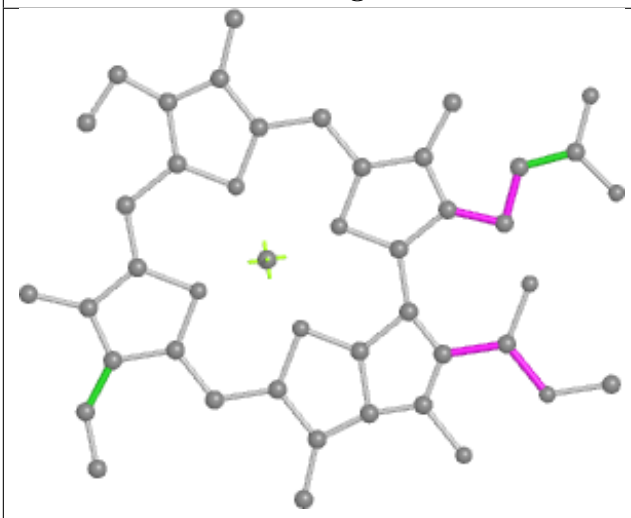

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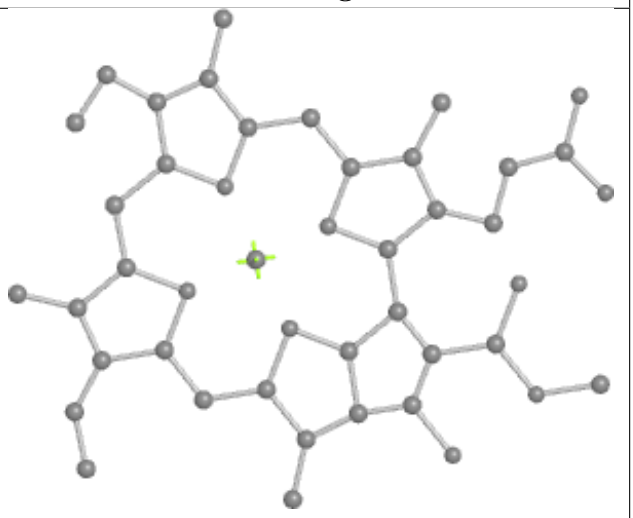
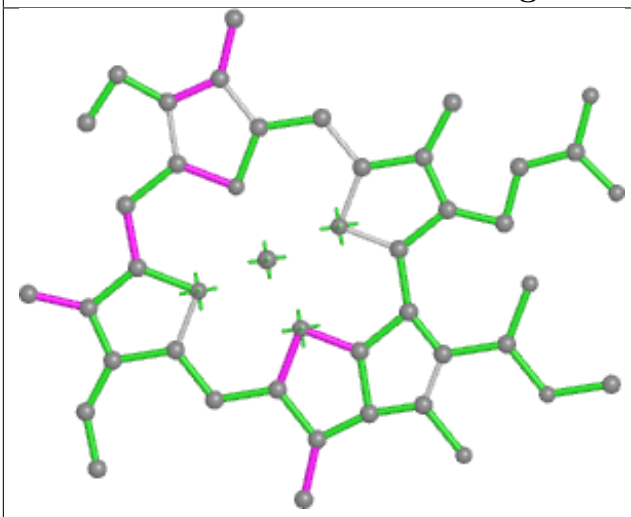


Rings

Ligand CLA 35 302



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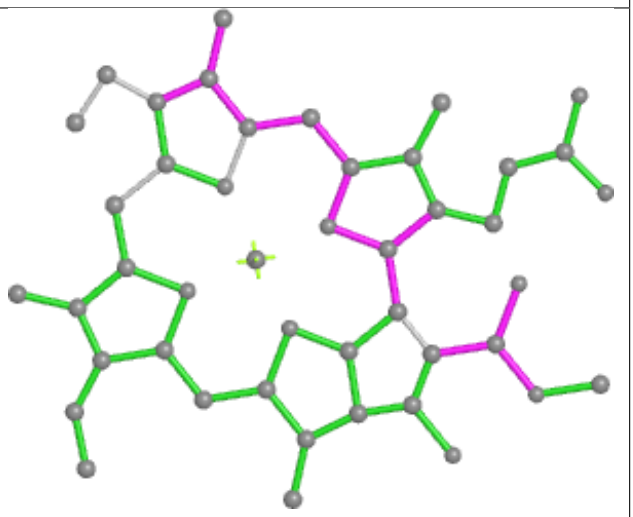

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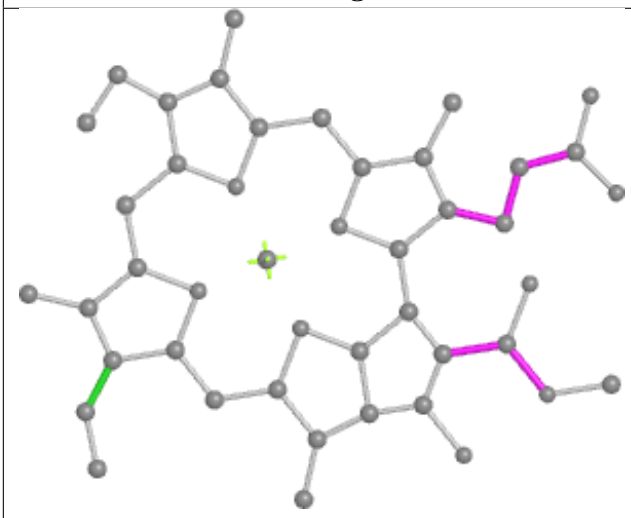

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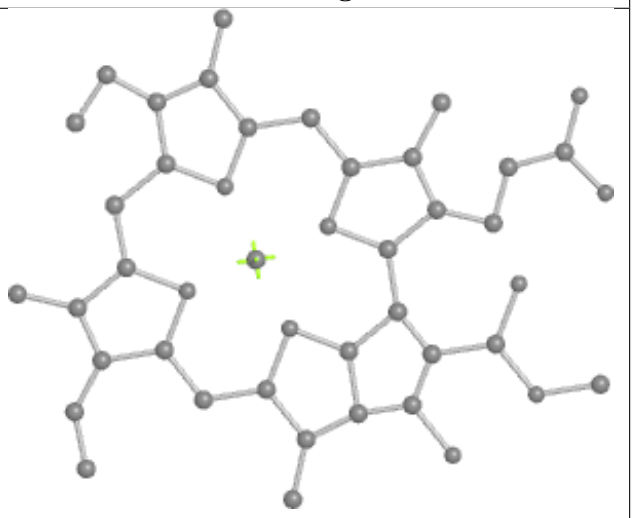
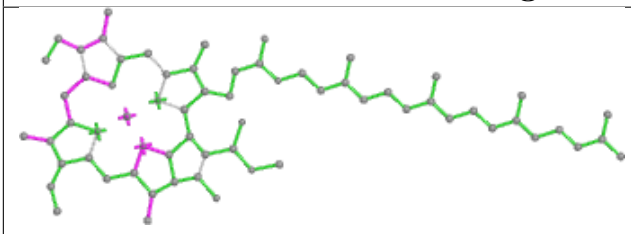


Rings

Ligand CLA 32 307



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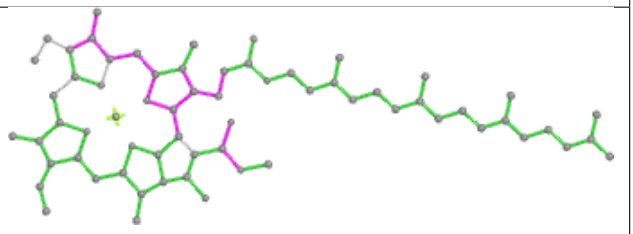

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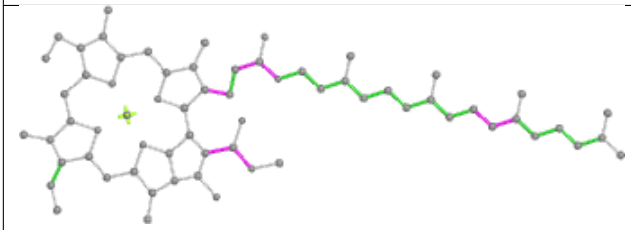

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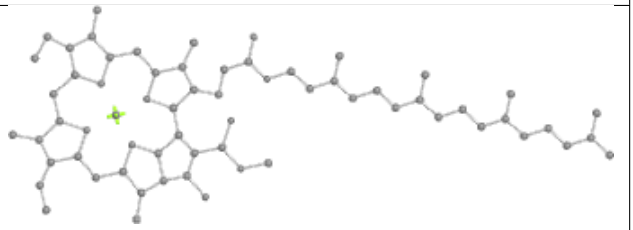
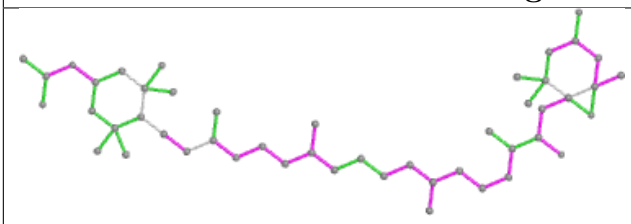


Rings

Ligand A86 40 210



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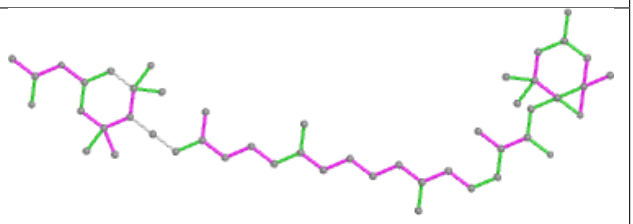

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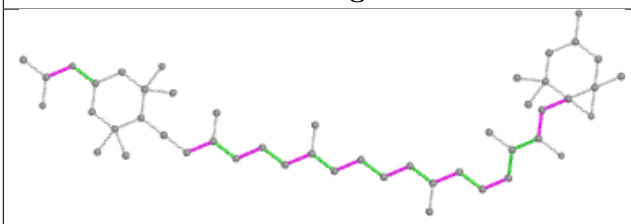

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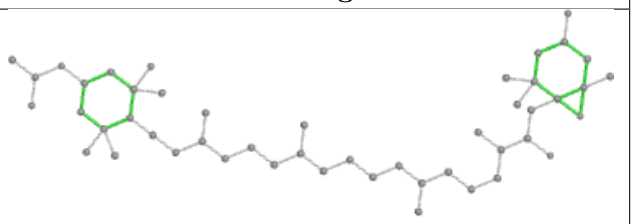
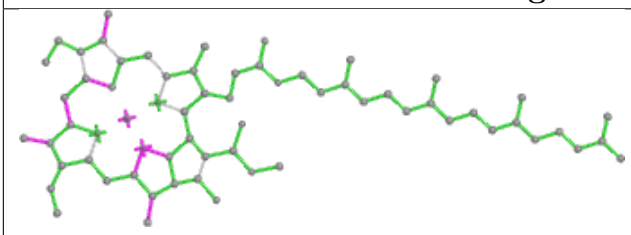


Rings

Ligand CLA a 402



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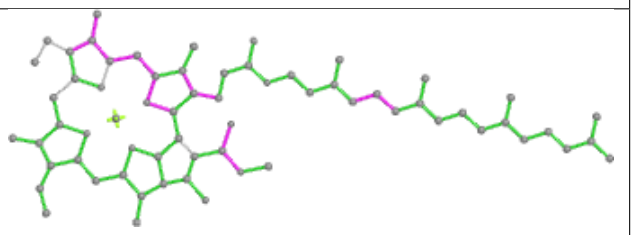

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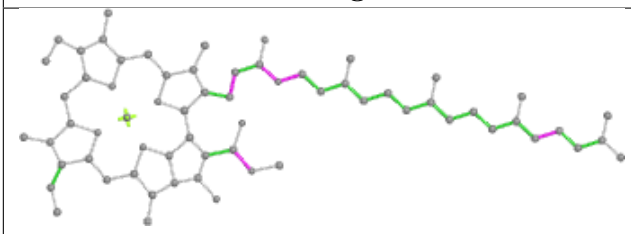

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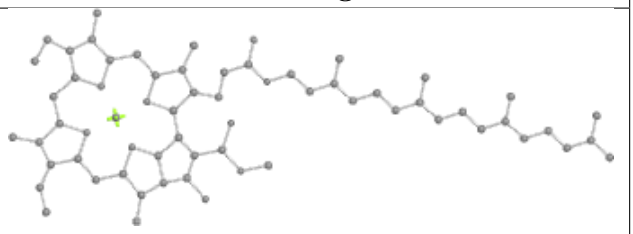
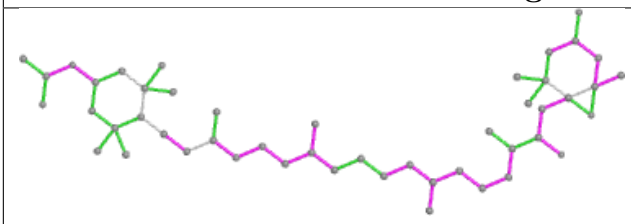


Rings

Ligand A86 16 313



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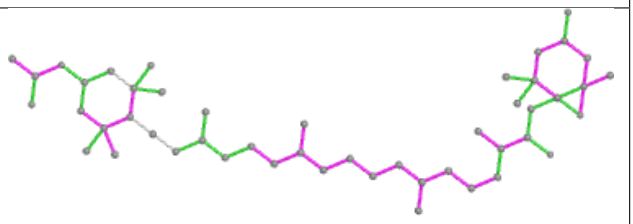

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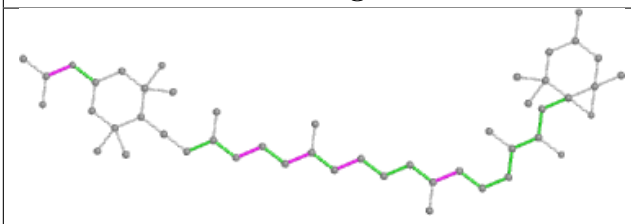

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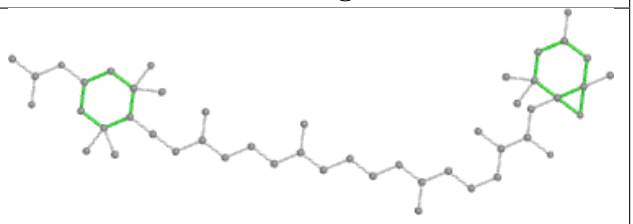
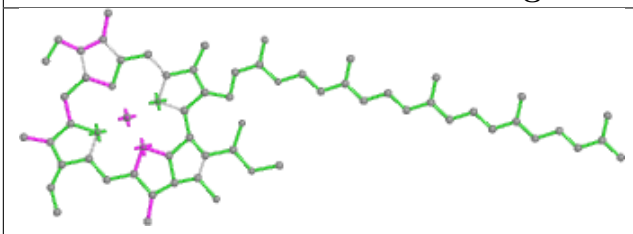


Rings

Ligand CLA A 404



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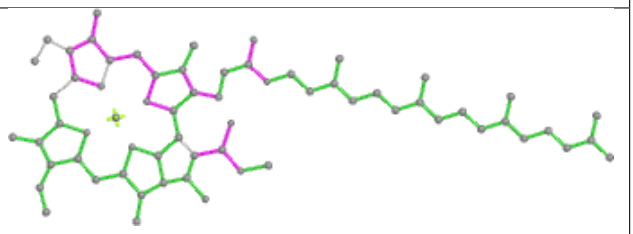

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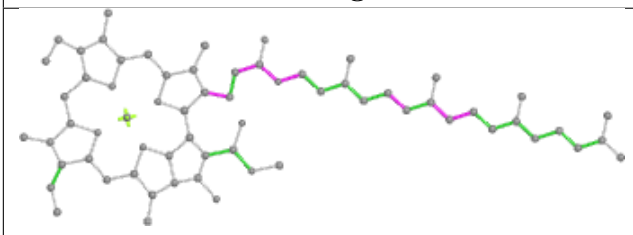

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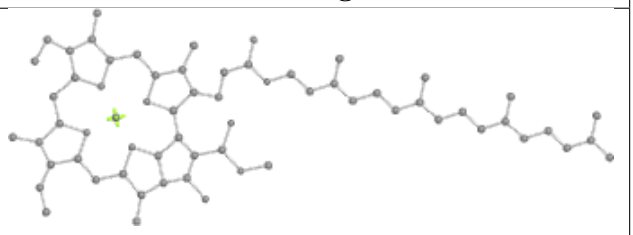
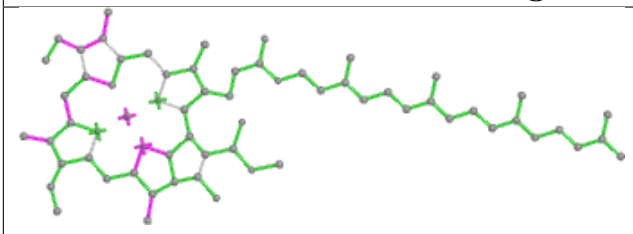


Rings

Ligand CLA b 609



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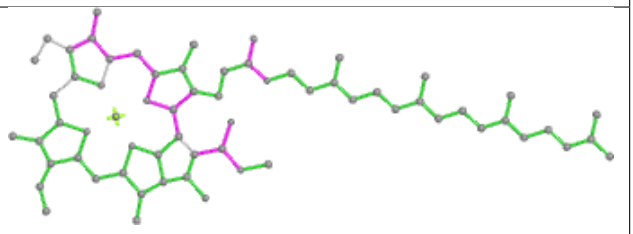

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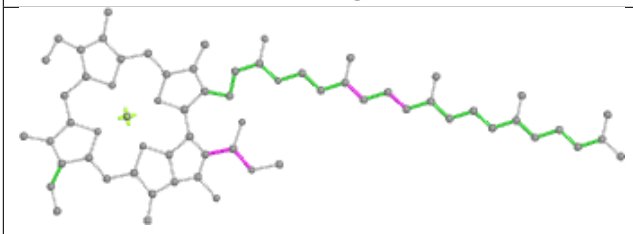

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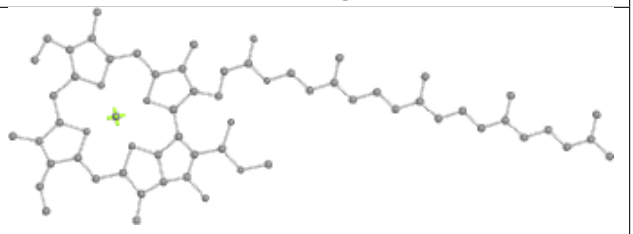
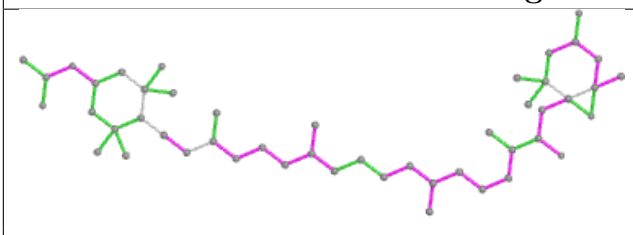


Rings

Ligand A86 21 314



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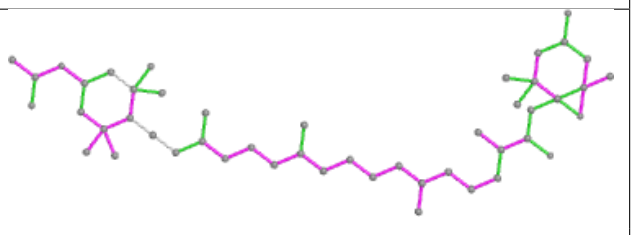

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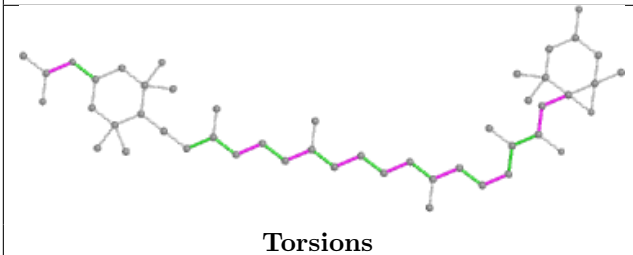

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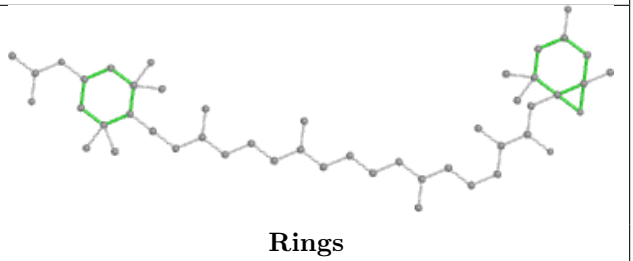
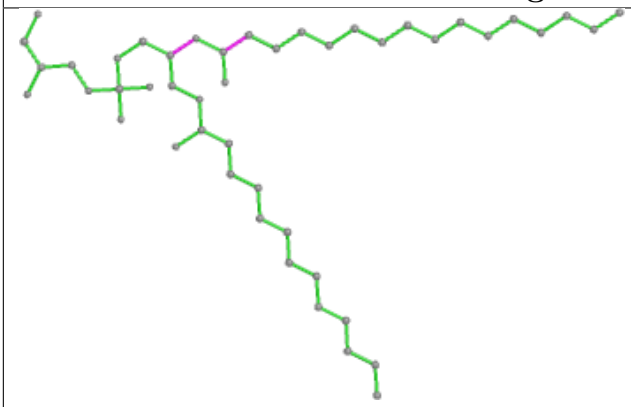


Rings

Ligand LHG a 407



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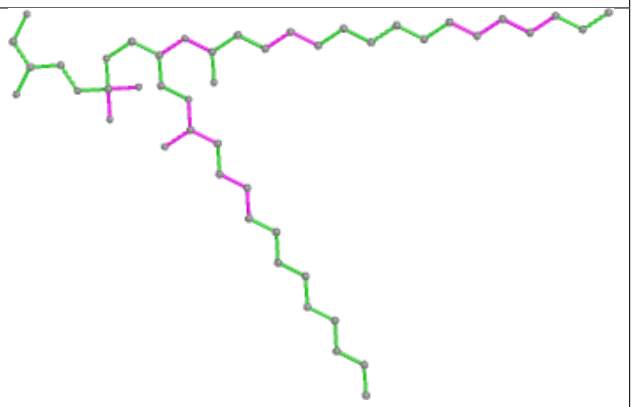
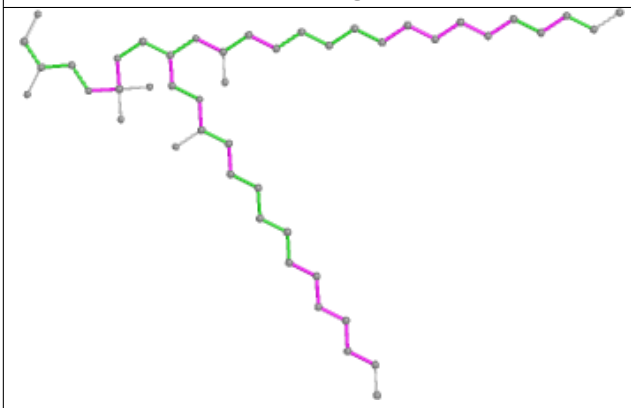


Bond angles



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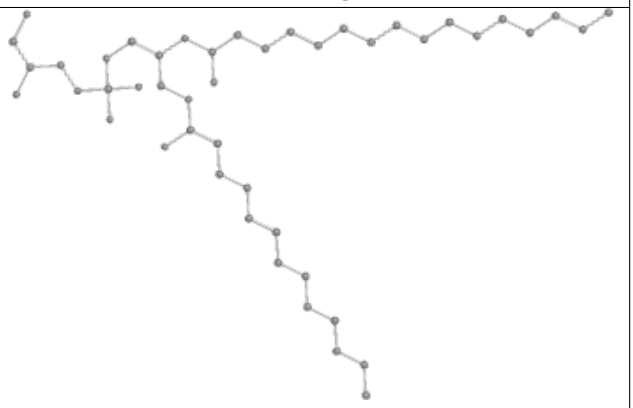
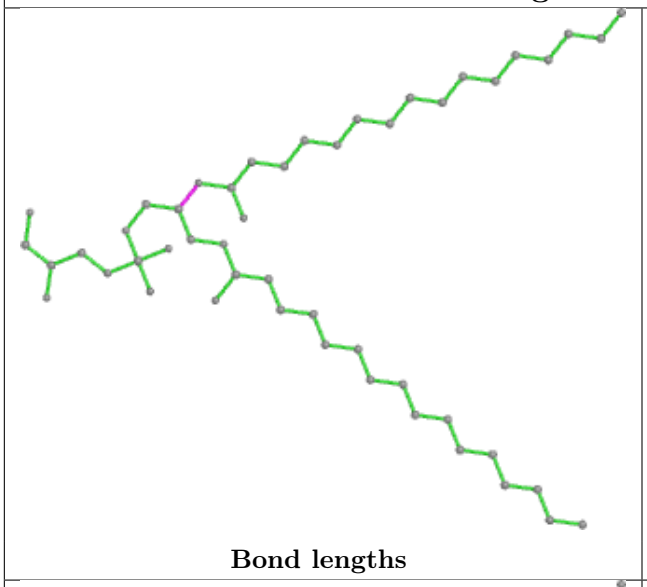


Rings

Ligand LHG l 102



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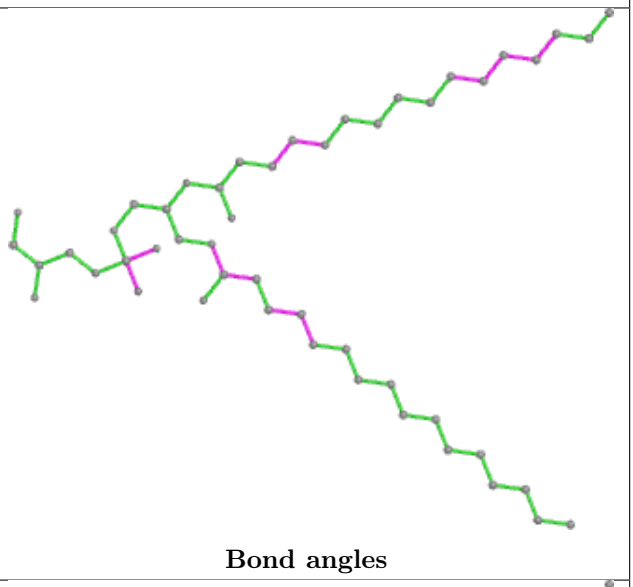
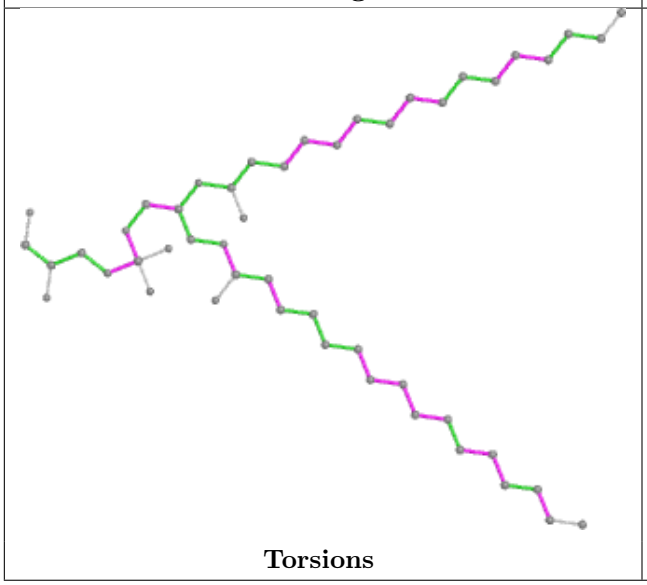
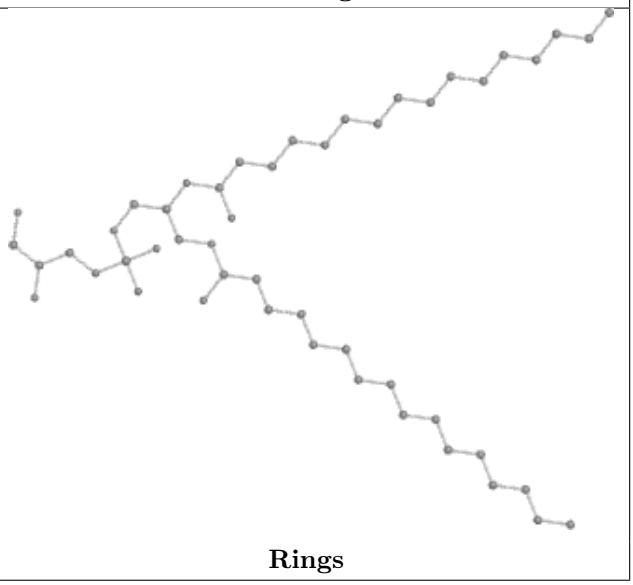


Bond angles

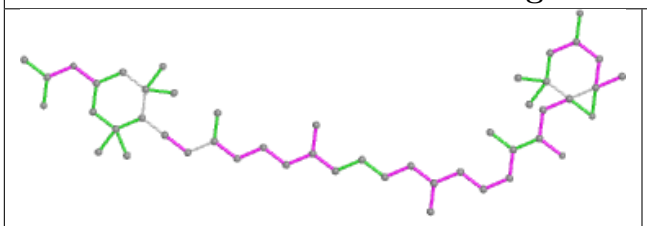


Torsions



Rings

Ligand A86 38 315



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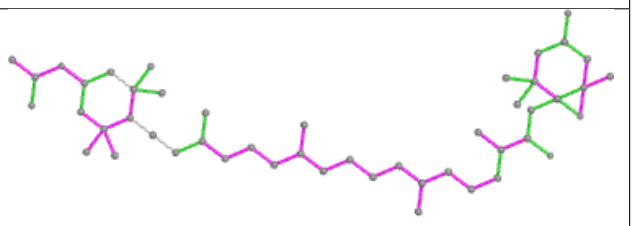
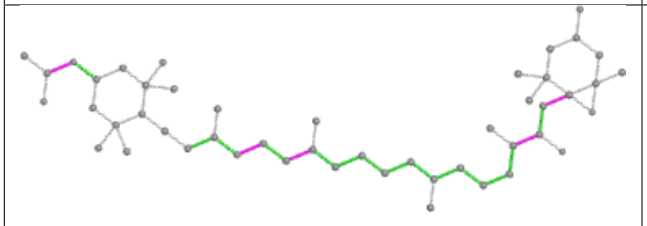
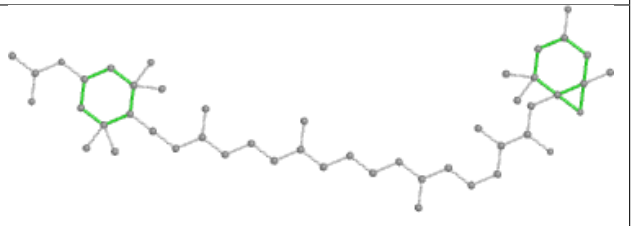


Bond angles

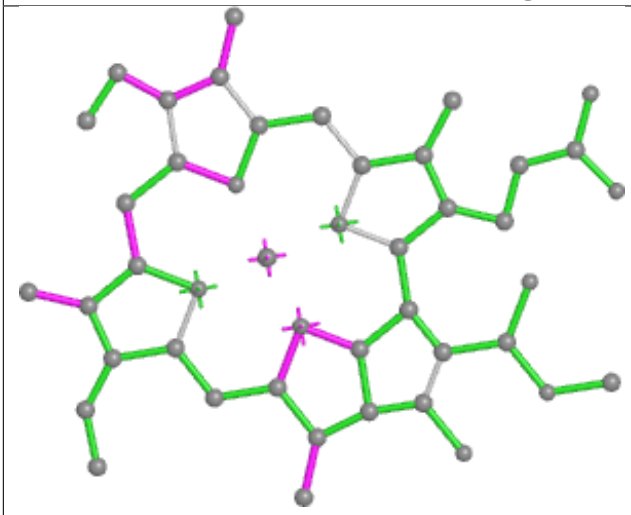


Torsions



Rings

Ligand CLA 36 307



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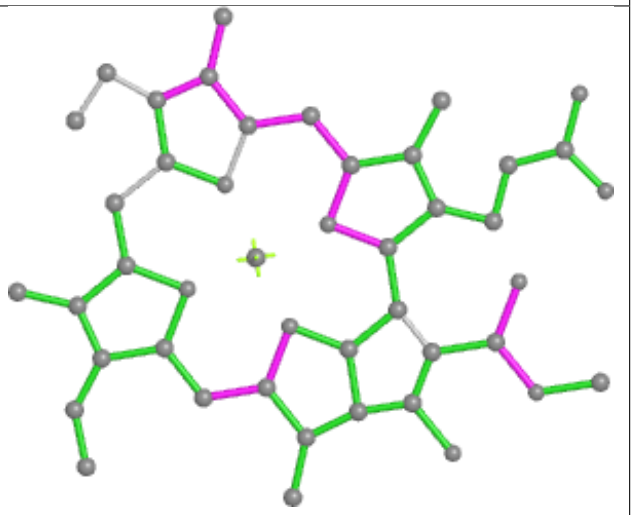

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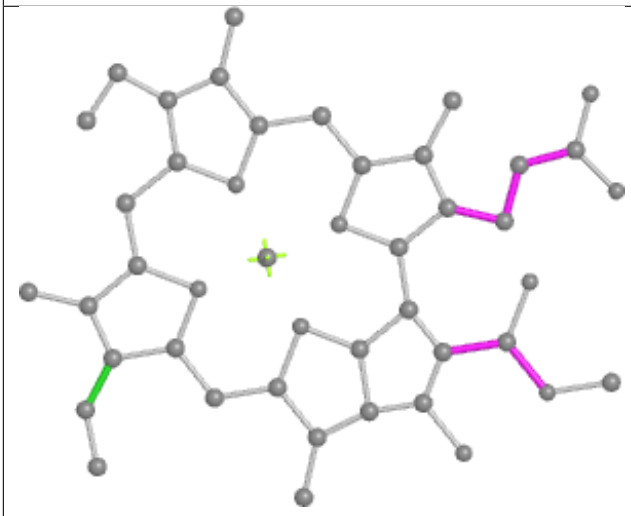
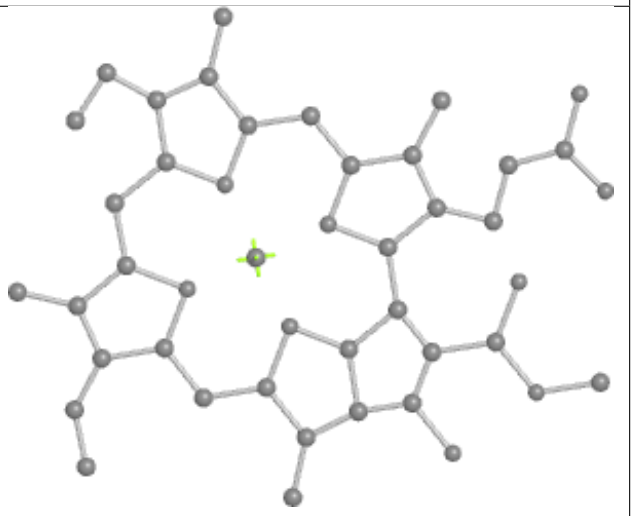
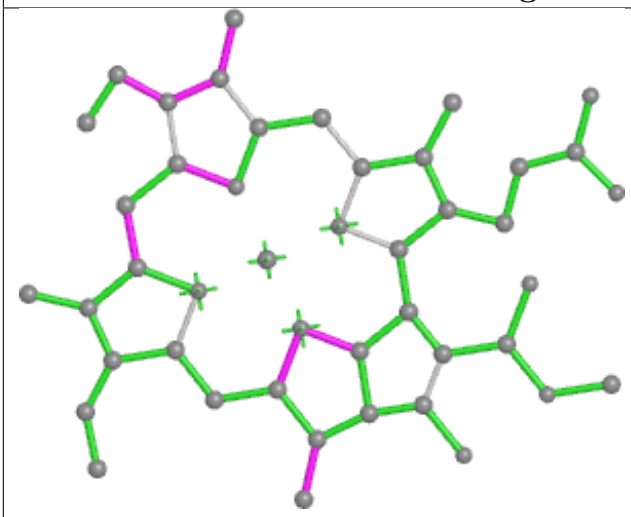


Torsions



Rings

Ligand CLA 12 310



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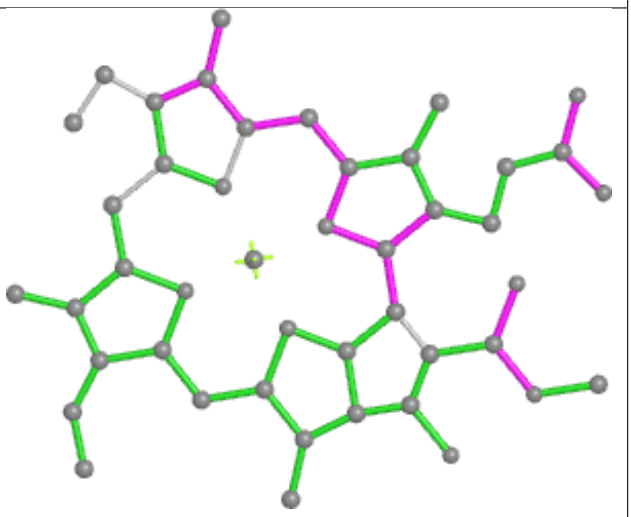

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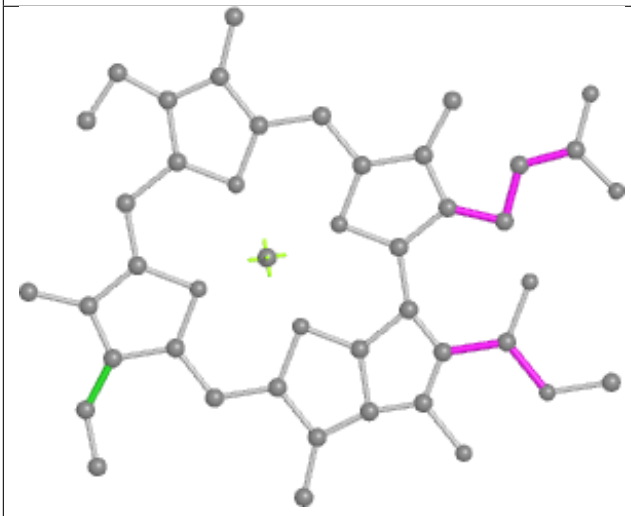

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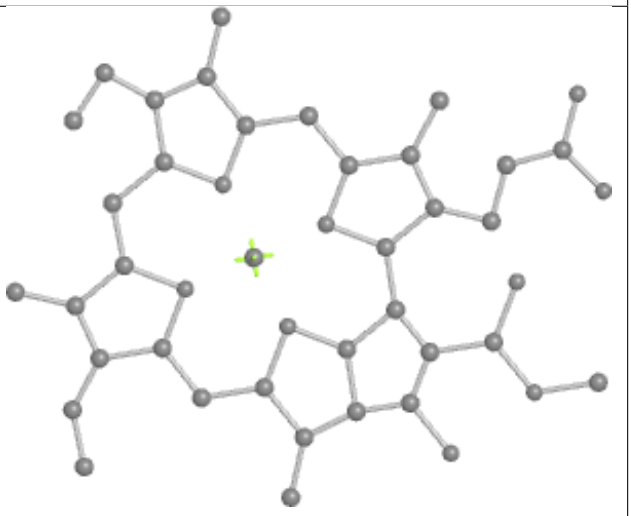
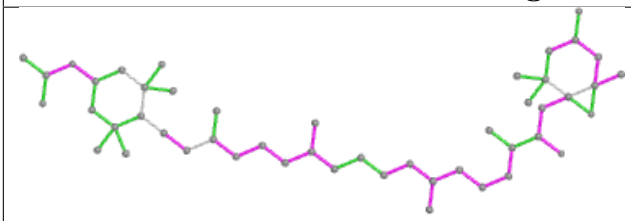


Rings

Ligand A86 35 311



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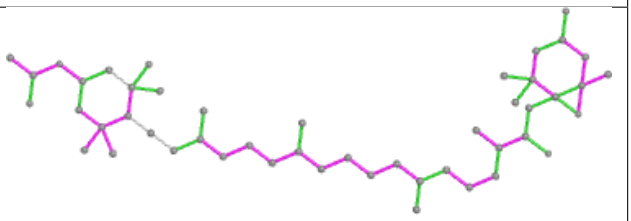

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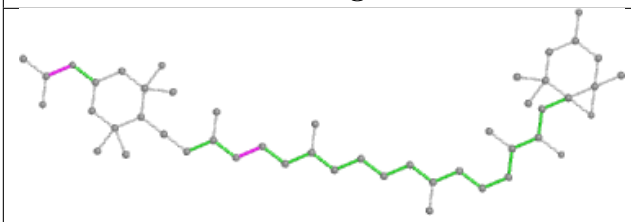

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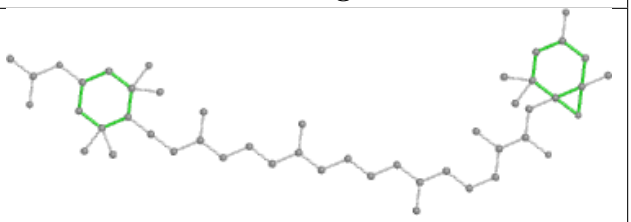
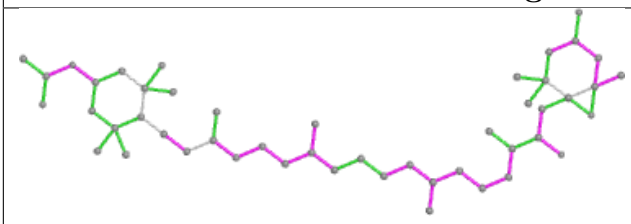


Rings

Ligand A86 37 311



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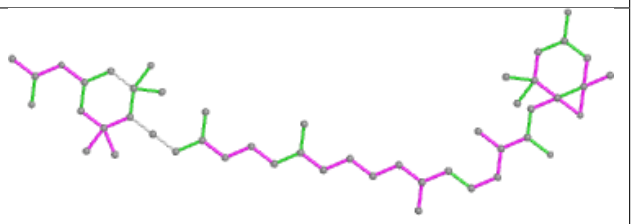

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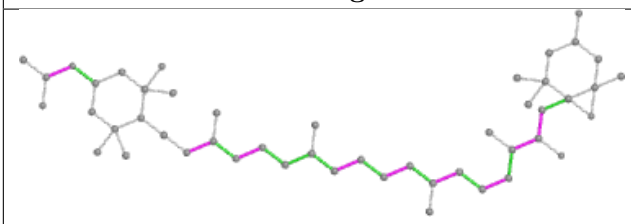

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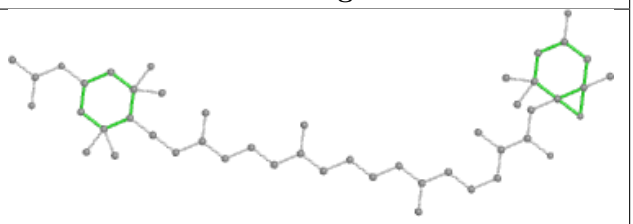
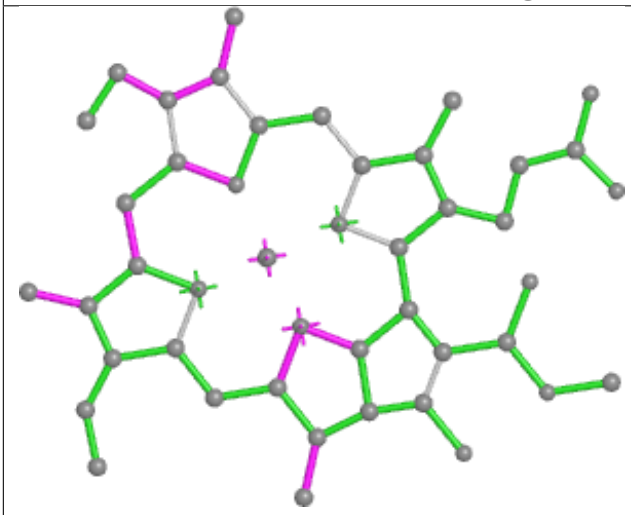


Rings

Ligand CLA 19 305



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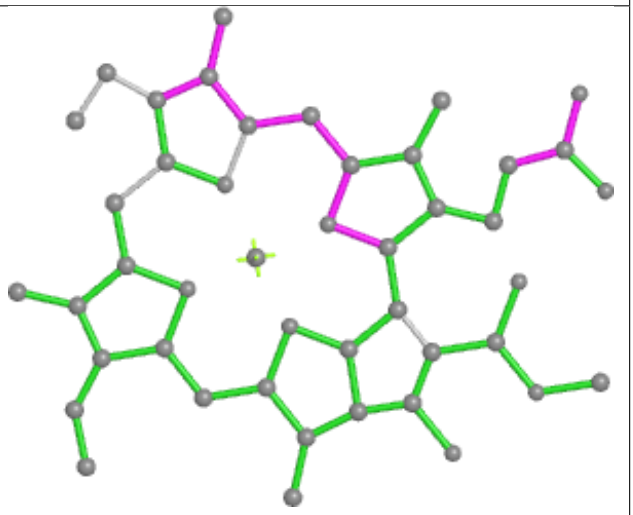

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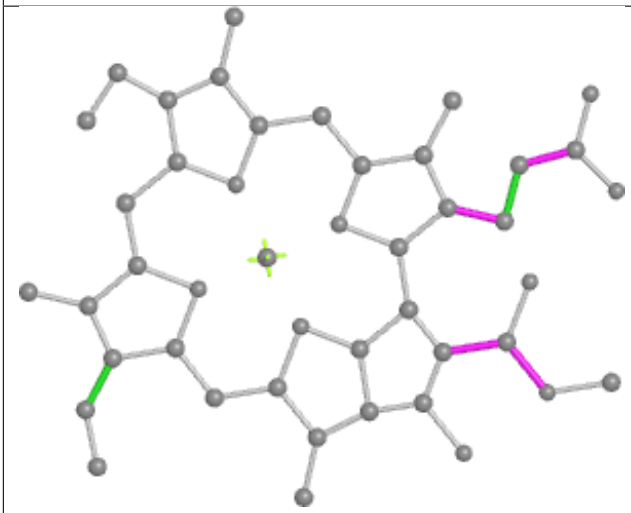

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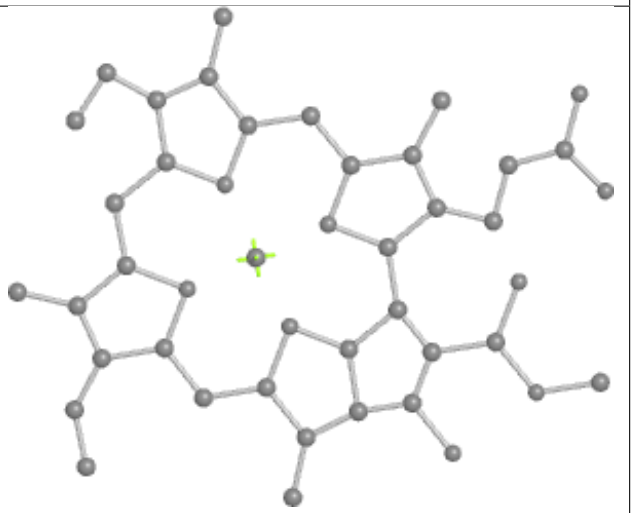

Rings

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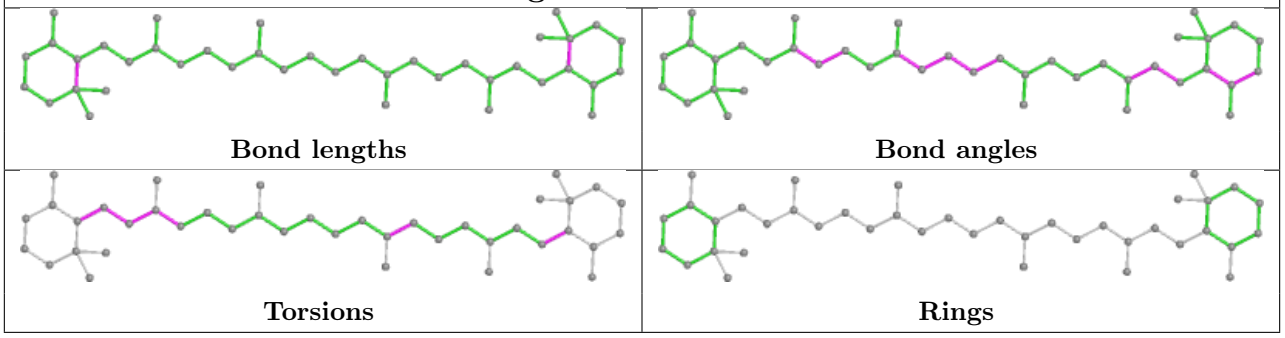

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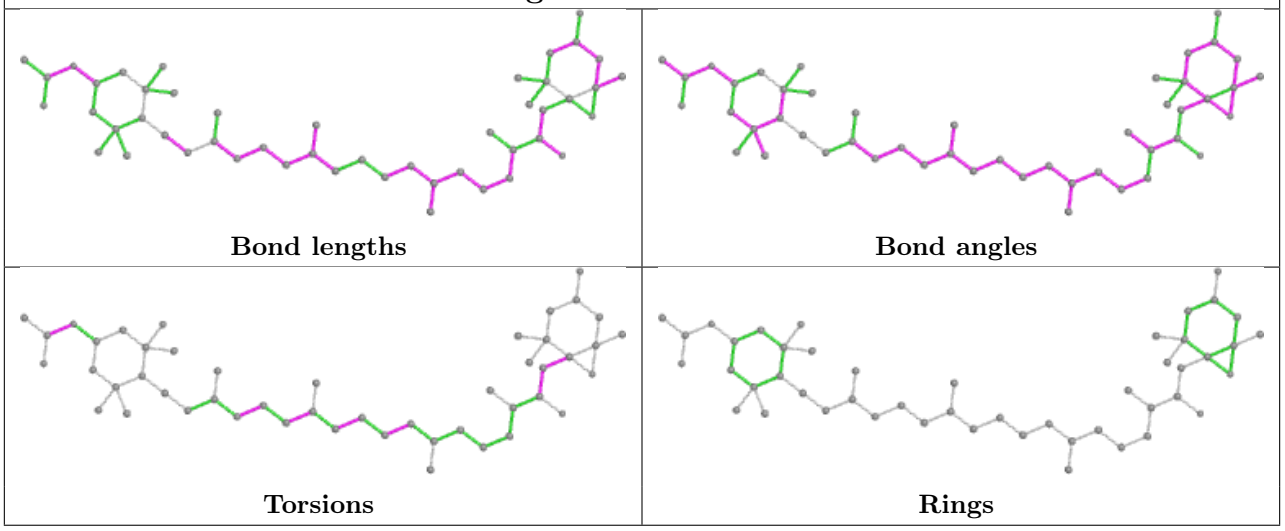

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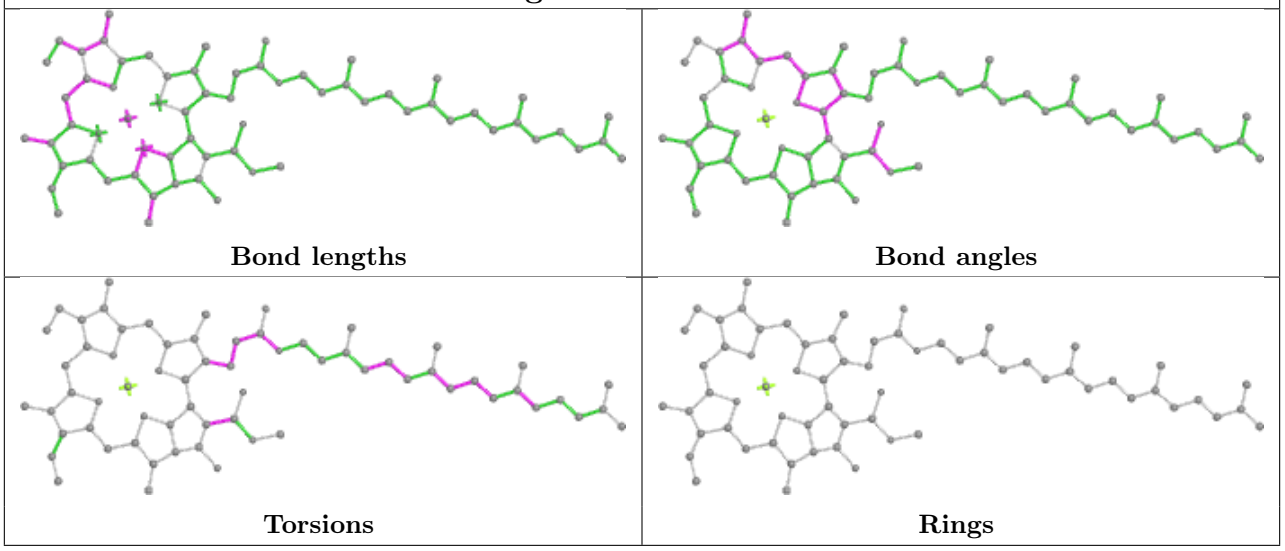

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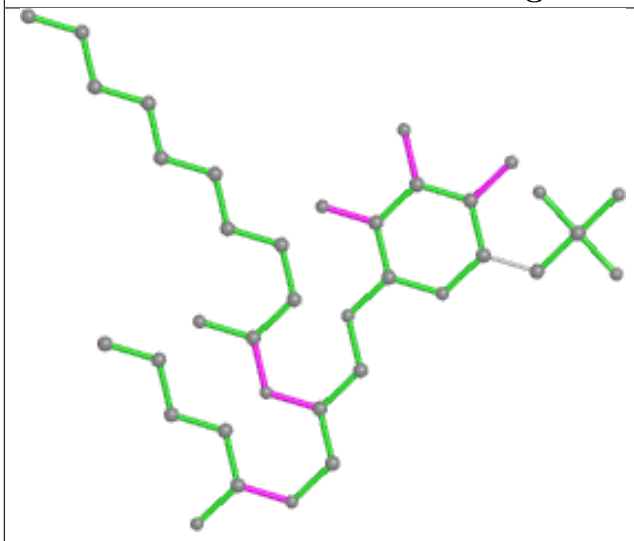
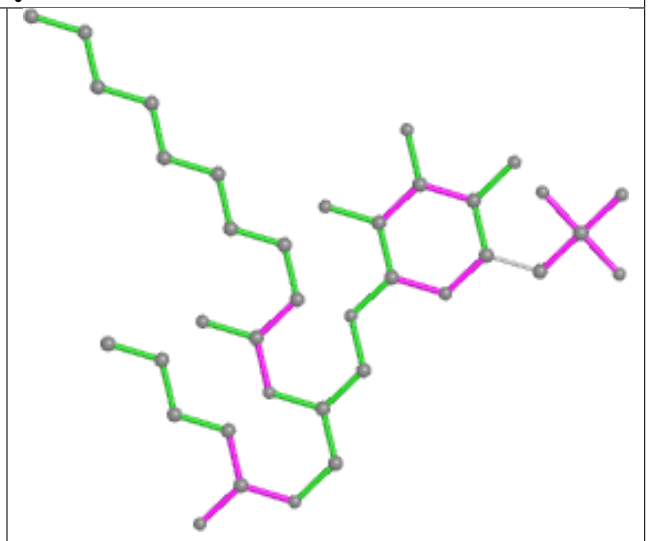
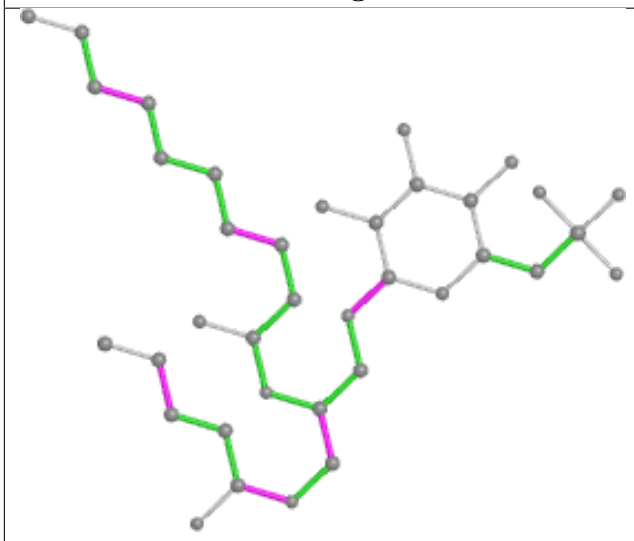


Bond lengths



Bond angles



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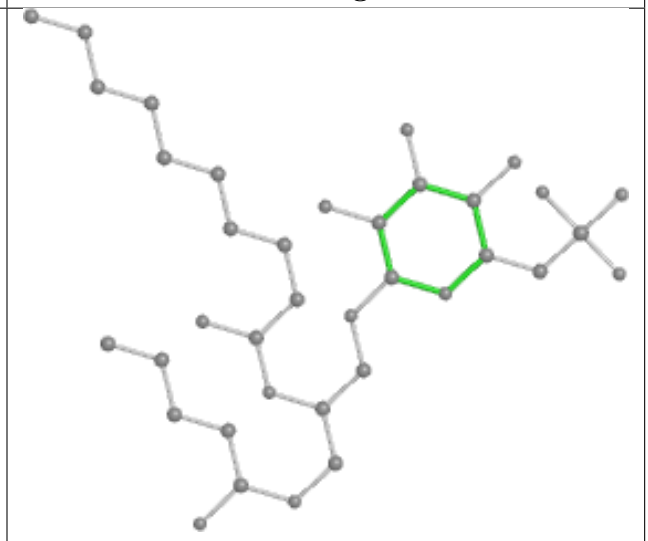
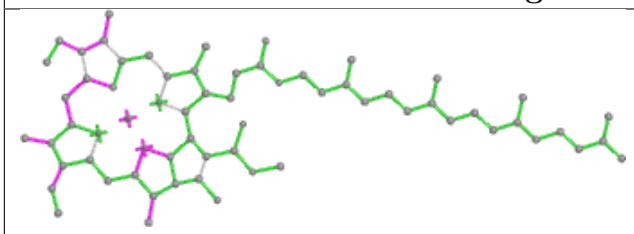


Rings

Ligand CLA B 615



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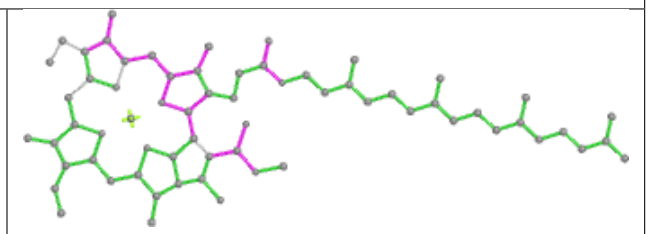

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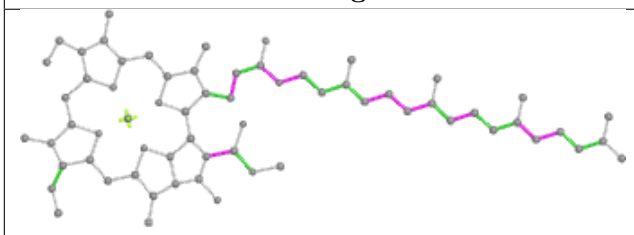

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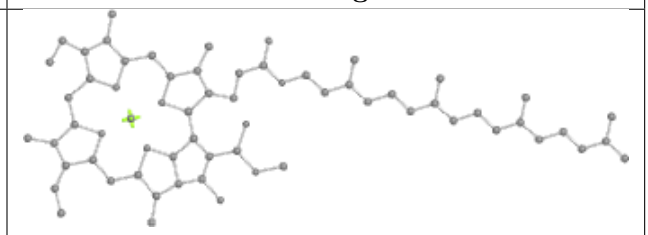
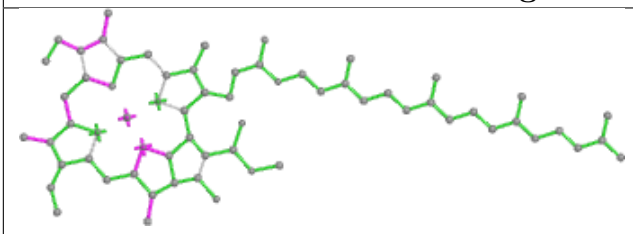


Rings

Ligand CLA 38 303



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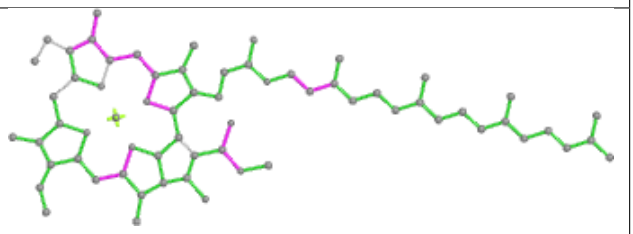

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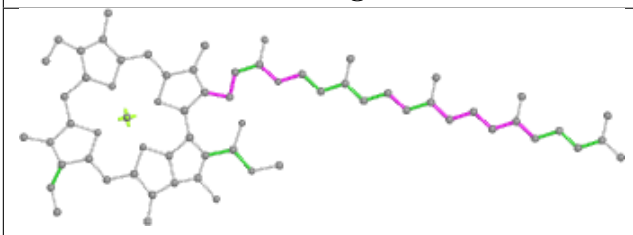

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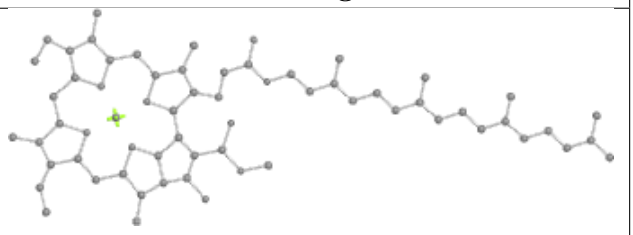
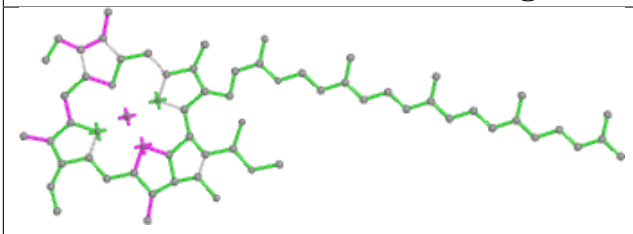


Rings

Ligand CLA 40 204



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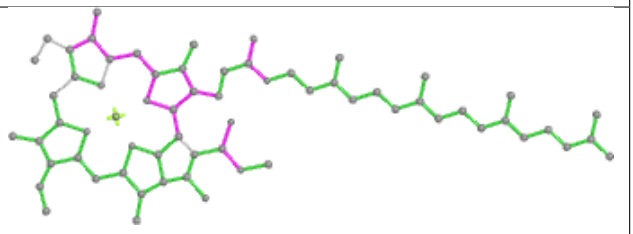

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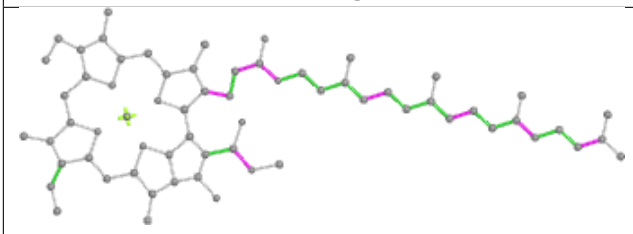

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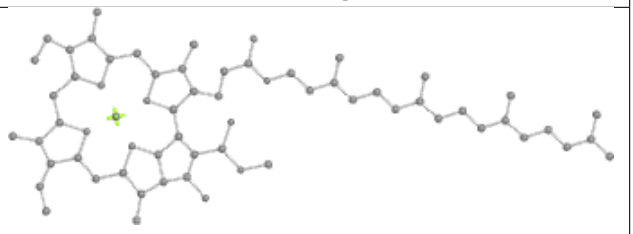
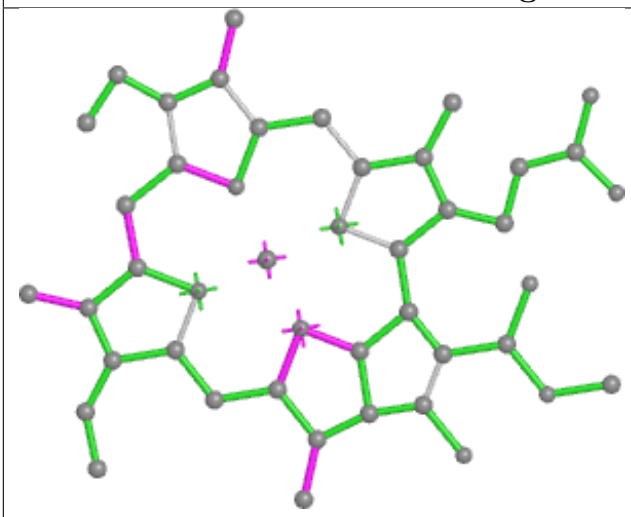


Rings

Ligand CLA 20 208



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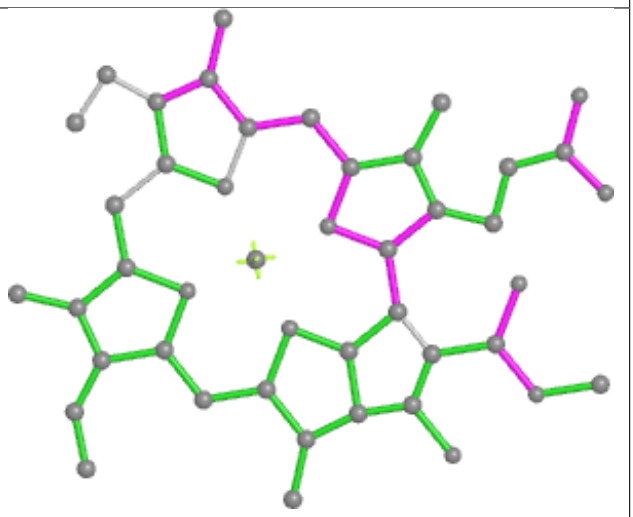

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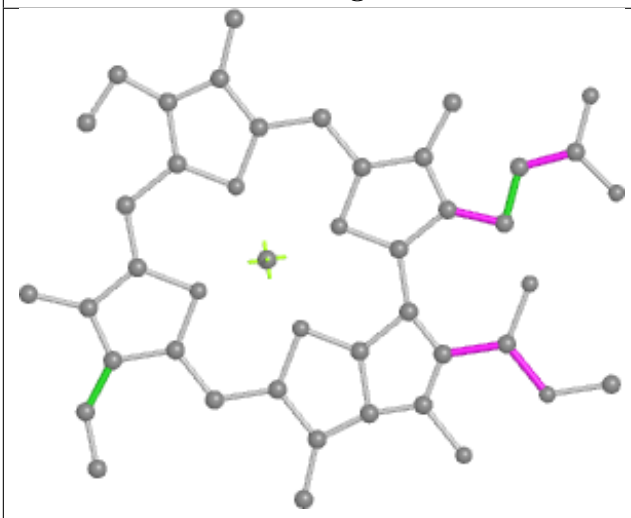

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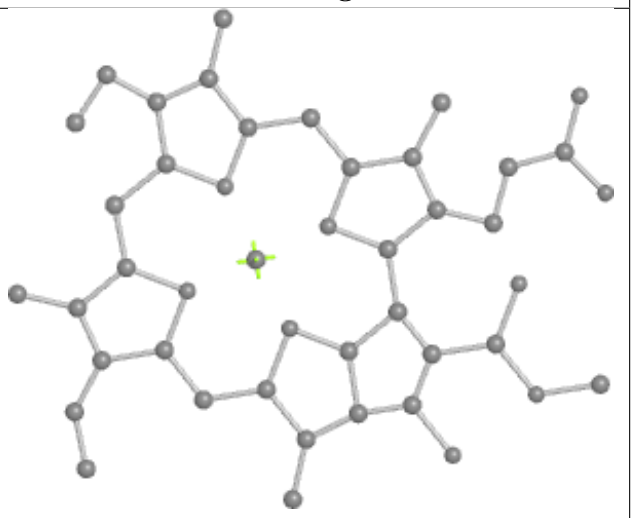
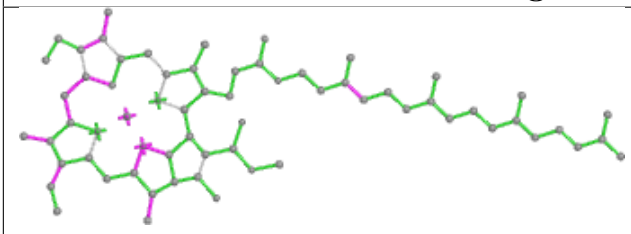


Rings

Ligand CLA b 606



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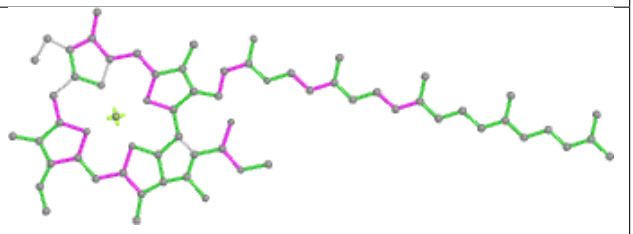

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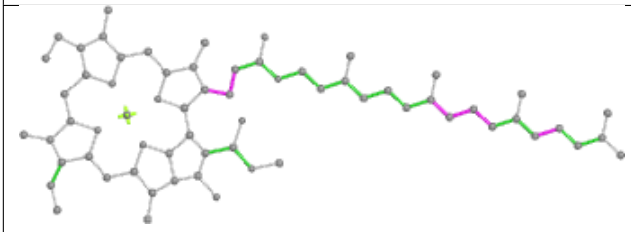

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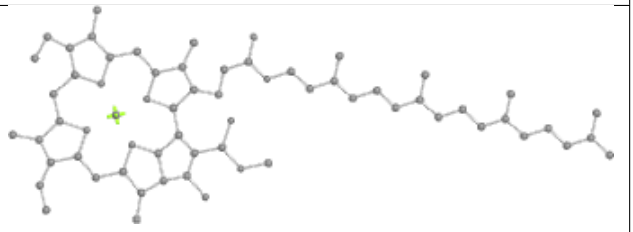
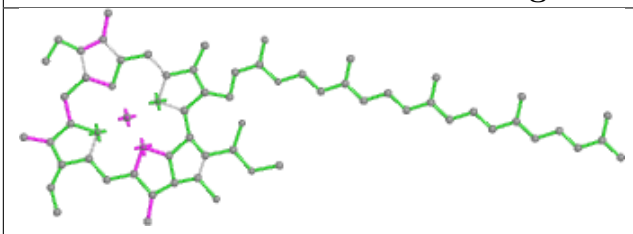


Rings

Ligand CLA c 523



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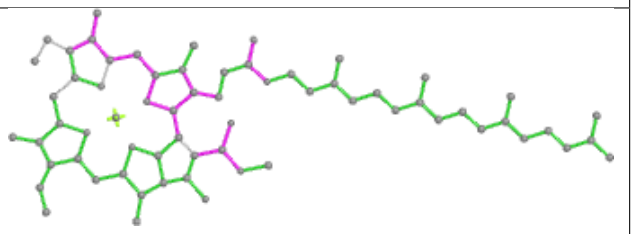

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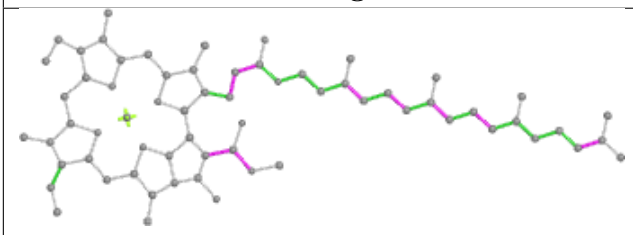

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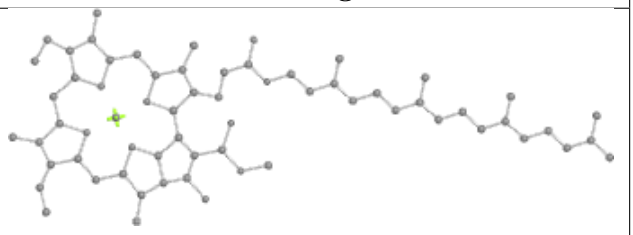
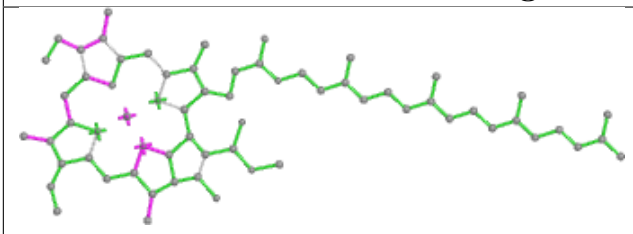


Rings

Ligand CLA 39 301



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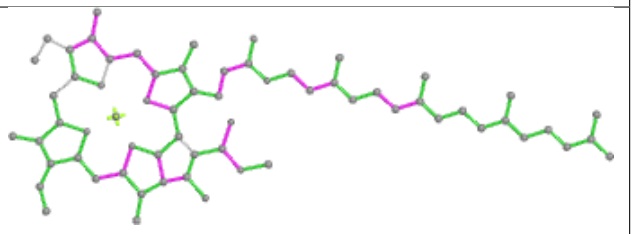
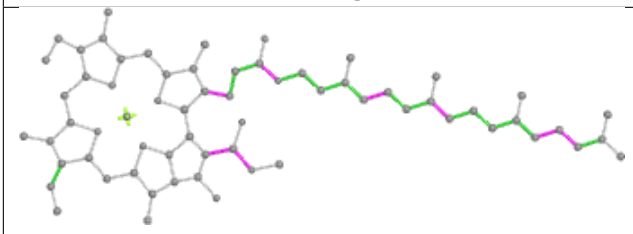


Bond angles



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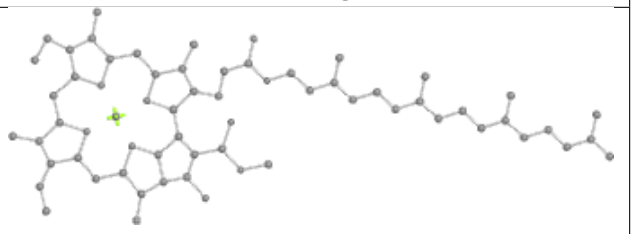
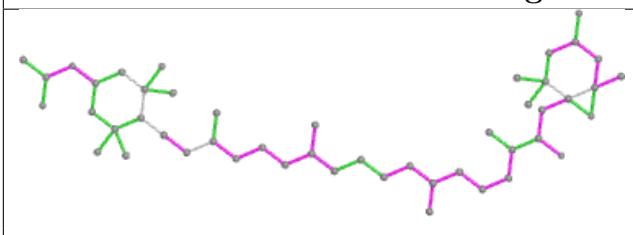


Rings

Ligand A86 13 311



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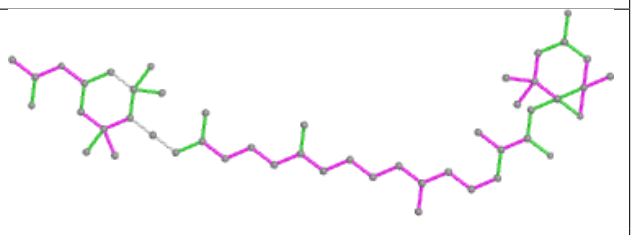
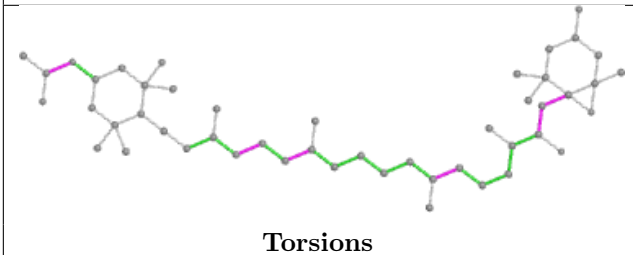


Bond angles



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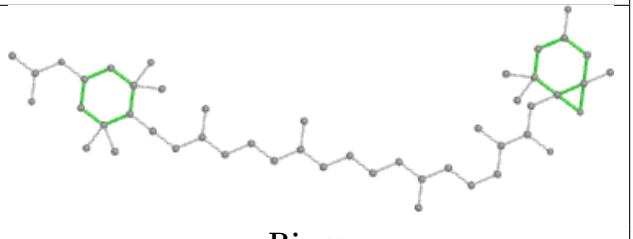
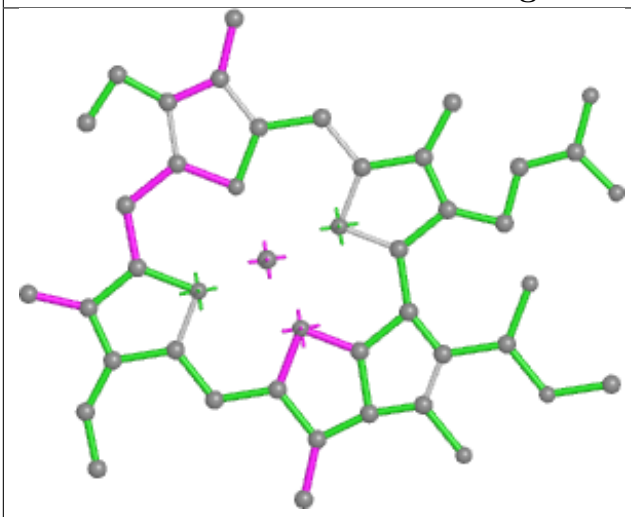


Rings

Ligand CLA 14 303



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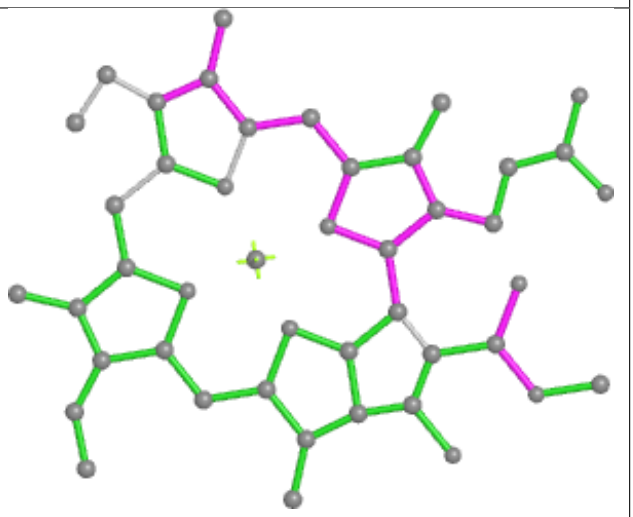

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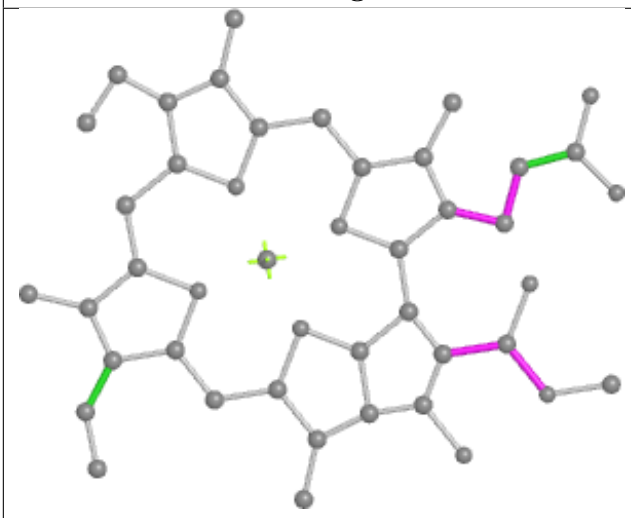
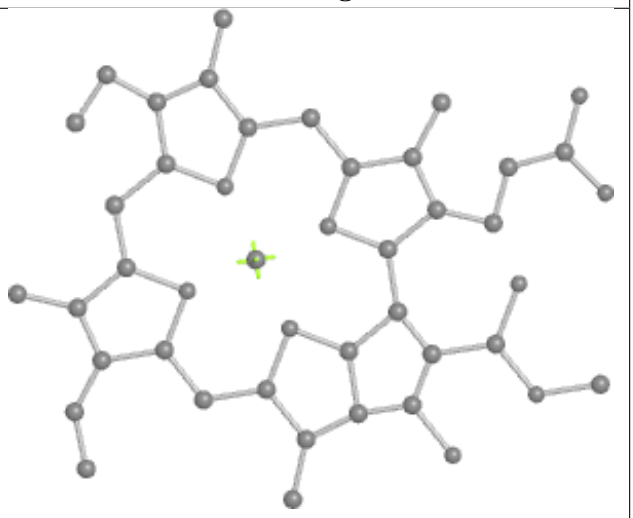
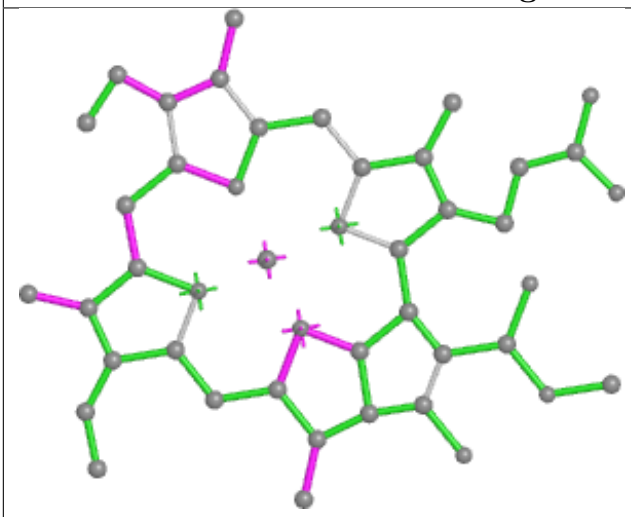


Torsions



Rings

Ligand CLA 39 305



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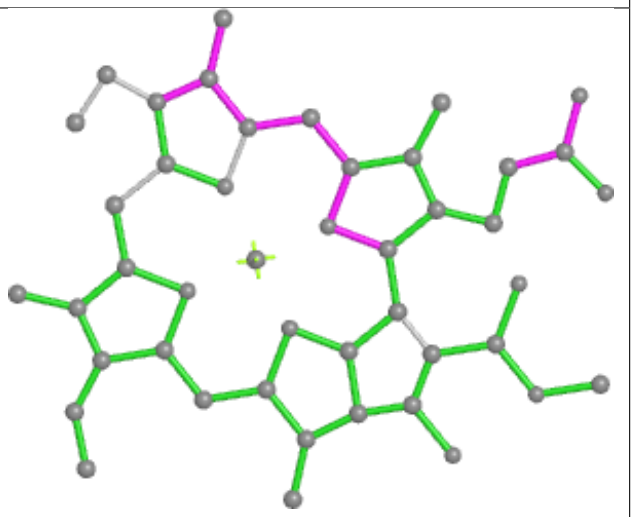

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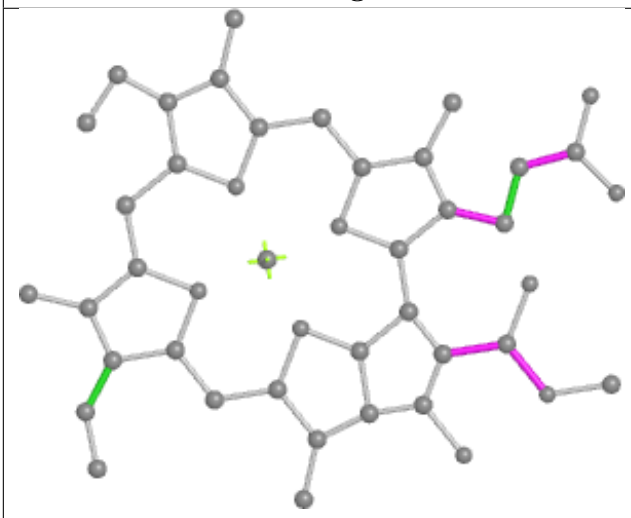

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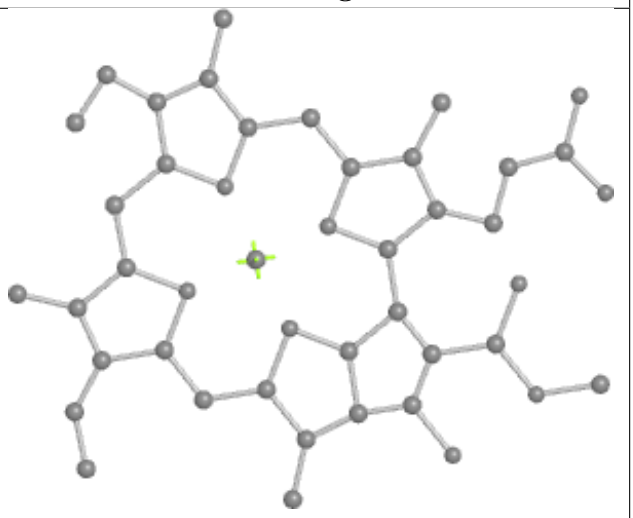
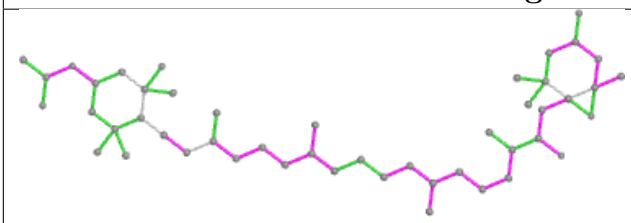


Rings

Ligand A86 35 316



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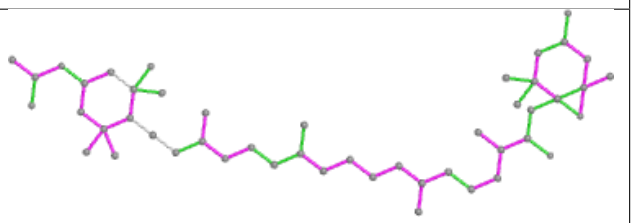

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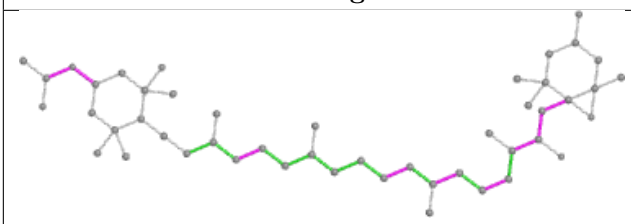

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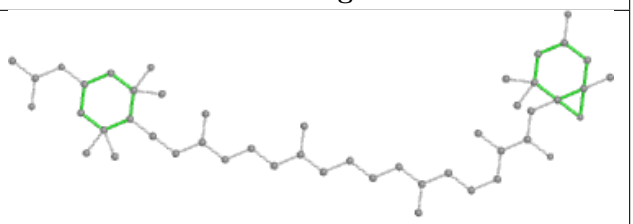
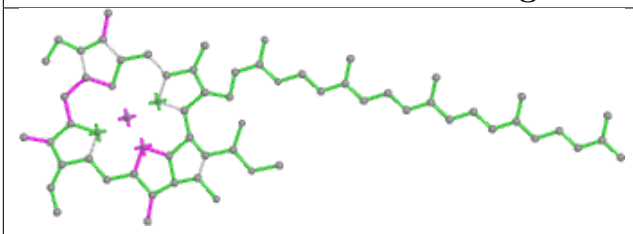


Rings

Ligand CLA 17 301



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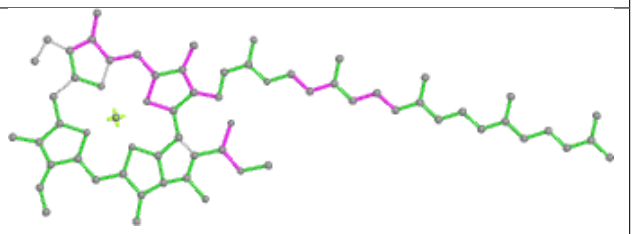

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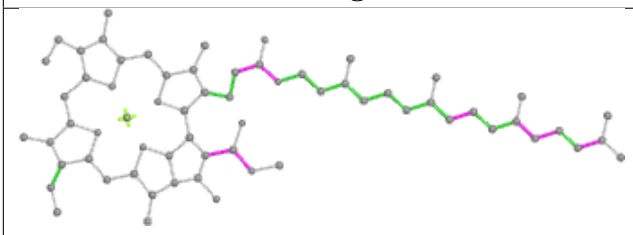

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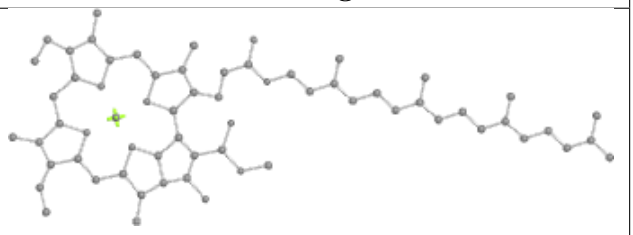
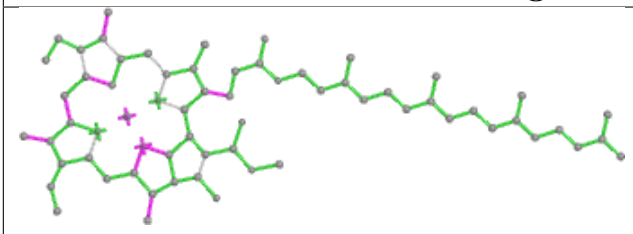


Rings

Ligand CLA d 406



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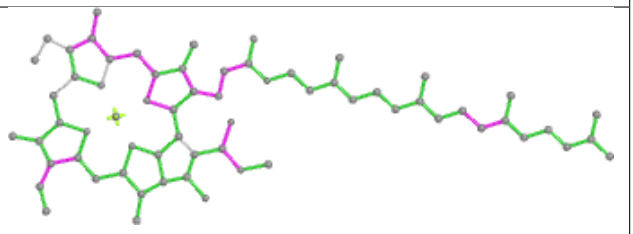

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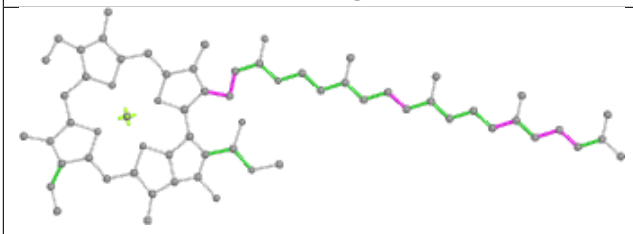

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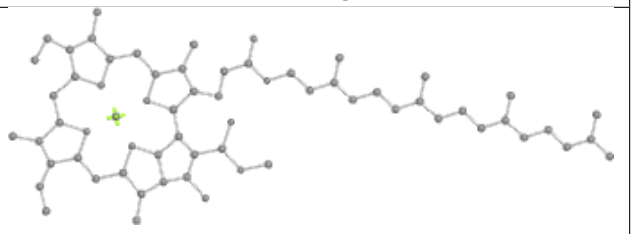
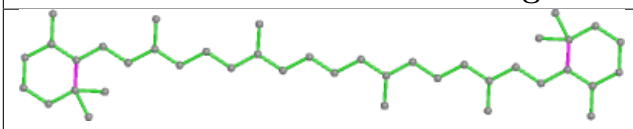


Rings

Ligand BCR B 617



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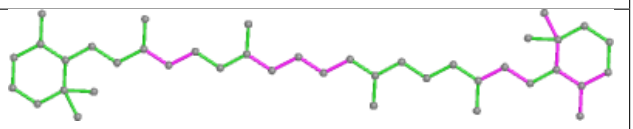

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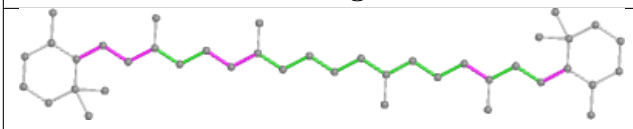
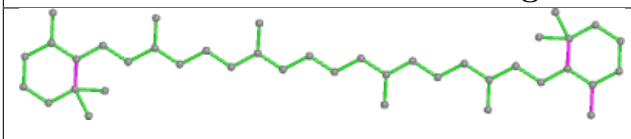


Torsions

Rings

Ligand BCR H 101



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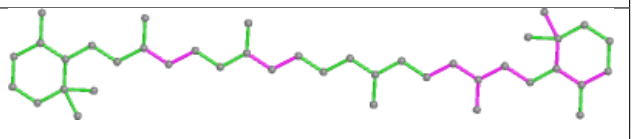

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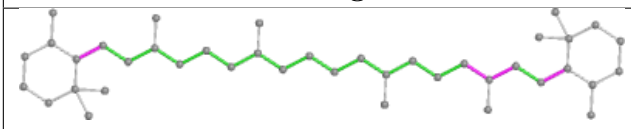

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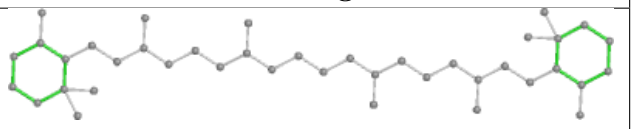
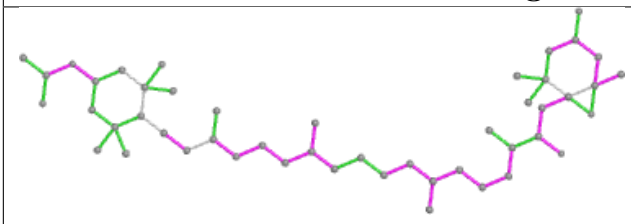


Rings

Ligand A86 33 302



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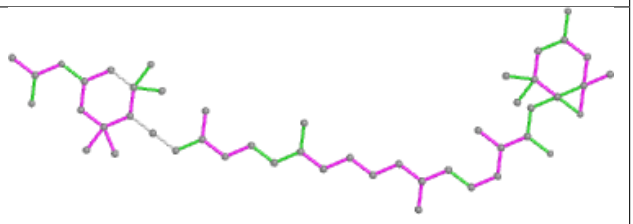

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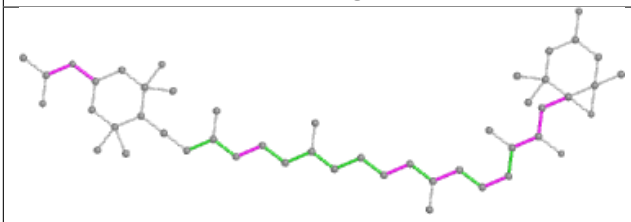

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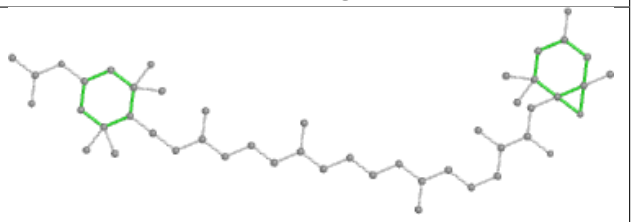
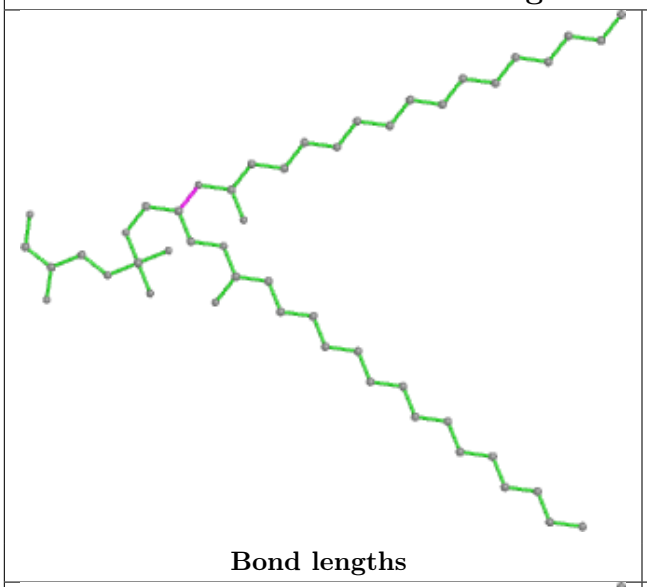


Rings

Ligand LHG L 102



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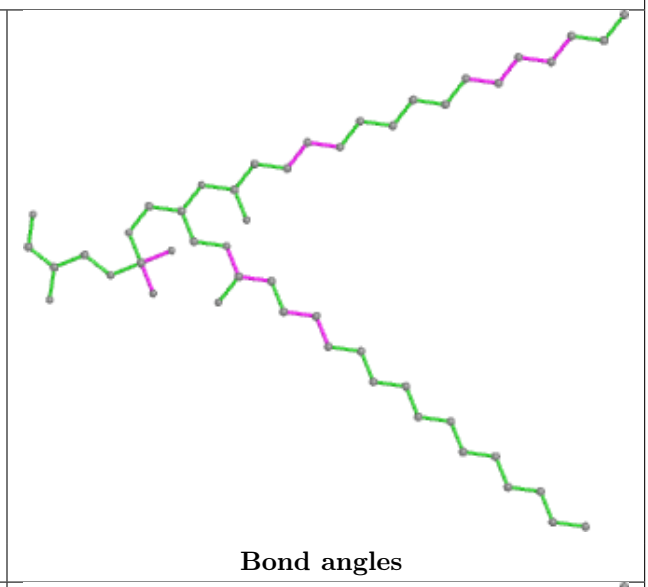

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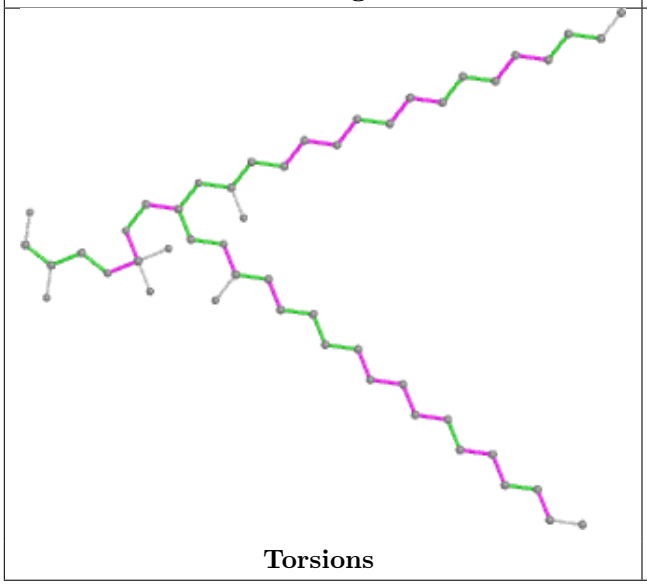

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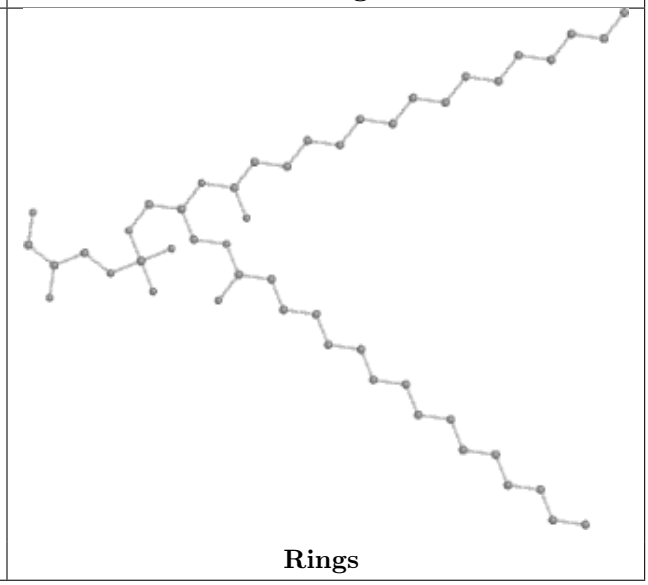
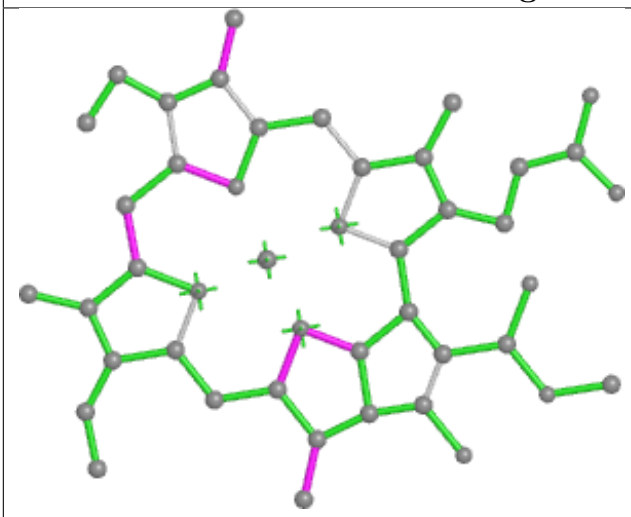


Rings

Ligand CLA 35 305



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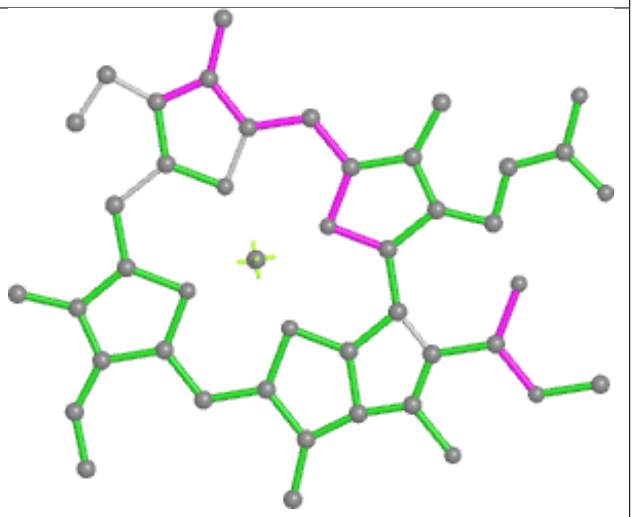

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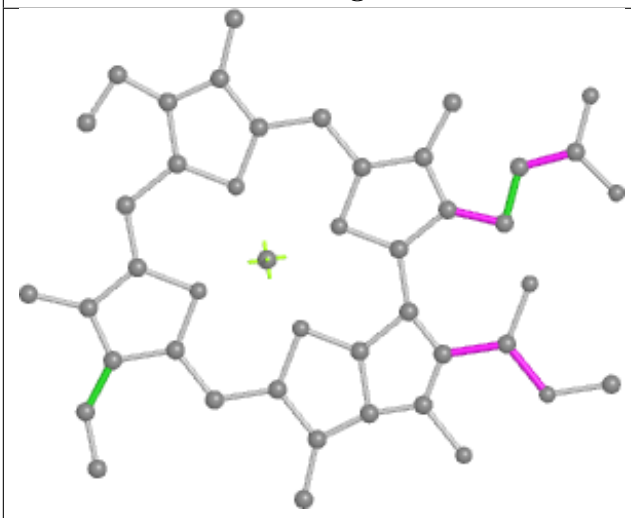

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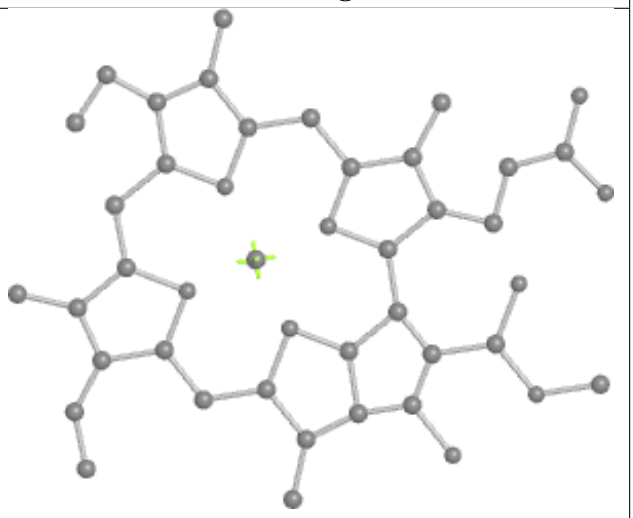

Rings

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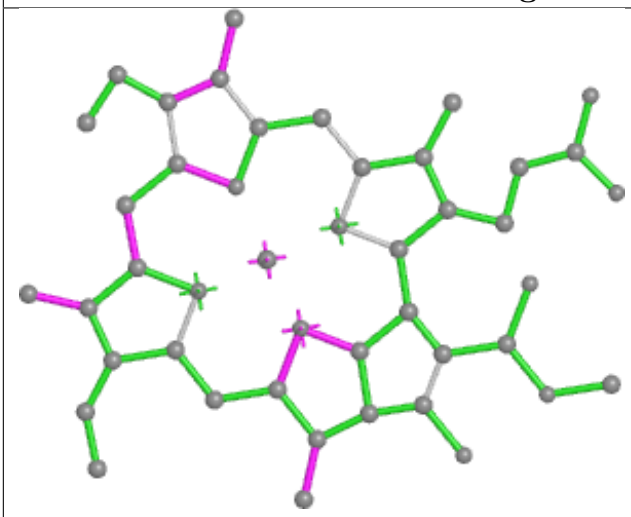

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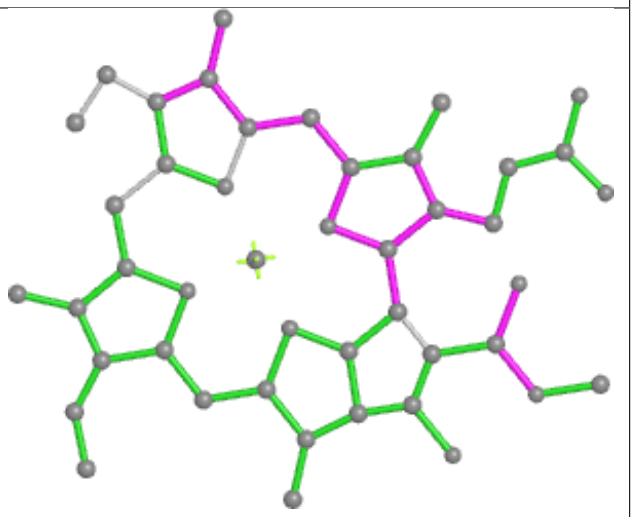

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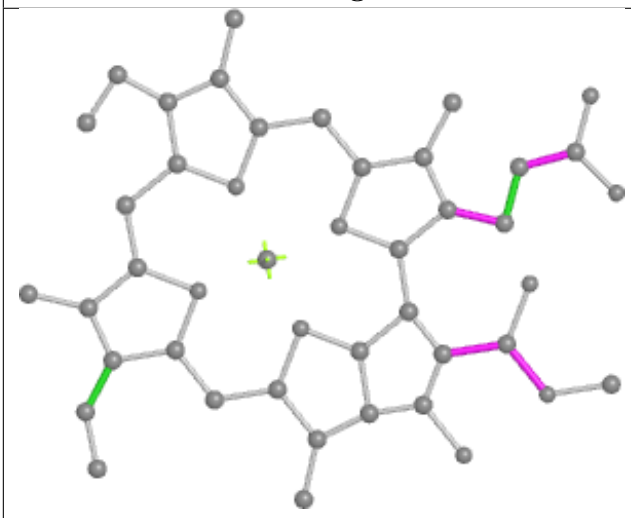

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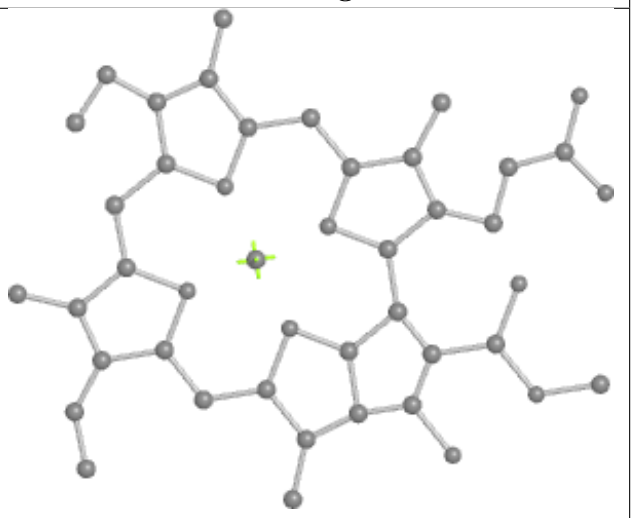
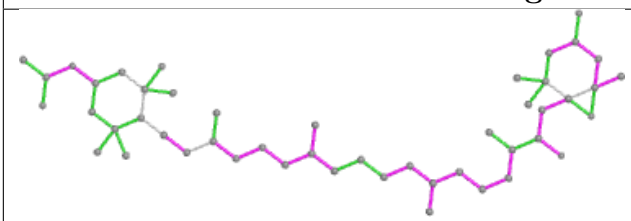


Rings

Ligand A86 20 211



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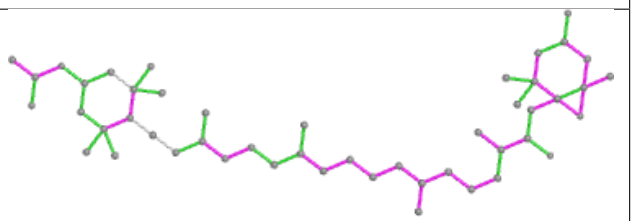

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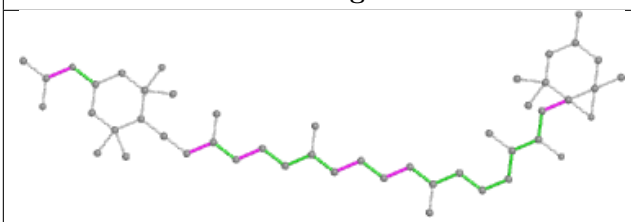

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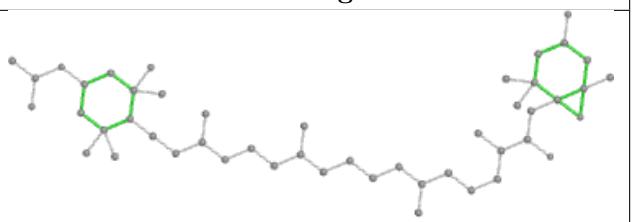
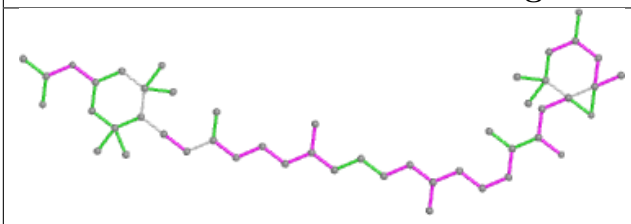


Rings

Ligand A86 14 314



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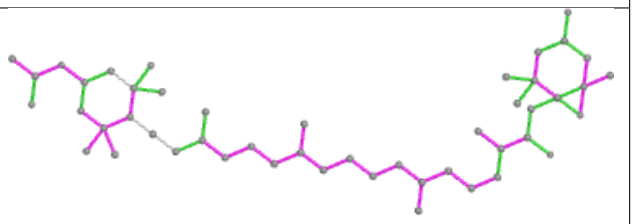
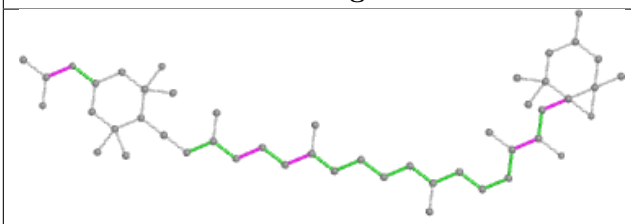


Bond angles



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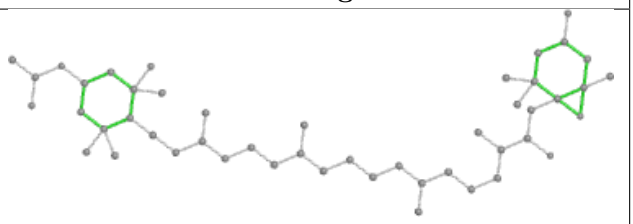
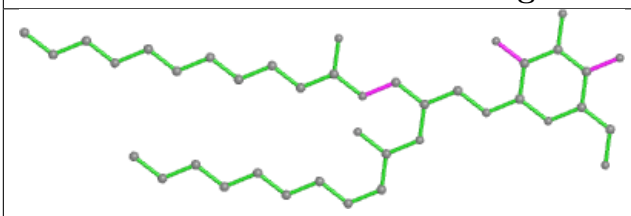


Rings

Ligand LMG m 102



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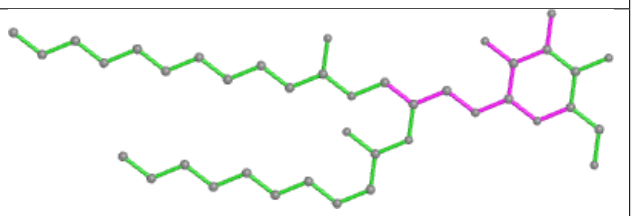
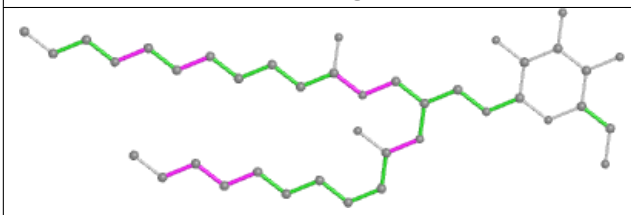


Bond angles



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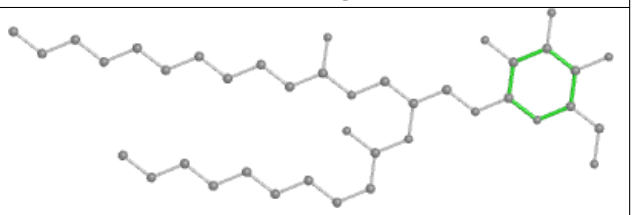
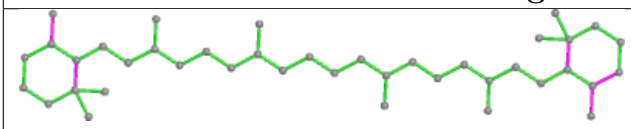


Rings

Ligand BCR c 516



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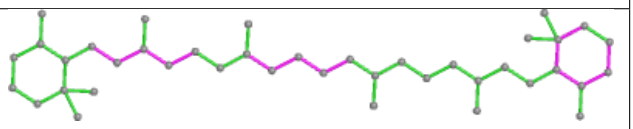
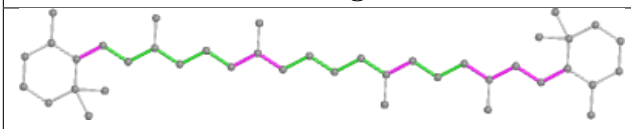
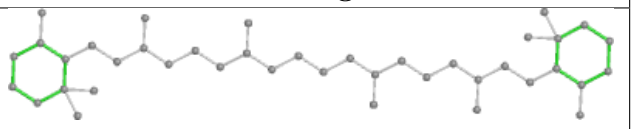


Bond angles

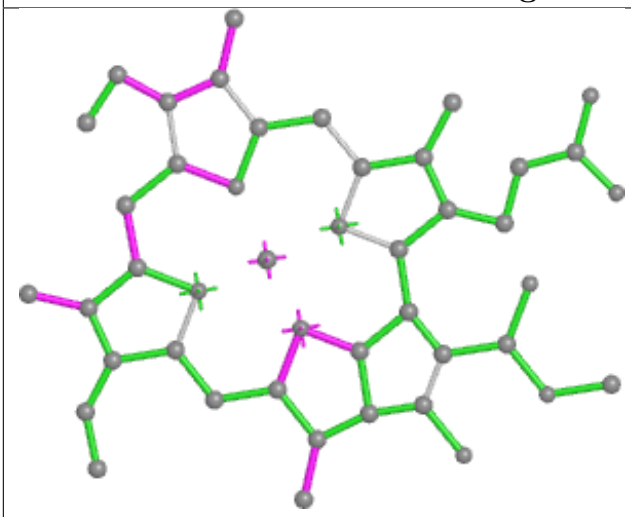


Torsions

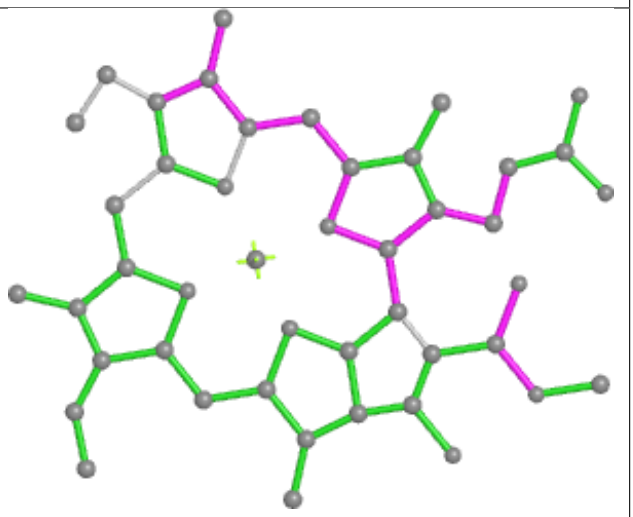


Rings

Ligand CLA 15 308



Bond lengths



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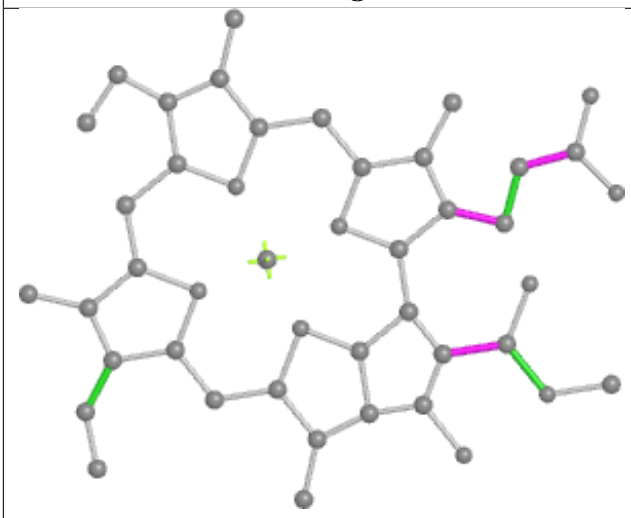

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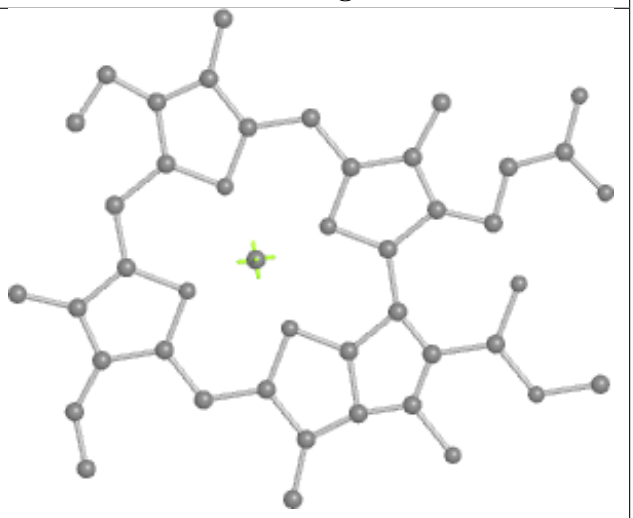
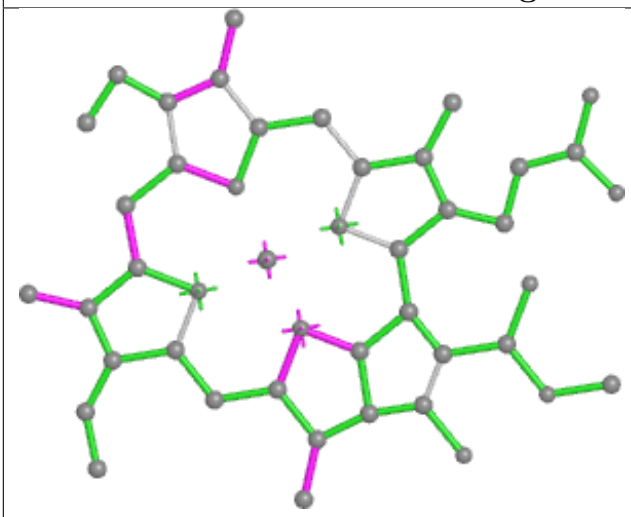


Rings

Ligand CLA 13 310



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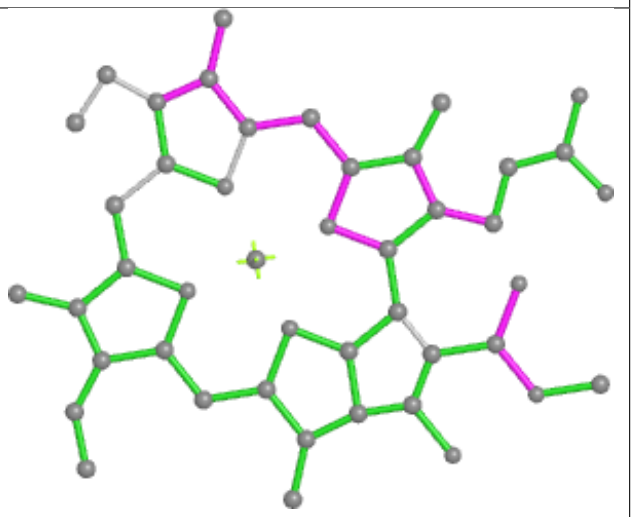

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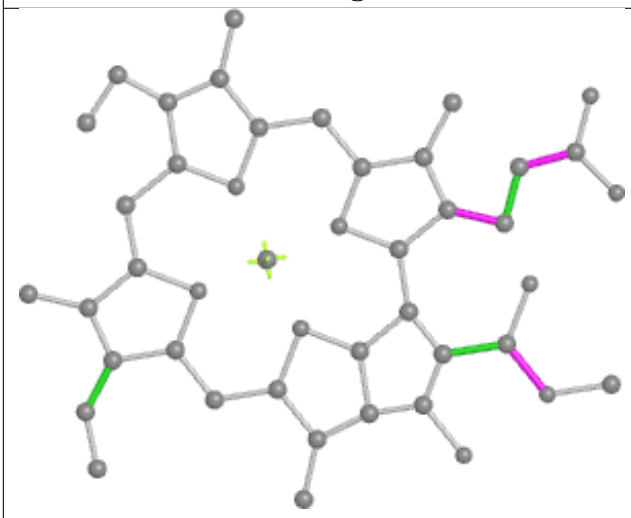

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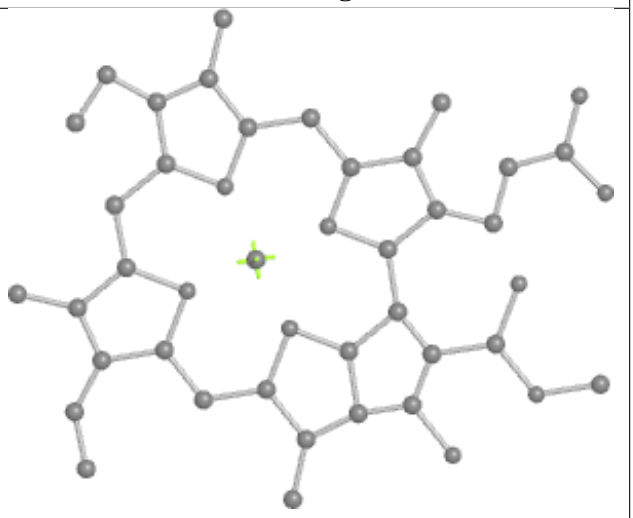
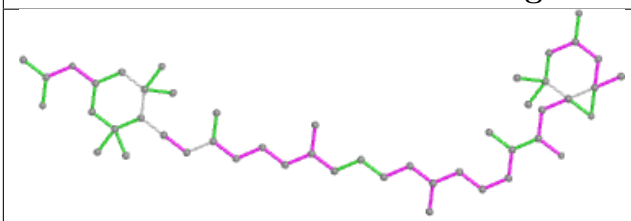


Rings

Ligand A86 15 316



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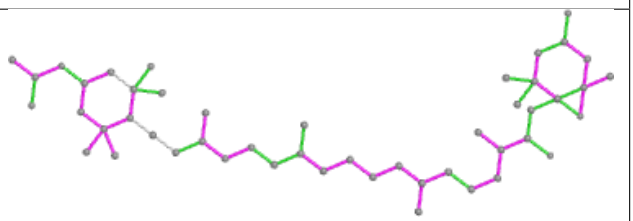

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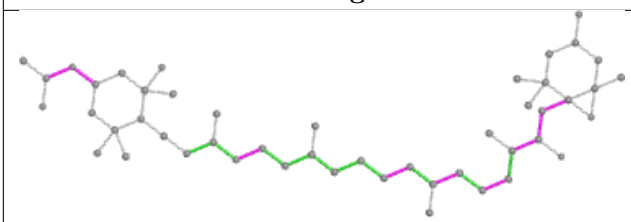

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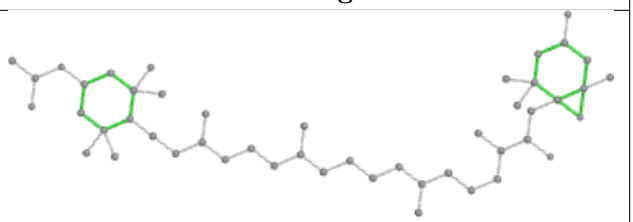
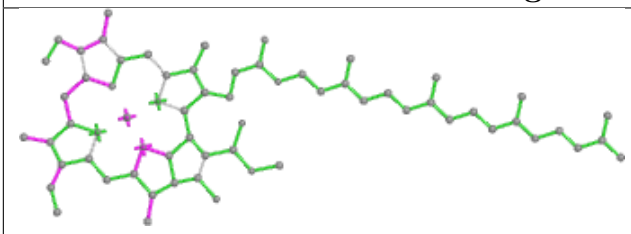


Rings

Ligand CLA B 611



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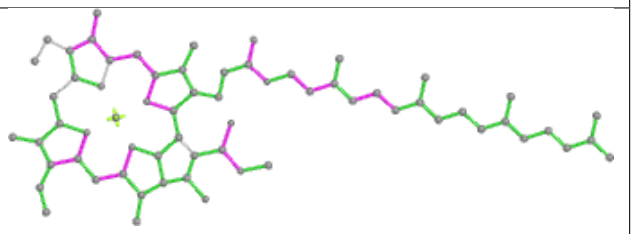
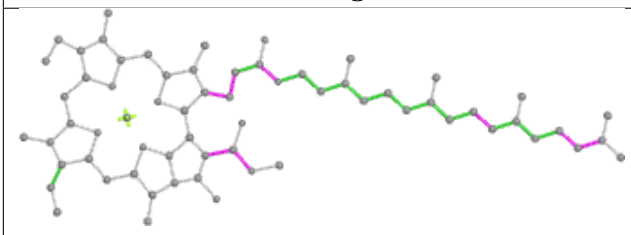


Bond angles



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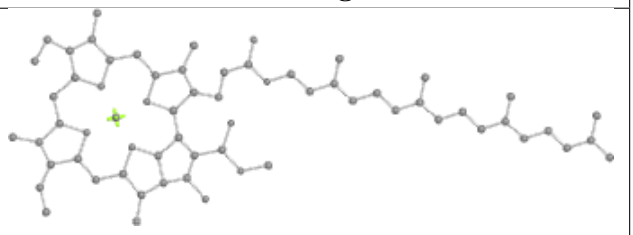
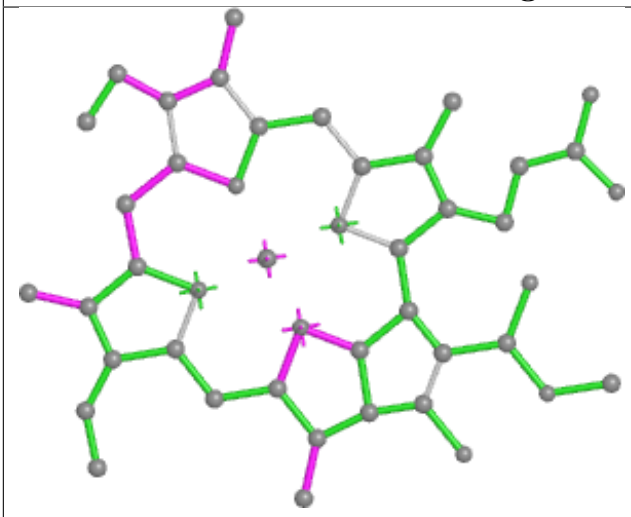


Rings

Ligand CLA 13 309



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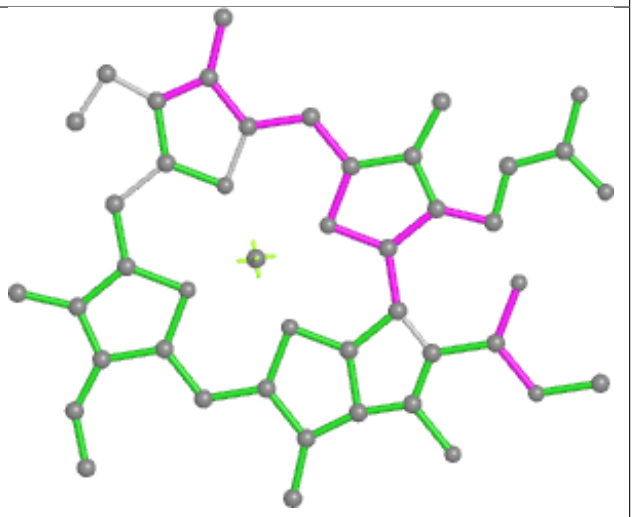
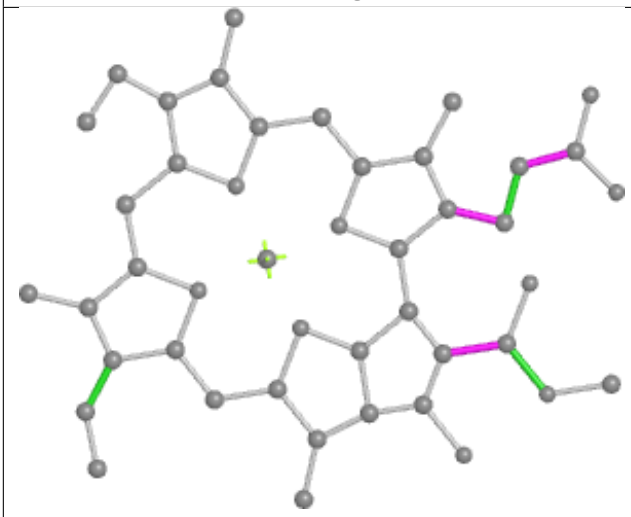


Bond angles



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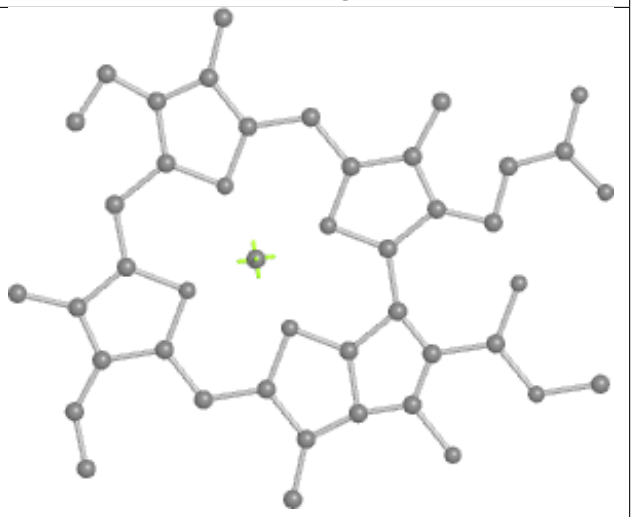
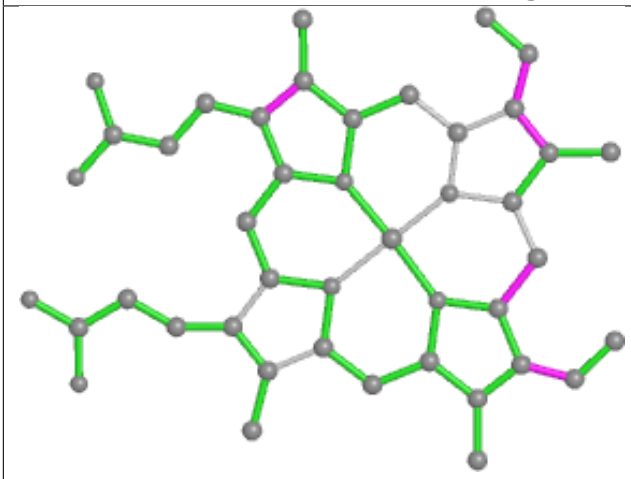


Rings

Ligand HEM v 201



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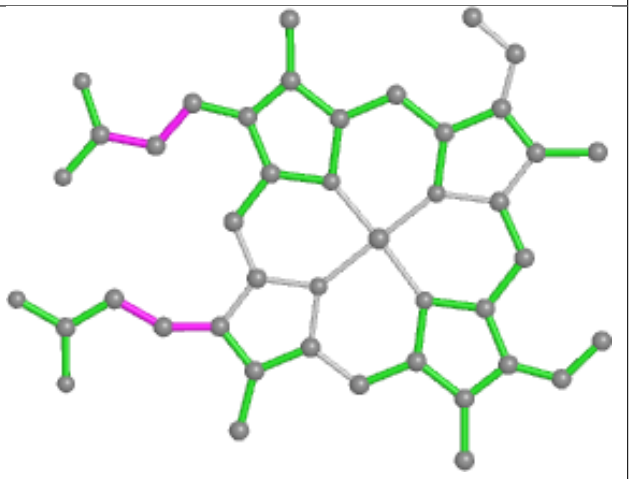
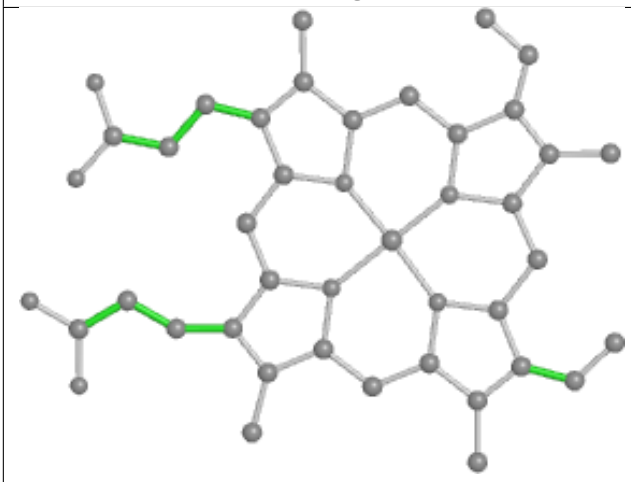


Bond angles



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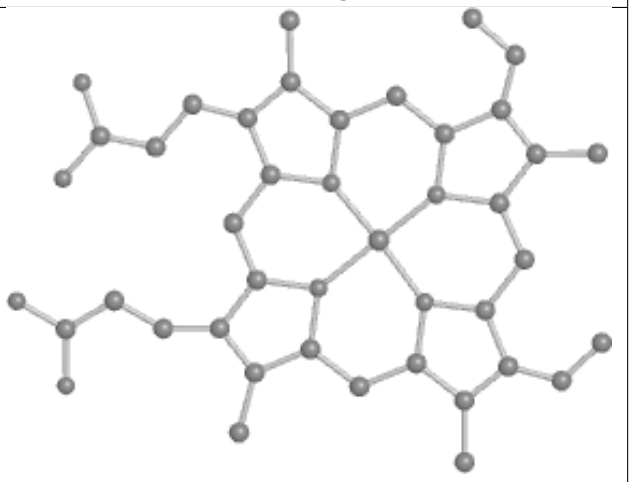
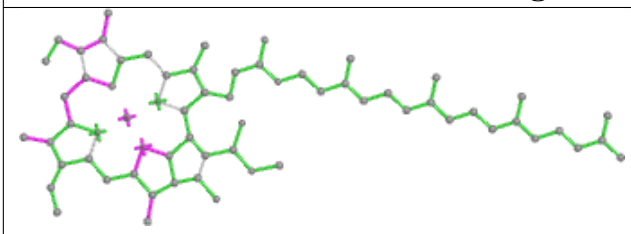


Rings

Ligand CLA c 507



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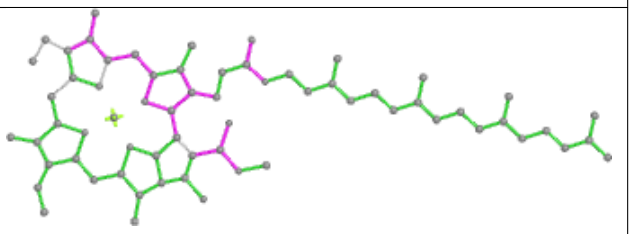
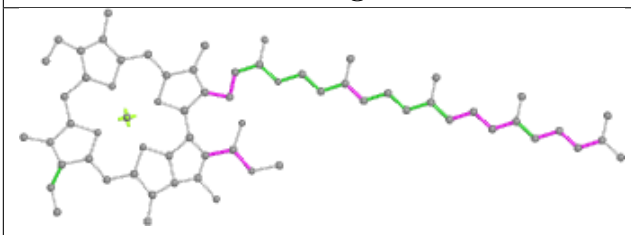


Bond angles



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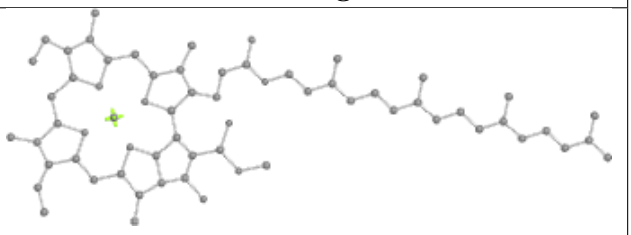
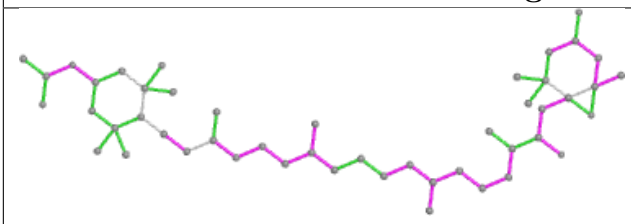


Rings

Ligand A86 32 318



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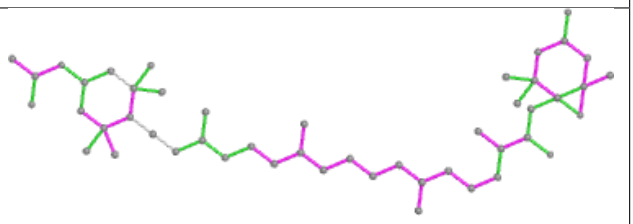
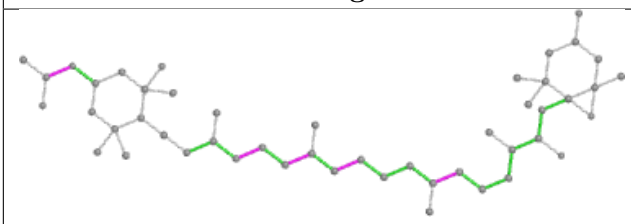
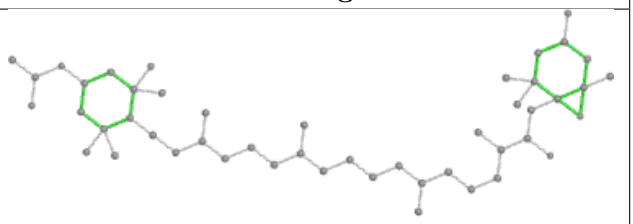


Bond angles

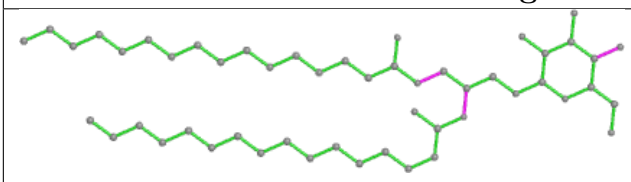


Torsions



Rings

Ligand LMG w 101



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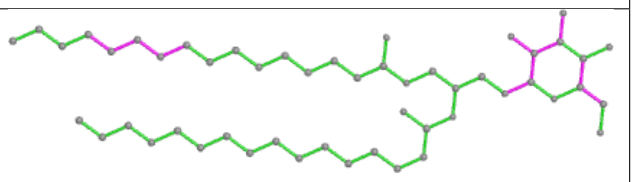
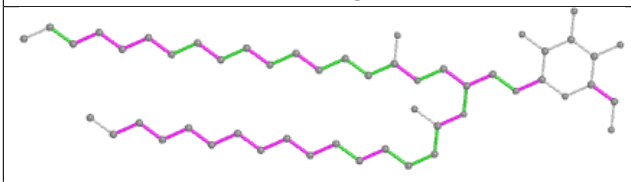
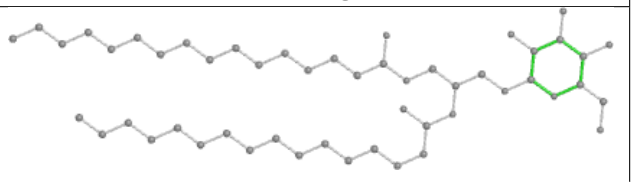


Bond angles

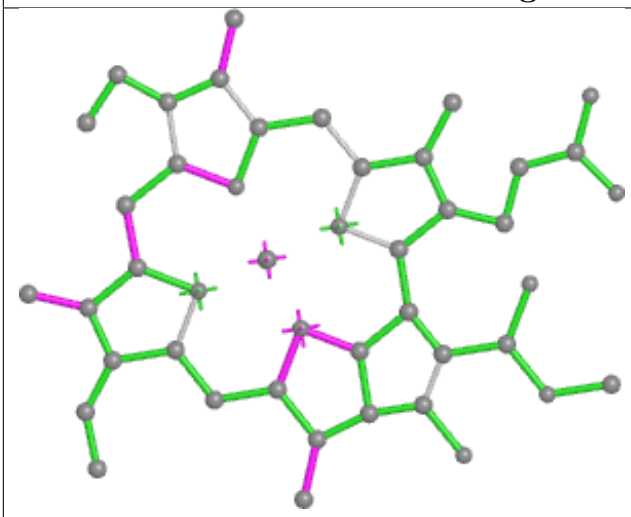


Torsions



Rings

Ligand CLA 31 309



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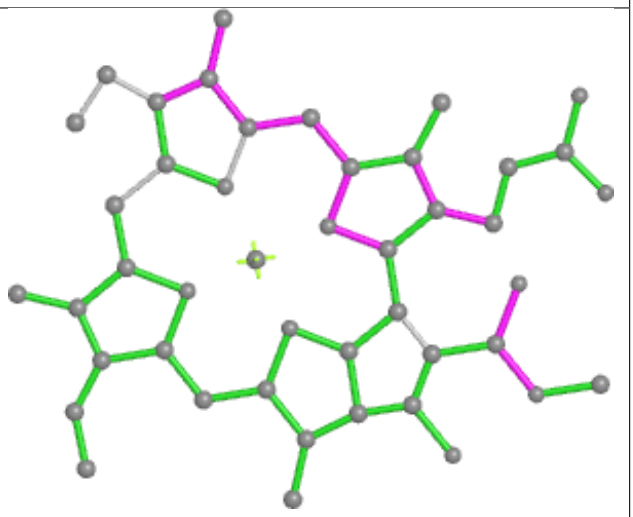
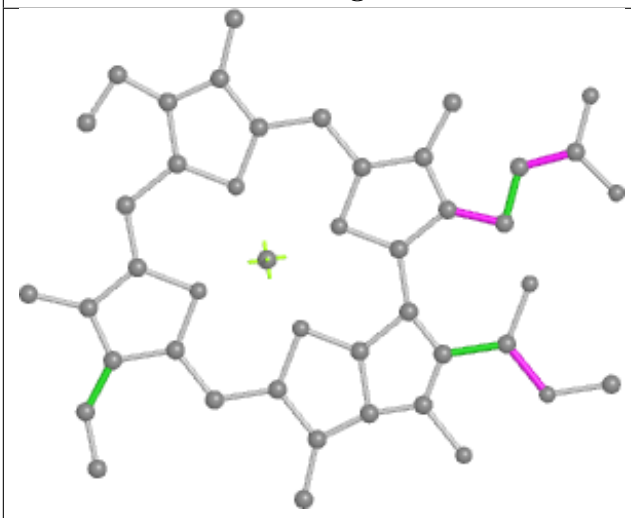


Bond angles



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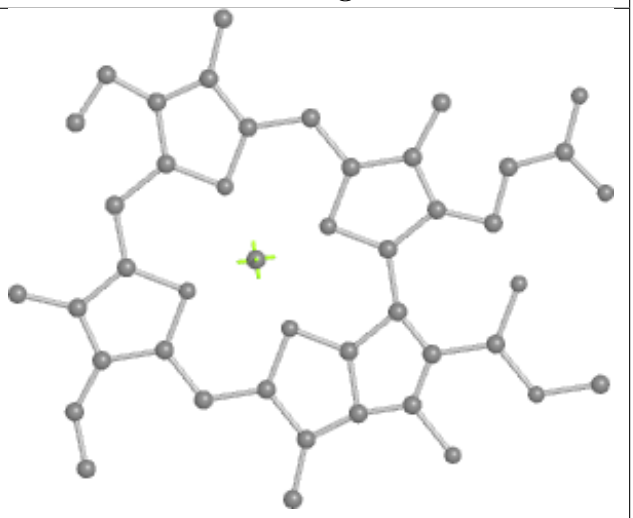
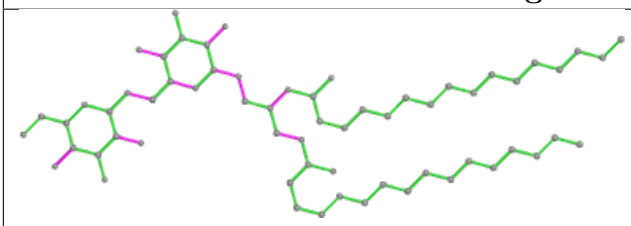


Rings

Ligand DGD c 518



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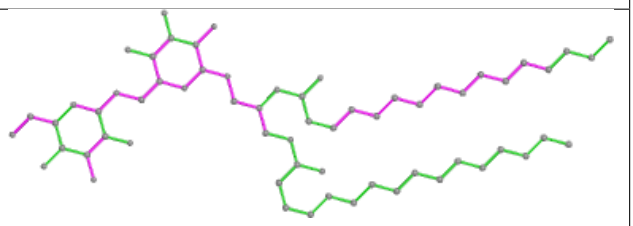
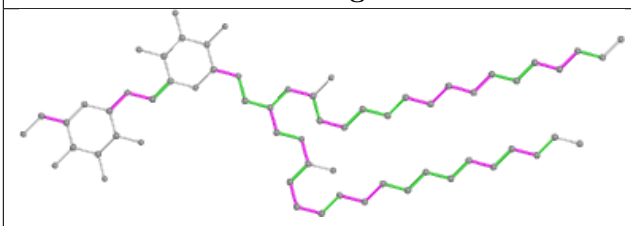
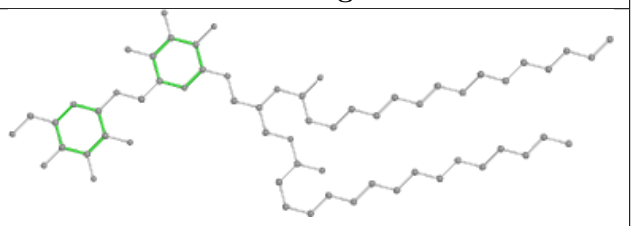


Bond angles

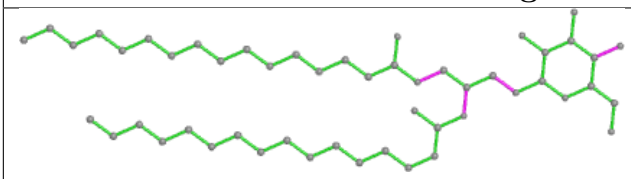


Torsions

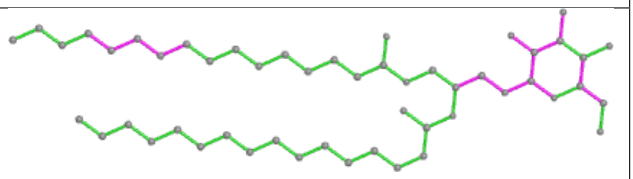


Rings

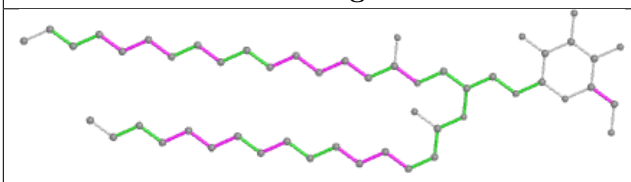
Ligand LMG B 619



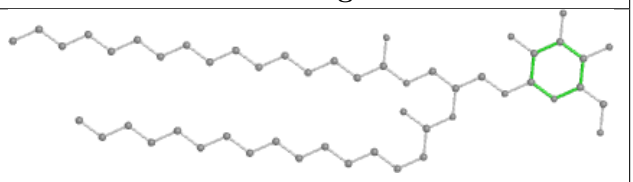
Bond lengths



Bond angles

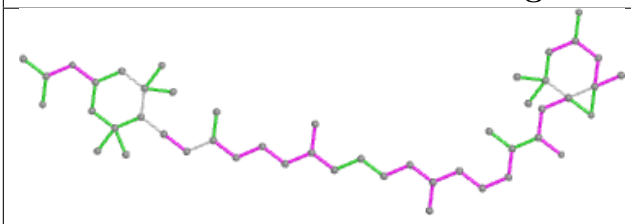


Torsions



Rings

Ligand A86 33 313



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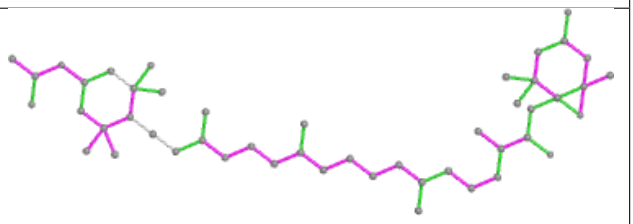
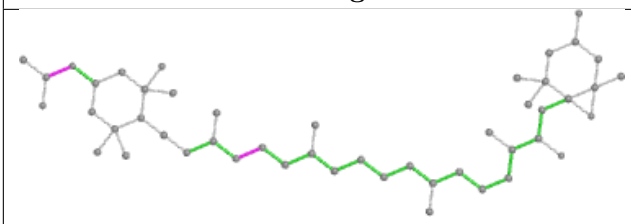
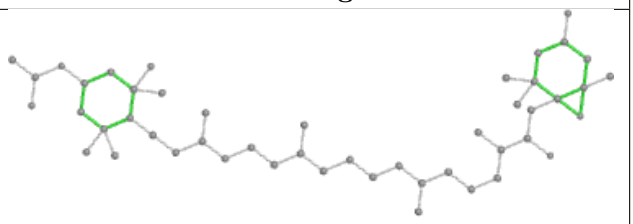


Bond angles

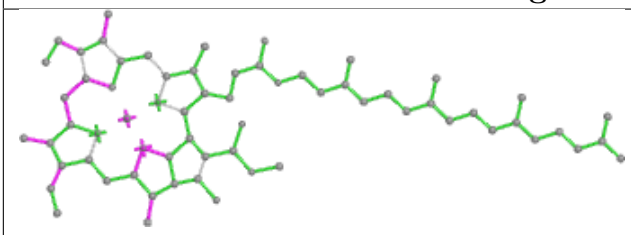


Torsions

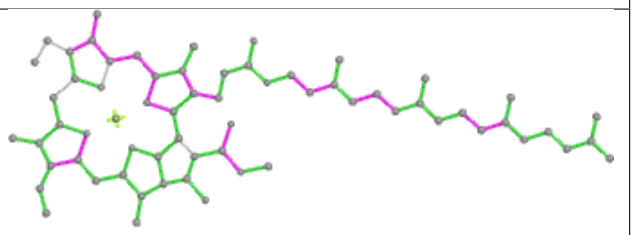


Rings

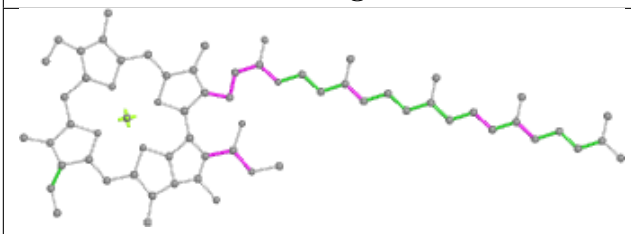
Ligand CLA c 502



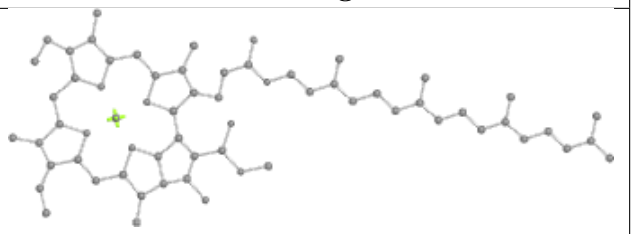
Bond lengths



Bond angles

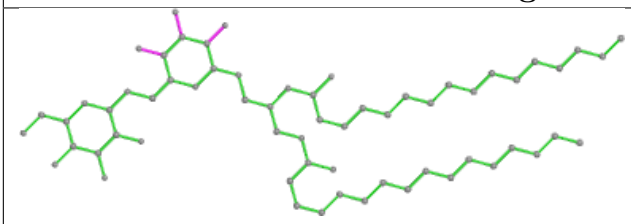


Torsions



Rings

Ligand DGD H 102



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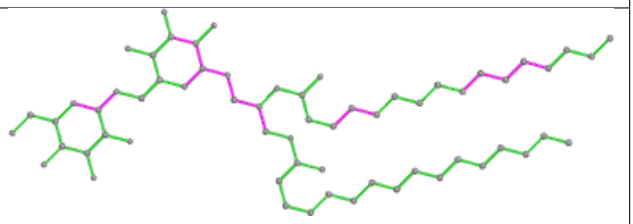

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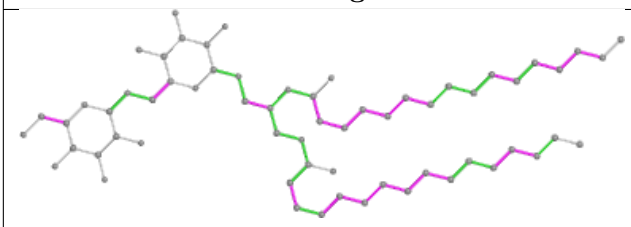

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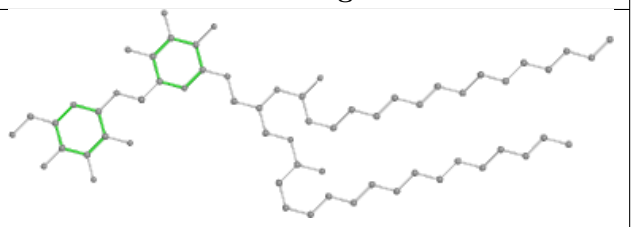
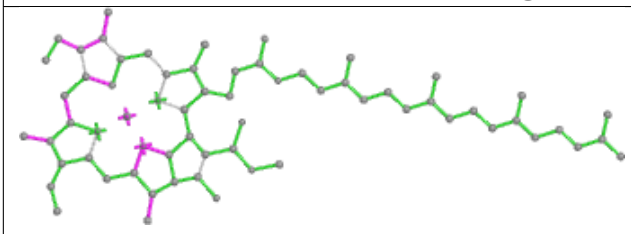


Rings

Ligand CLA 32 311



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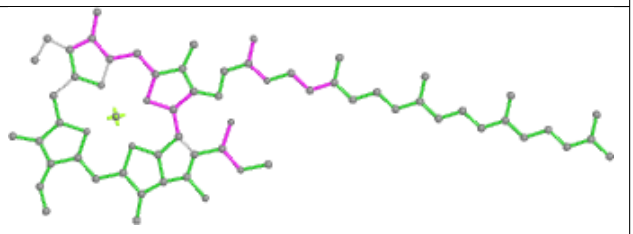

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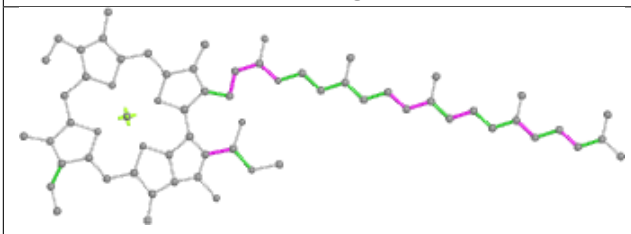

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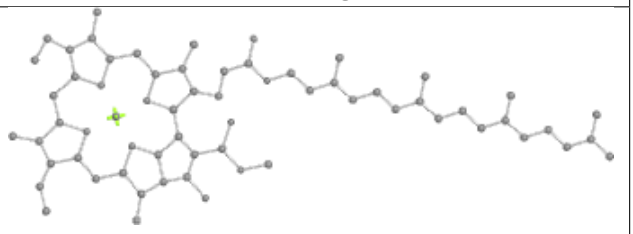
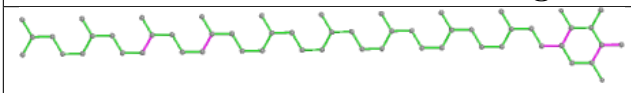


Rings

Ligand PL9 d 405



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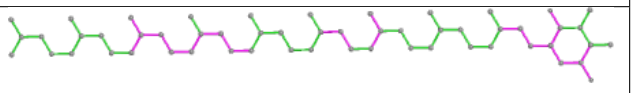

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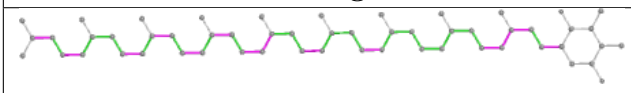

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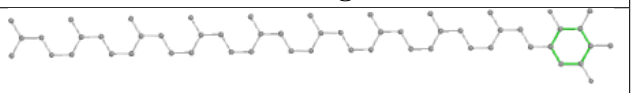
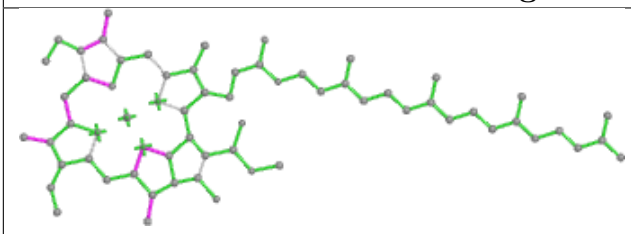


Rings

Ligand CLA 19 303



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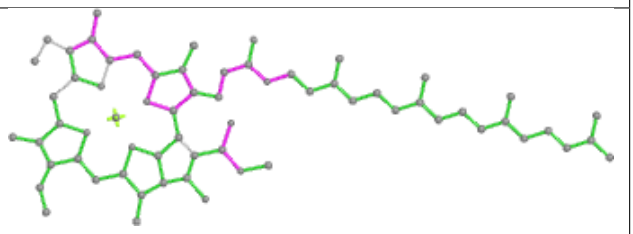

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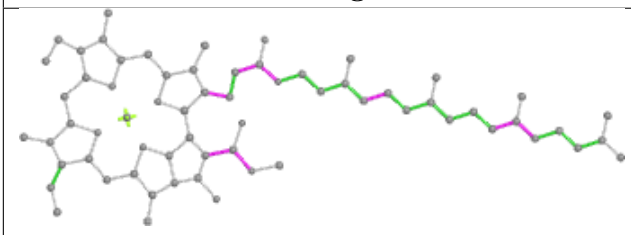

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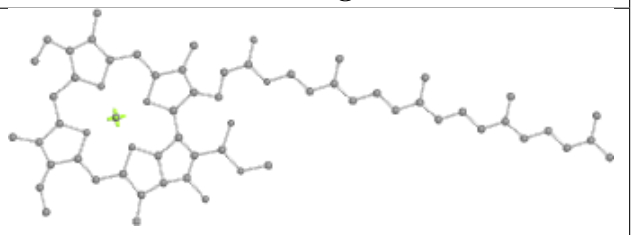
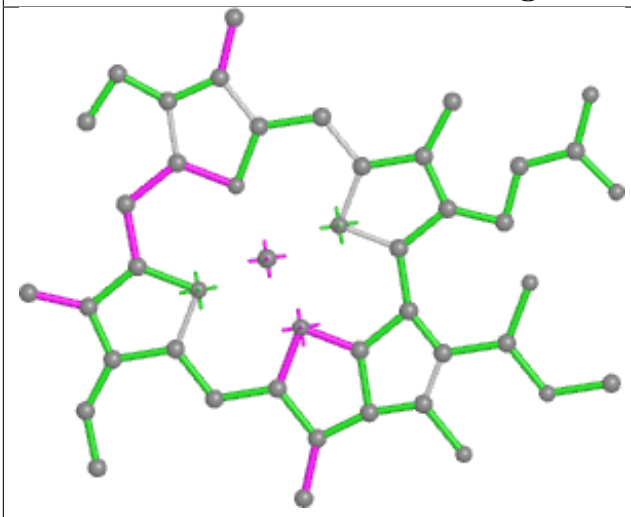


Rings

Ligand CLA 16 305



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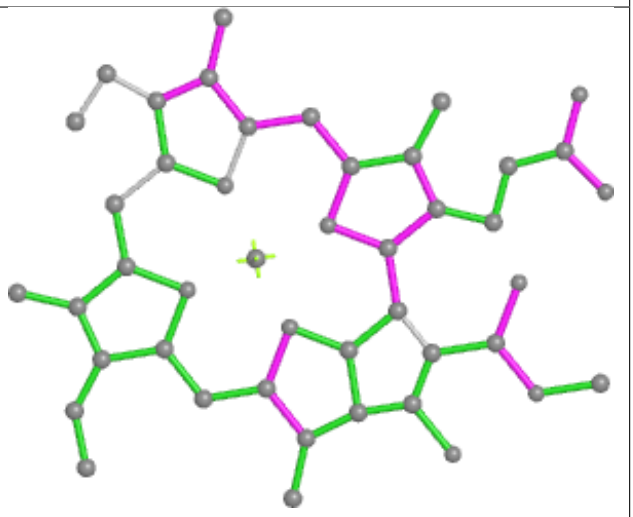

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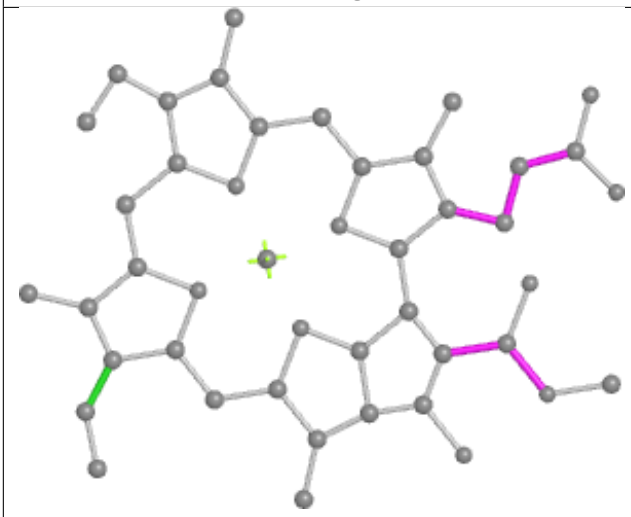

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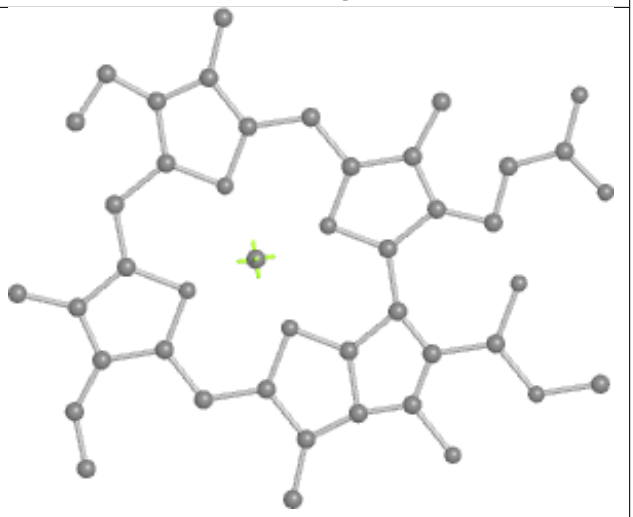
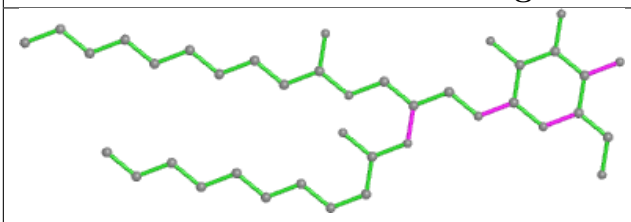


Rings

Ligand LMG 12 301



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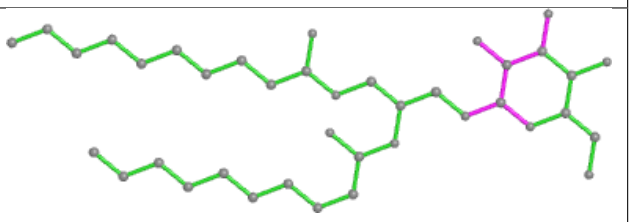
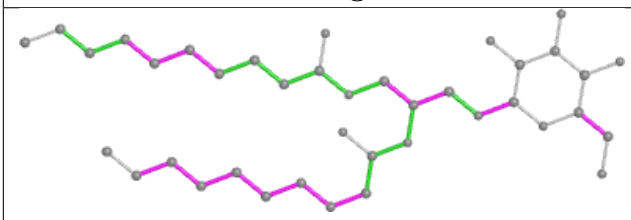


Bond angles



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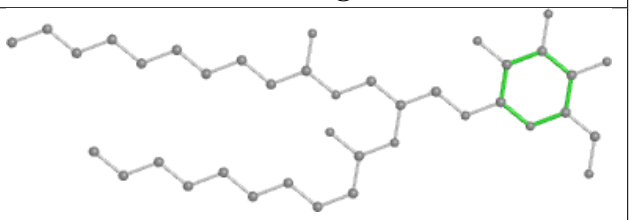
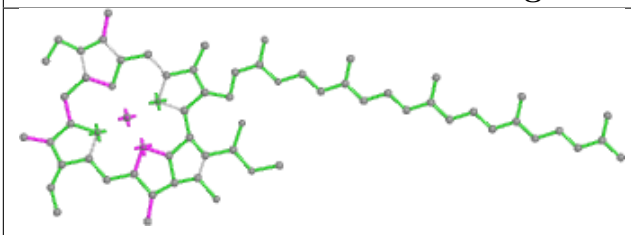


Rings

Ligand CLA C 514



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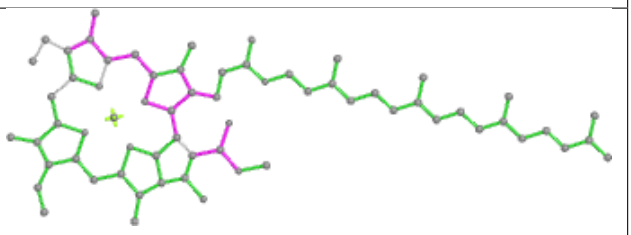

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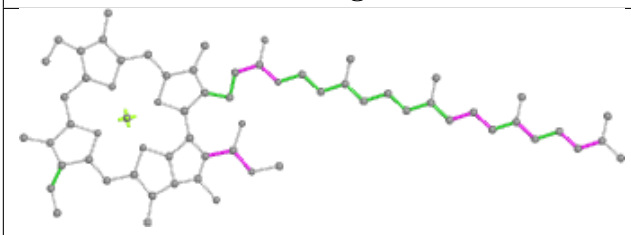

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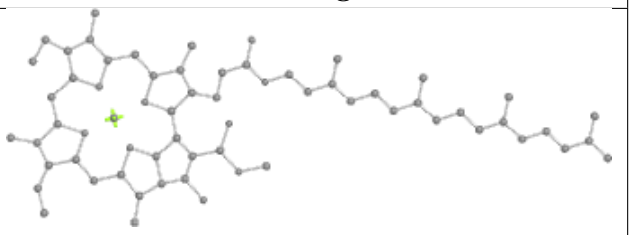
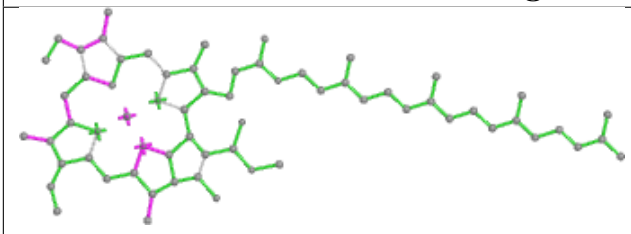


Rings

Ligand CLA B 608



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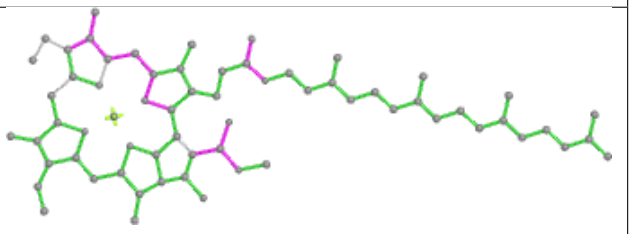

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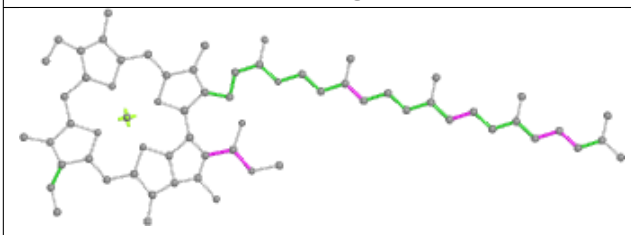

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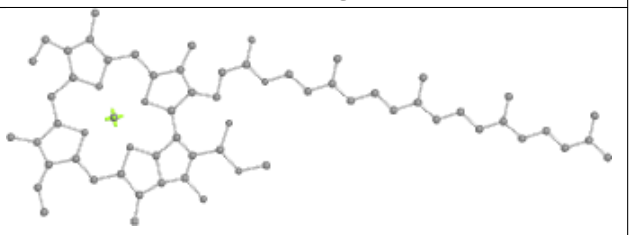
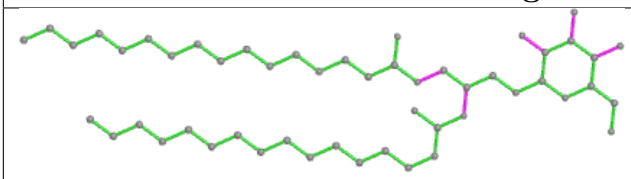


Rings

Ligand LMG b 619



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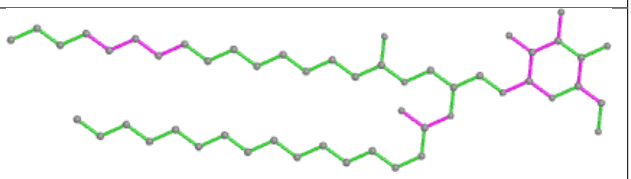

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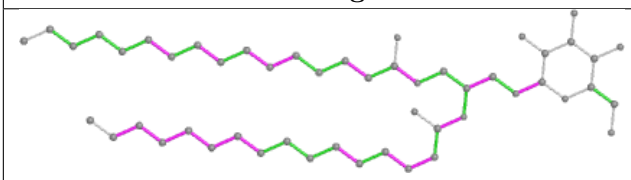

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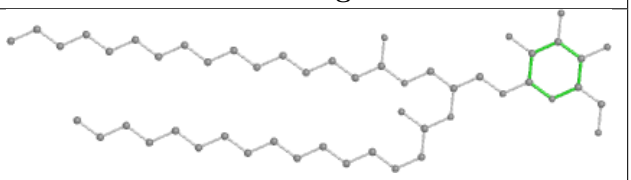
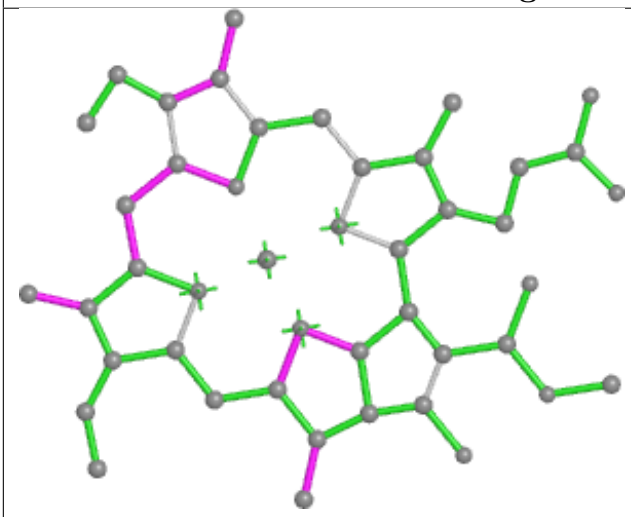


Rings

Ligand CLA 16 306



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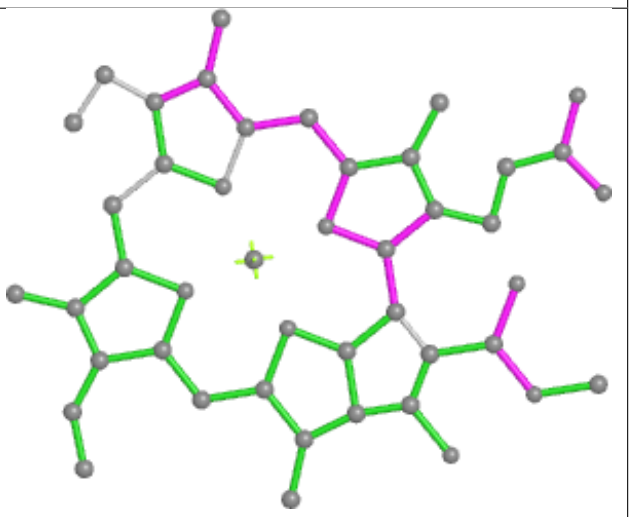
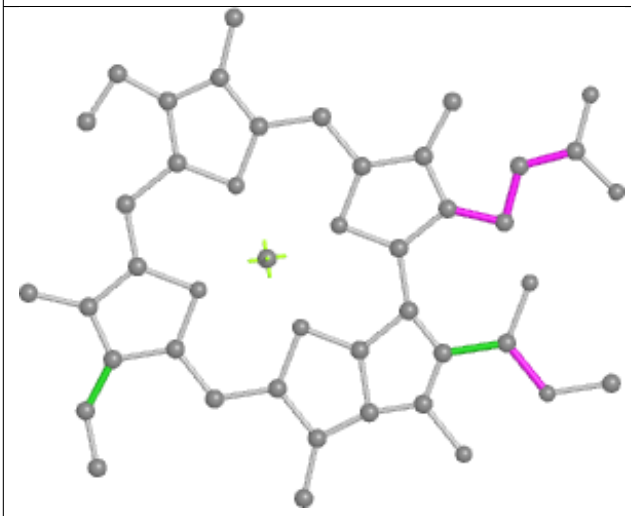


Bond angles



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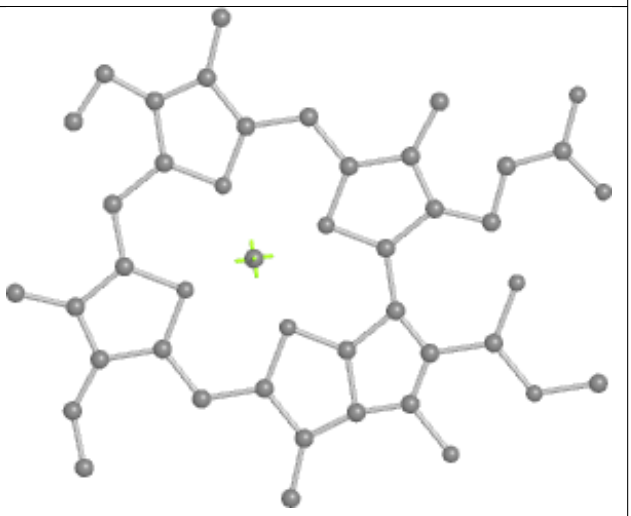
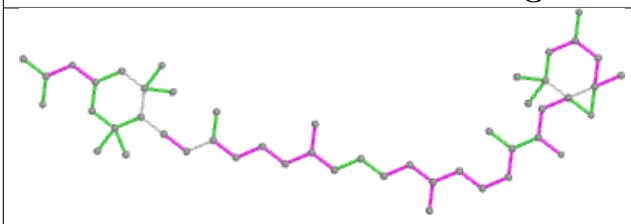


Rings

Ligand A86 13 316



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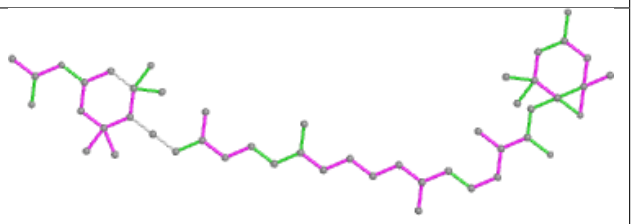

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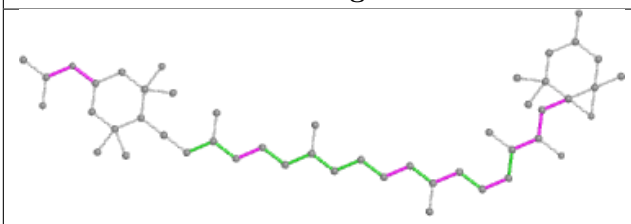

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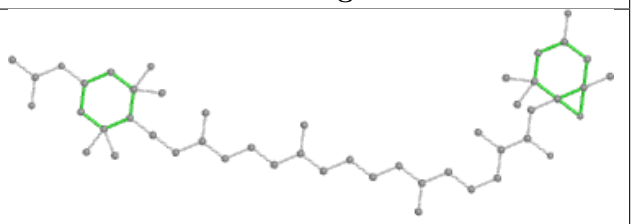
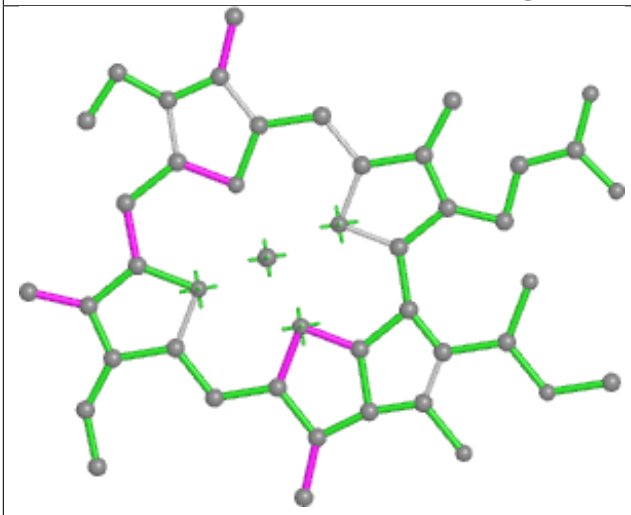


Rings

Ligand CLA 41 302



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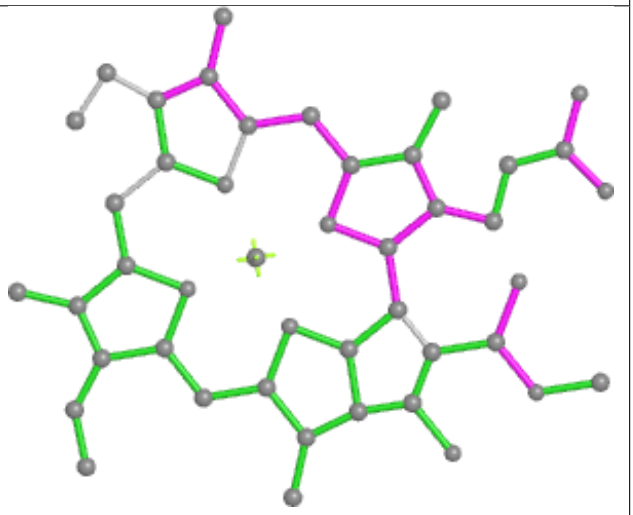

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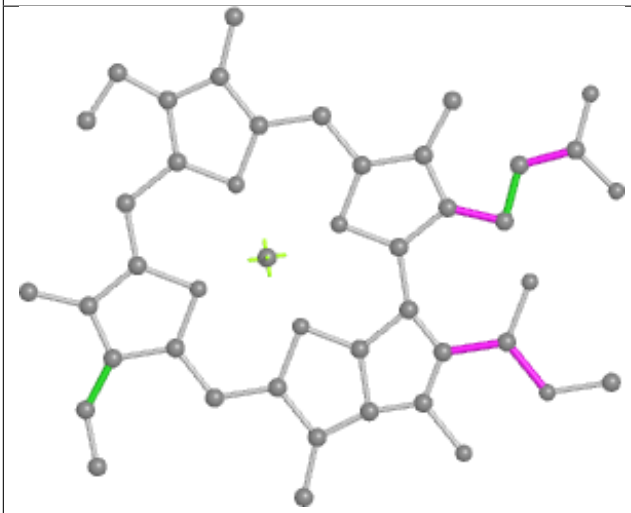

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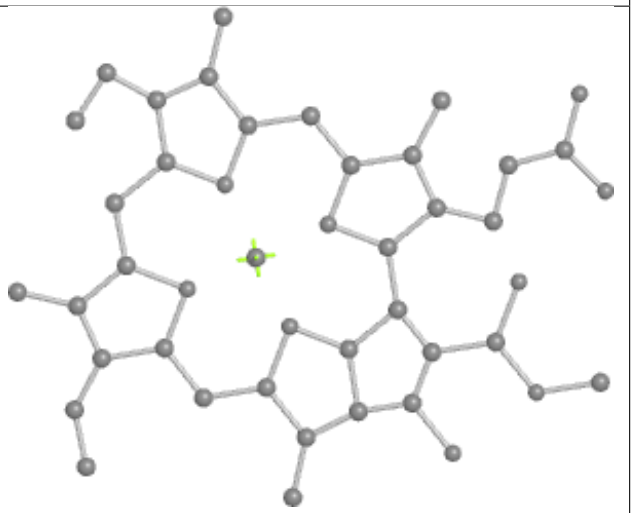
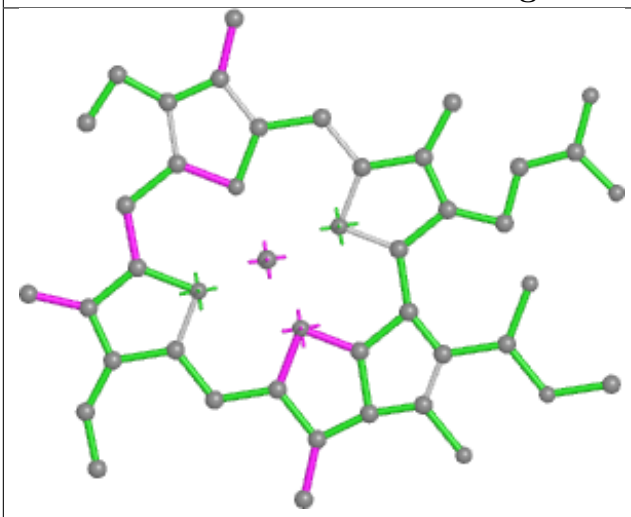


Rings

Ligand CLA 14 306



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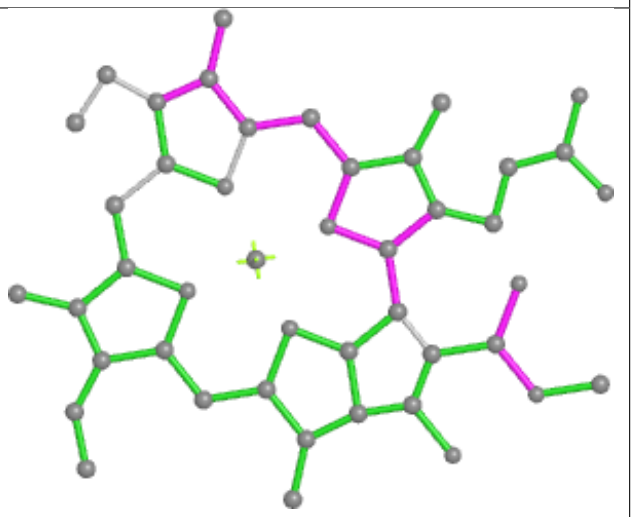
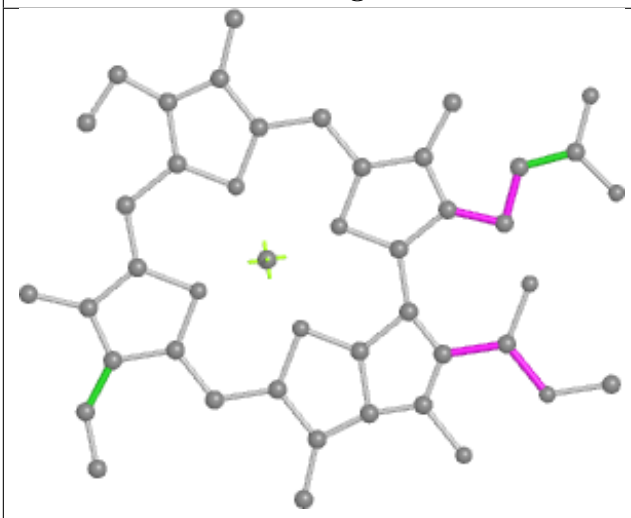


Bond angles



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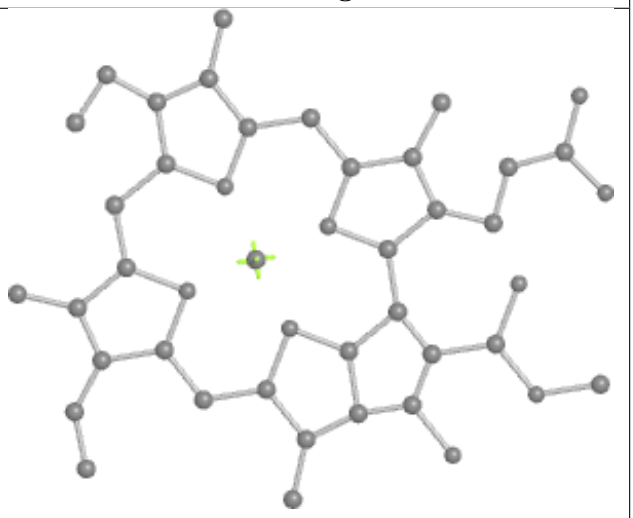
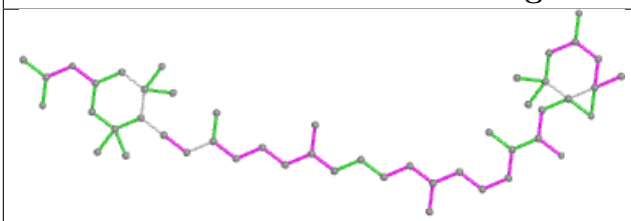


Rings

Ligand A86 17 311



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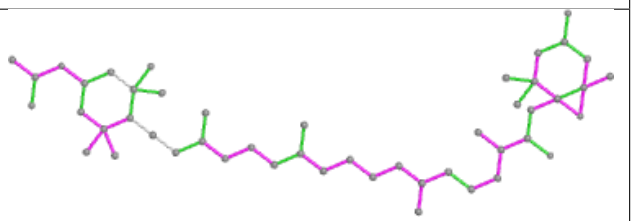
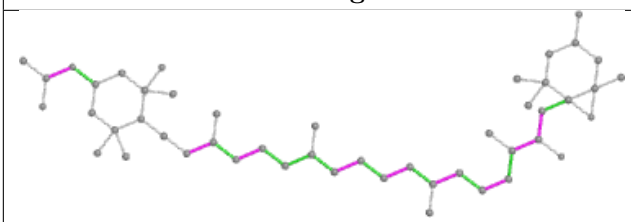
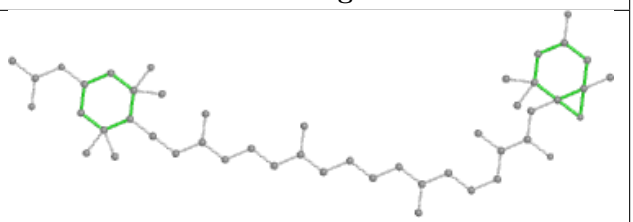


Bond angles

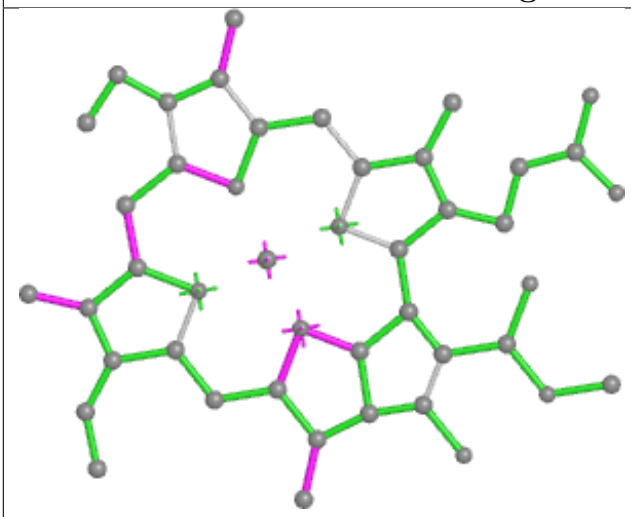


Torsions



Rings

Ligand CLA 21 304



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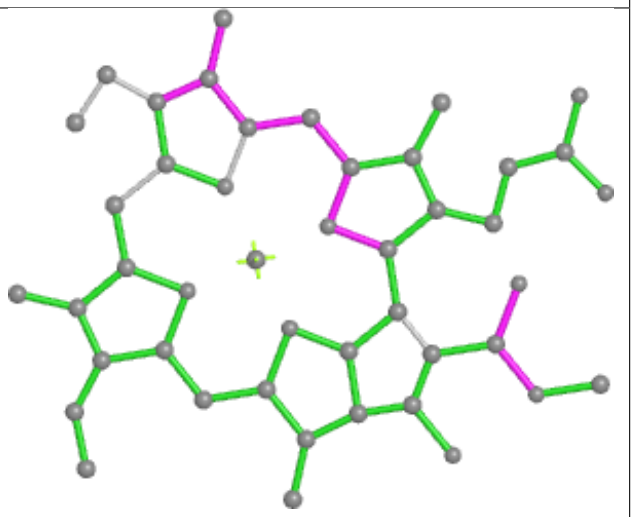
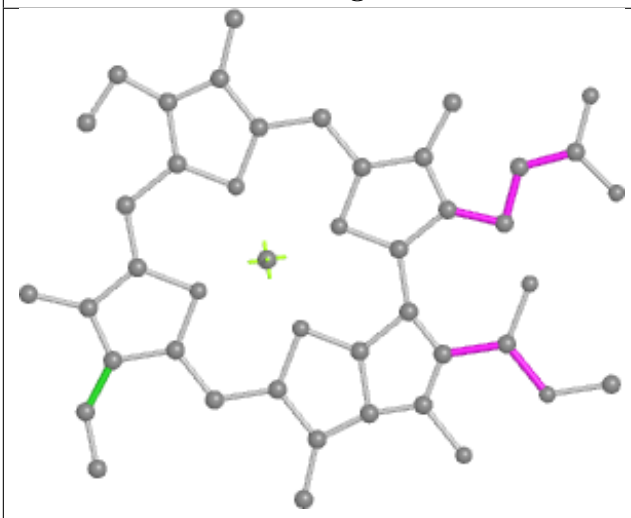


Bond angles



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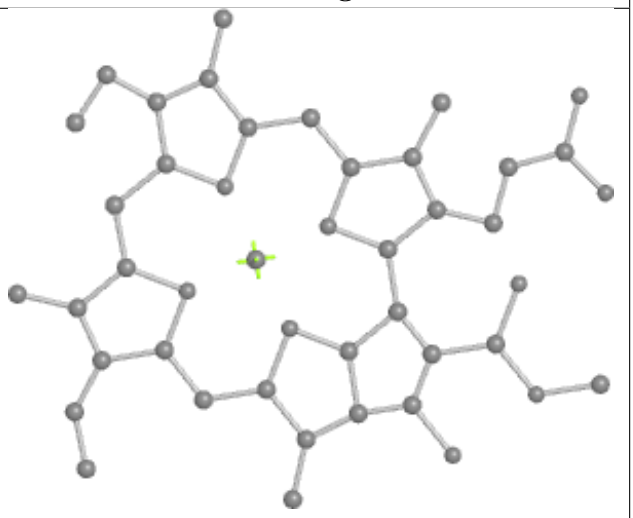
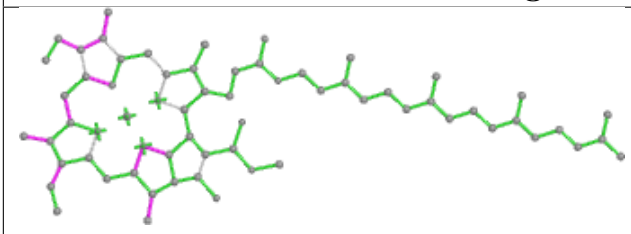


Rings

Ligand CLA B 602



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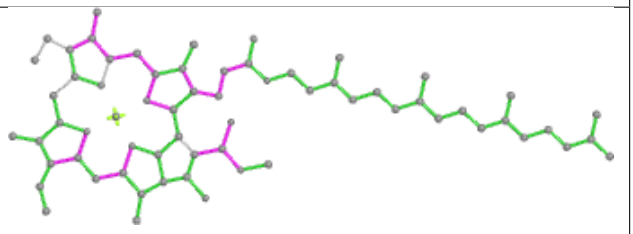

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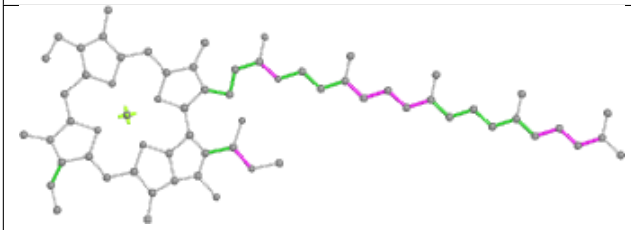

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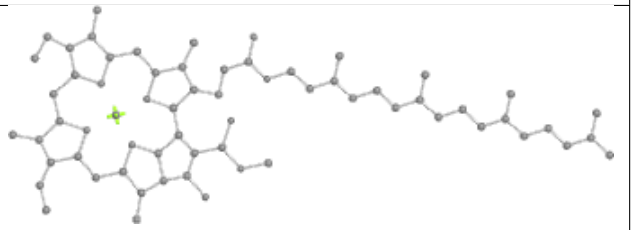
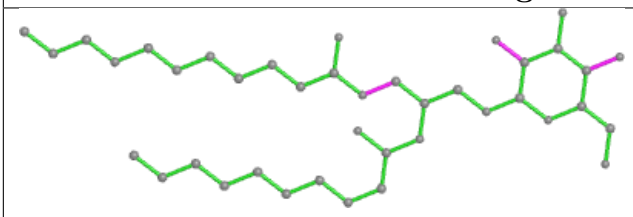


Rings

Ligand LMG M 102



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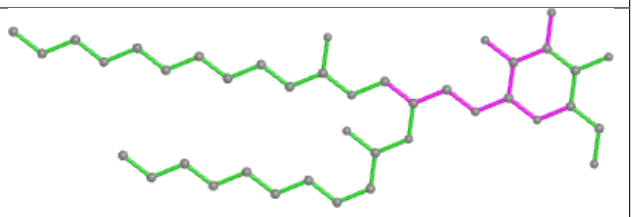

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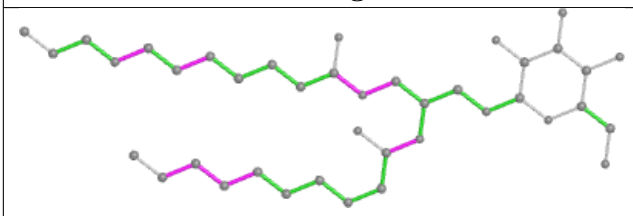

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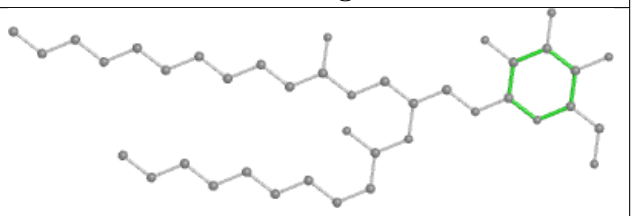
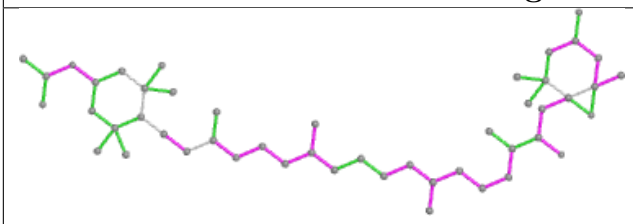


Rings

Ligand A86 31 313



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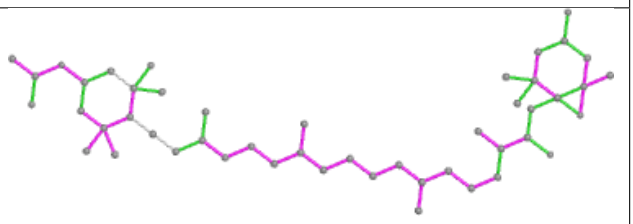

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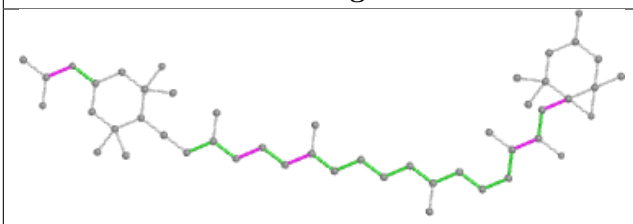

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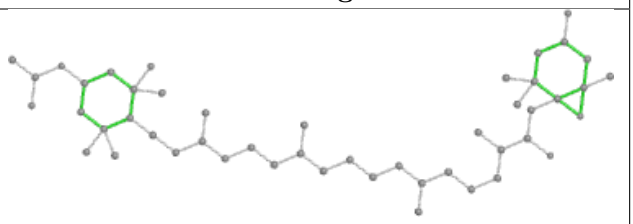
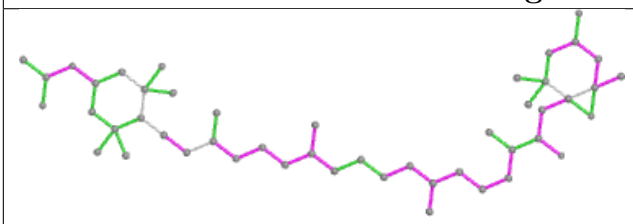


Rings

Ligand A86 33 312



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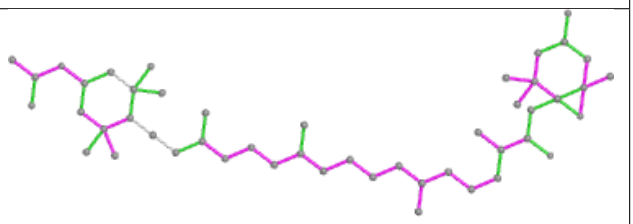

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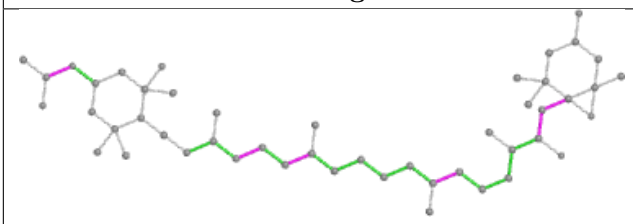

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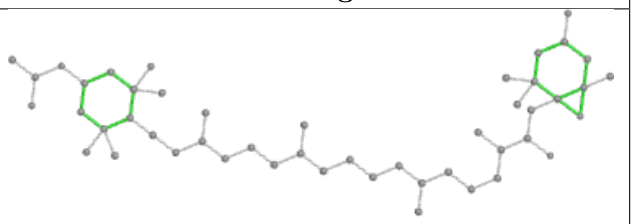
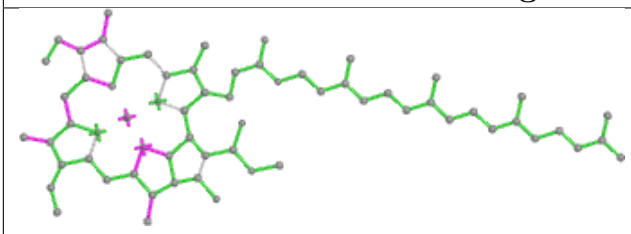


Rings

Ligand CLA 17 305



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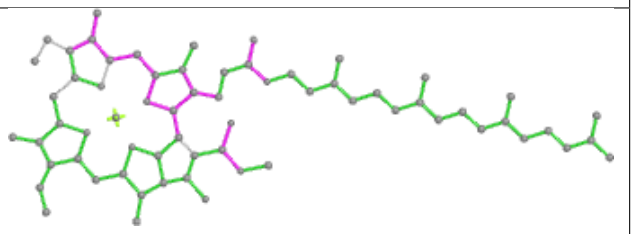
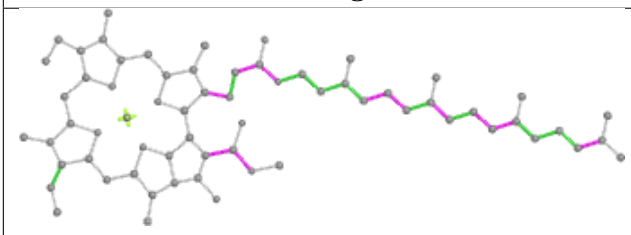


Bond angles



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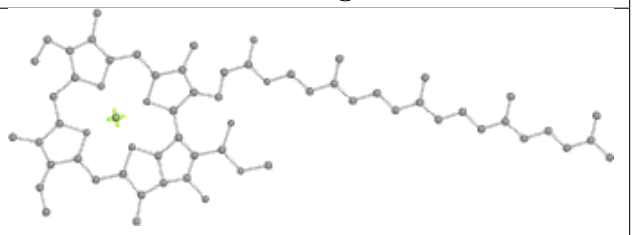
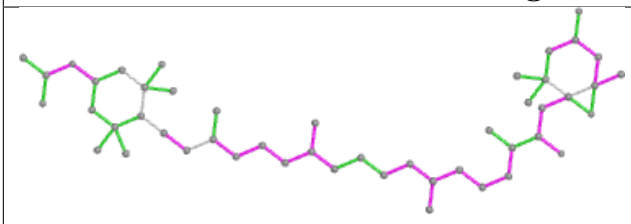


Rings

Ligand A86 13 315



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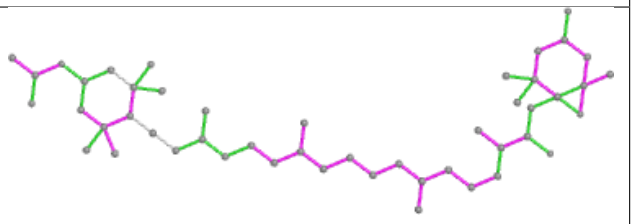

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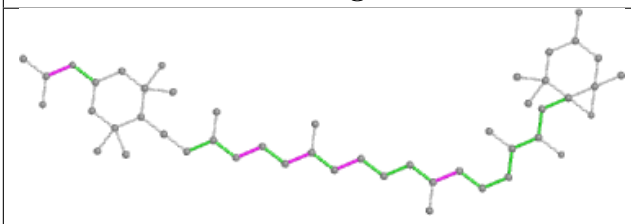

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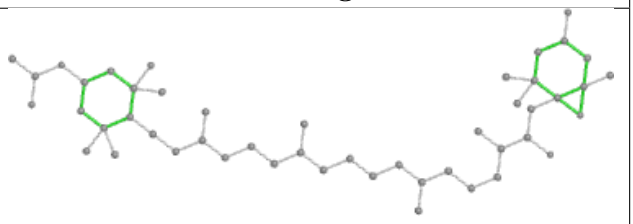
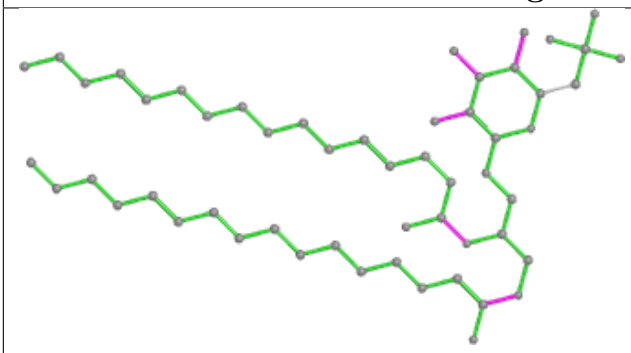


Rings

Ligand SQD L 103



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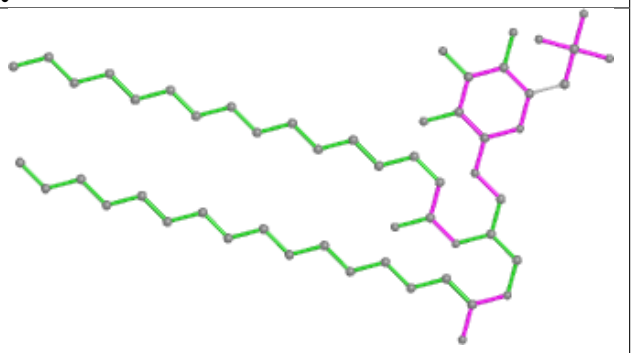

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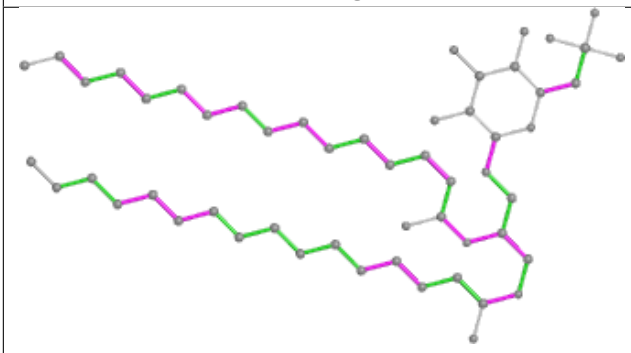

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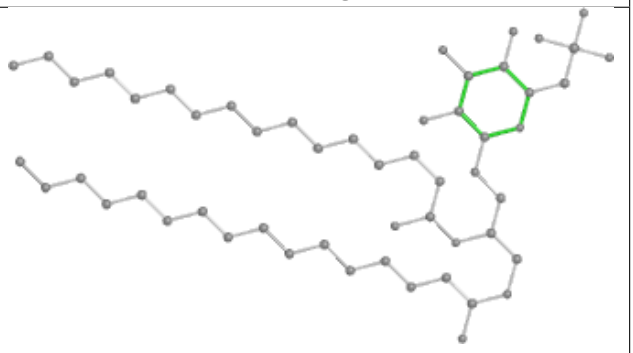
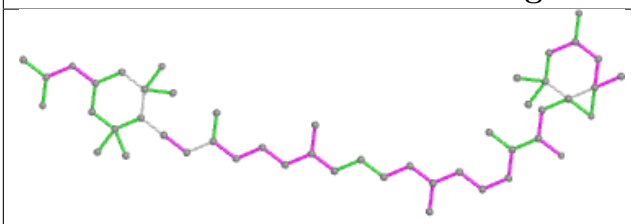


Rings

Ligand A86 40 201



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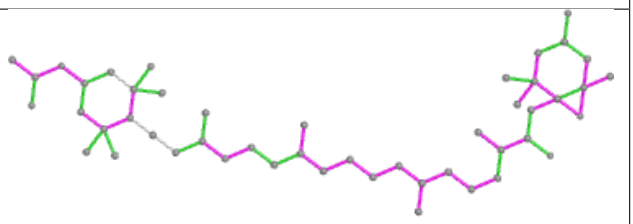

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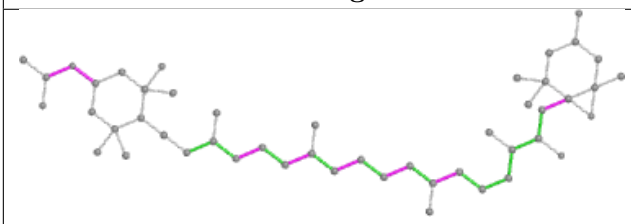

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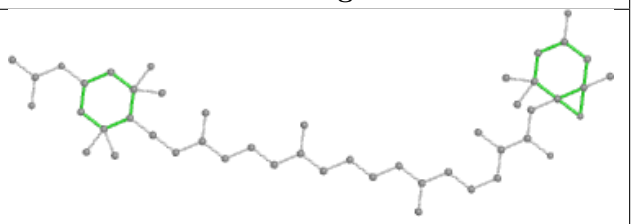
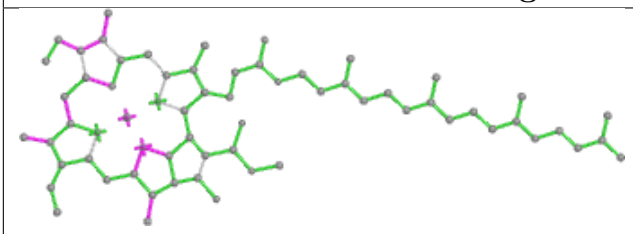


Rings

Ligand CLA 16 304



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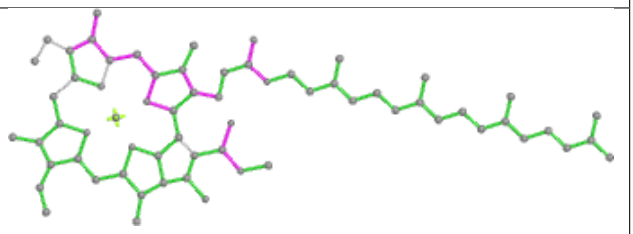
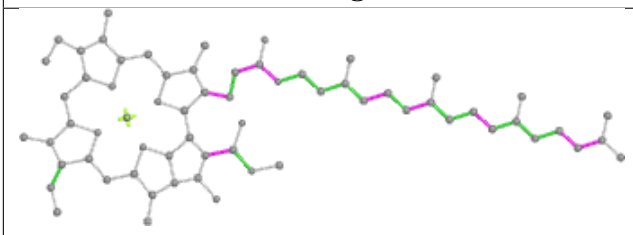


Bond angles



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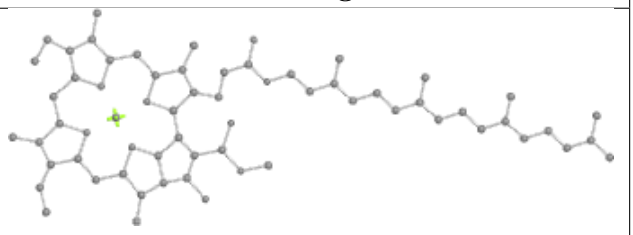
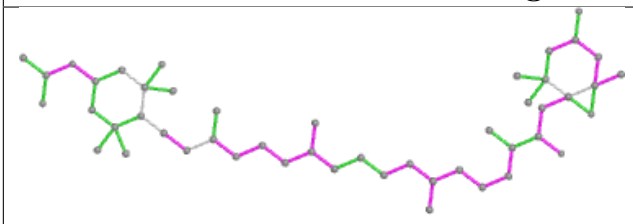


Rings

Ligand A86 11 316



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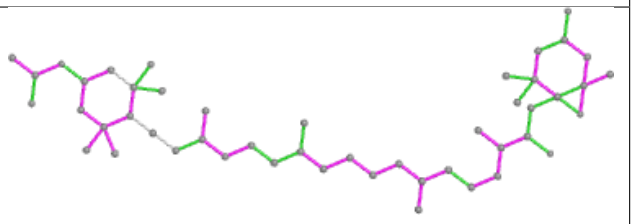
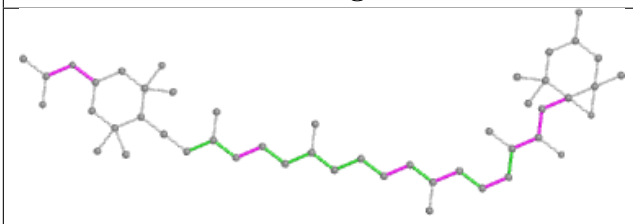
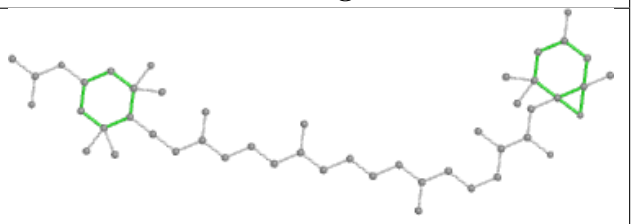


Bond angles

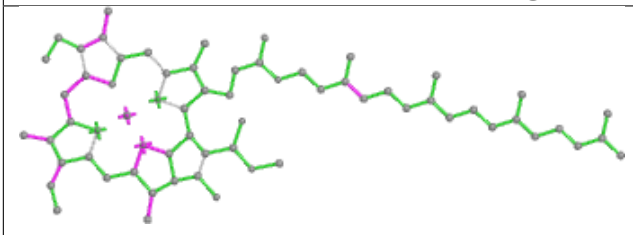


Torsions



Rings

Ligand CLA B 606



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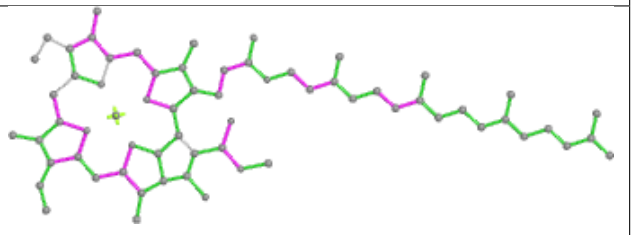
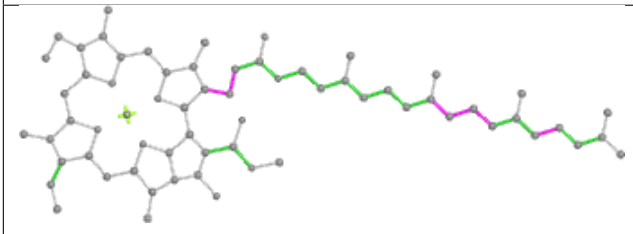


Bond angles



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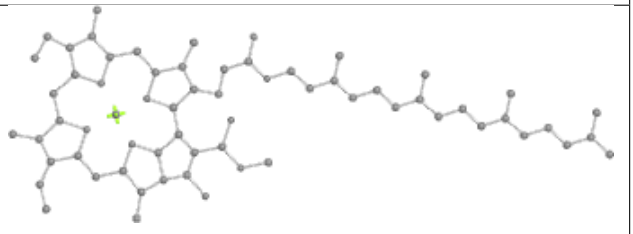
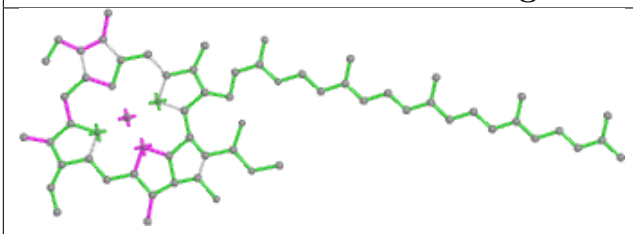


Rings

Ligand CLA 14 304



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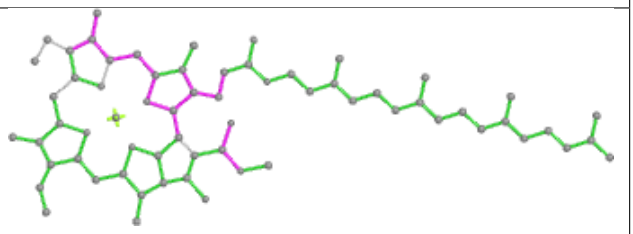
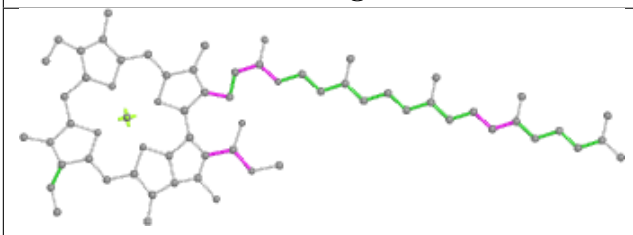
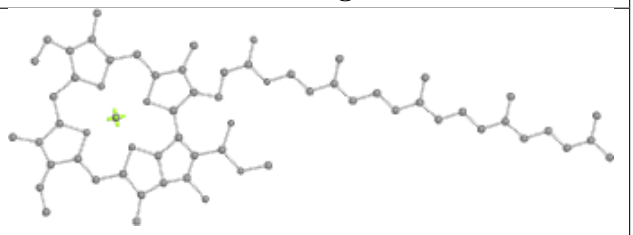


Bond angles

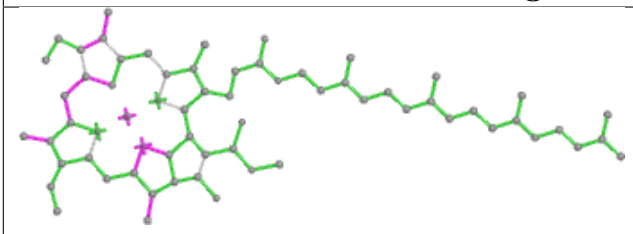


Torsions

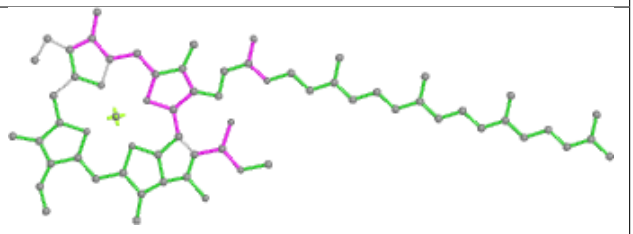


Rings

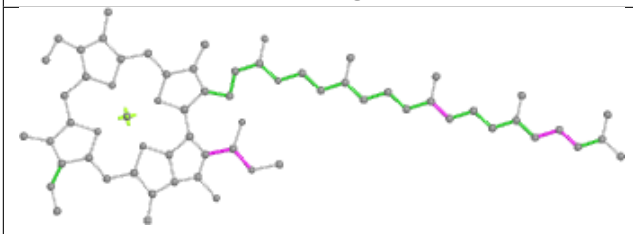
Ligand CLA B 614



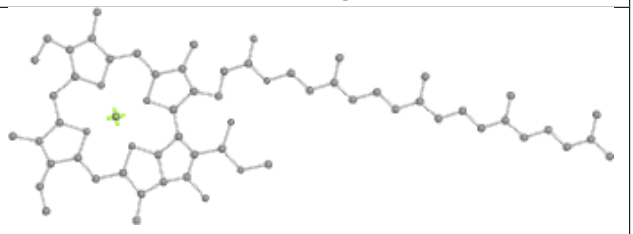
Bond lengths



Bond angles

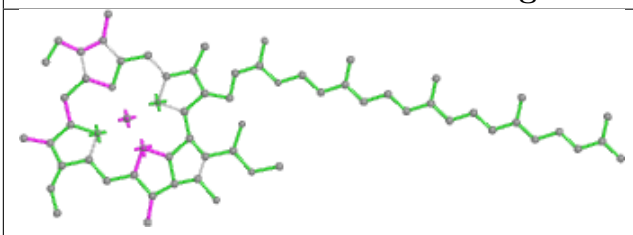


Torsions



Rings

Ligand CLA 37 305



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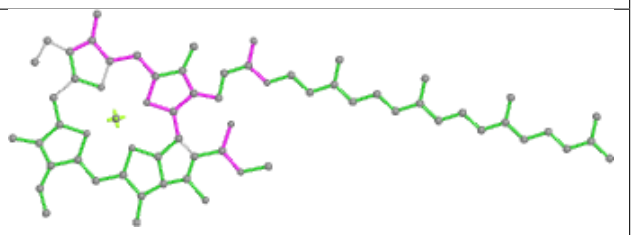

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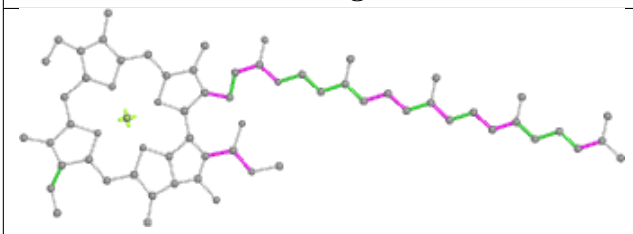

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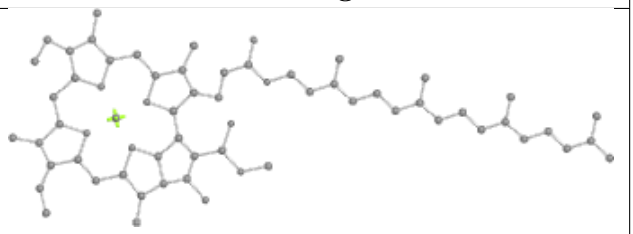
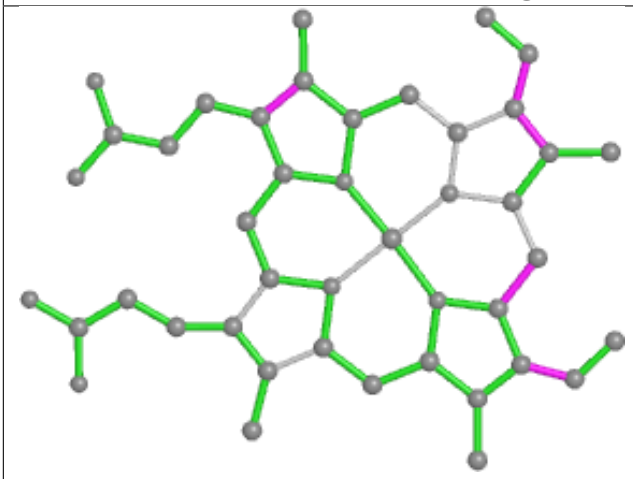


Rings

Ligand HEM V 201



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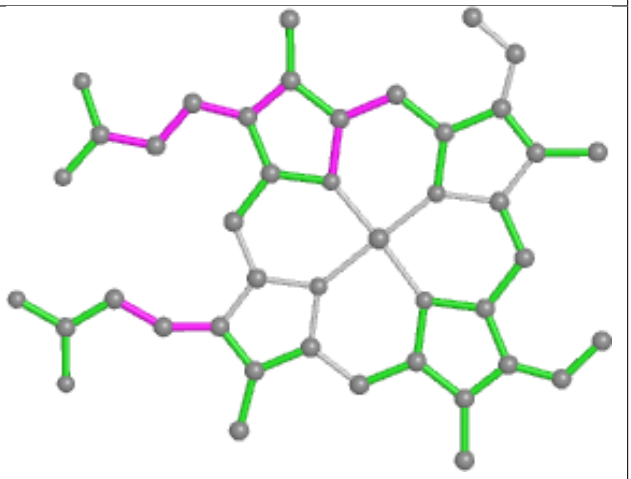

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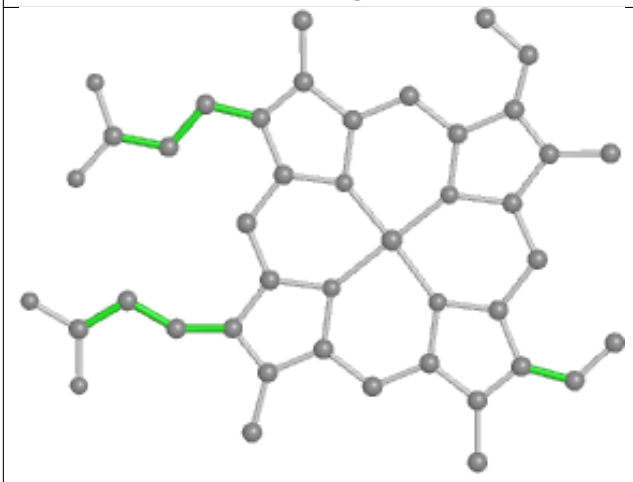

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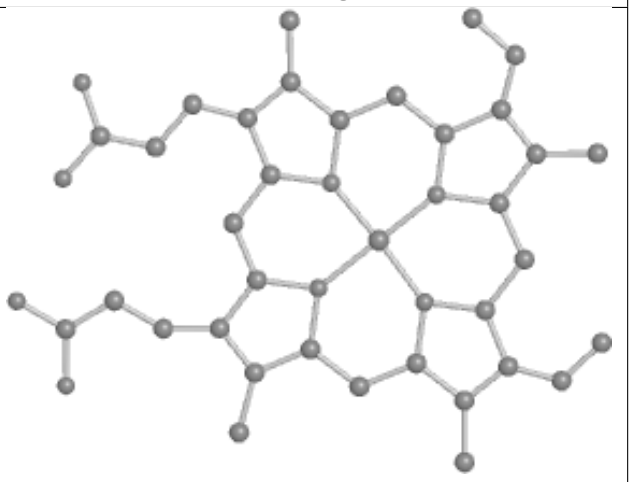
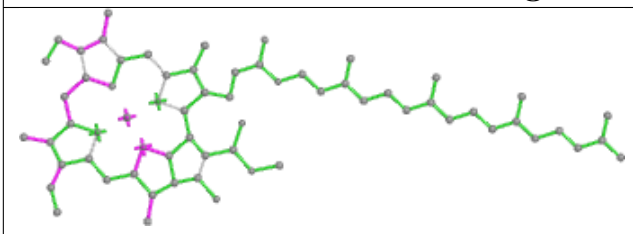


Rings

Ligand CLA B 604



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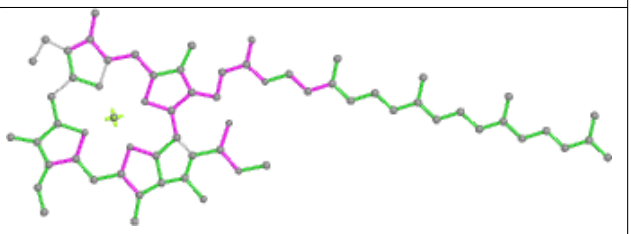

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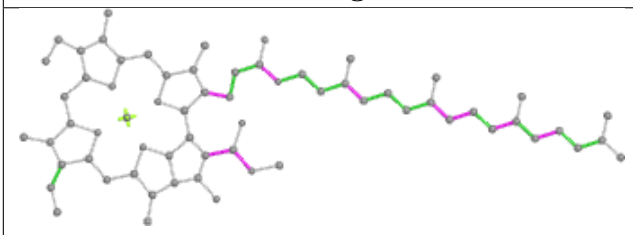

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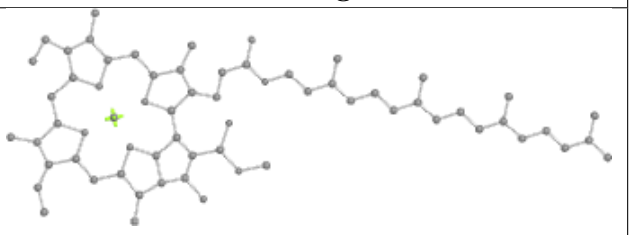
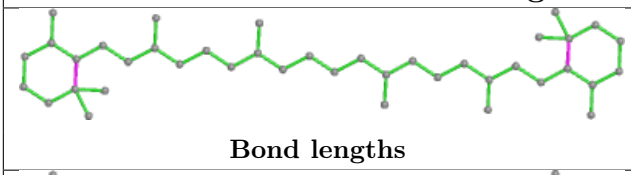


Rings

Ligand BCR c 521



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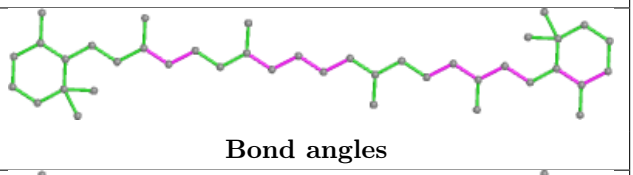

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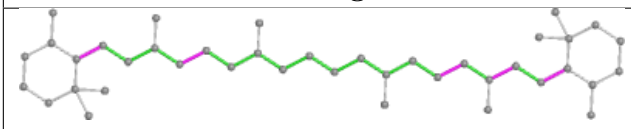

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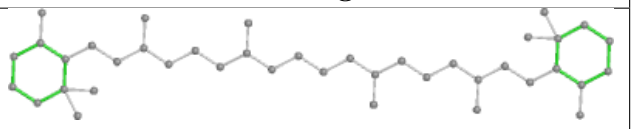
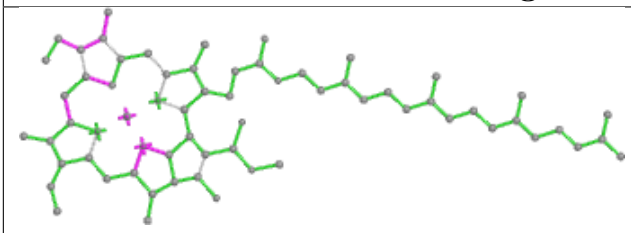


Rings

Ligand CLA 21 303



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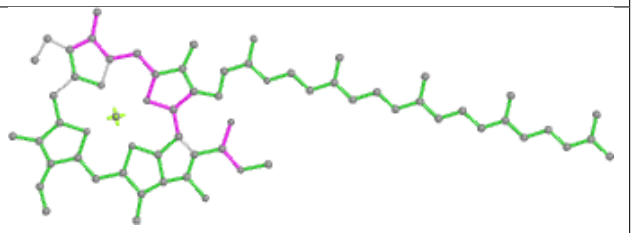

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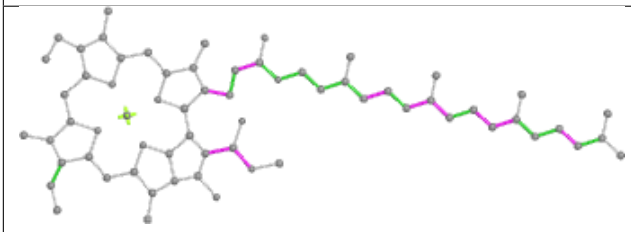

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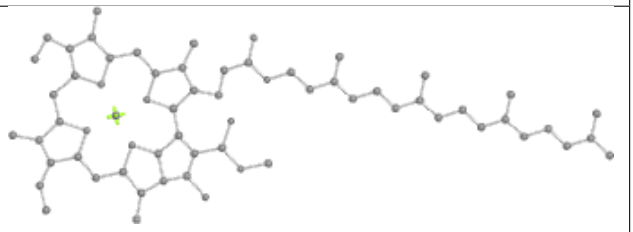
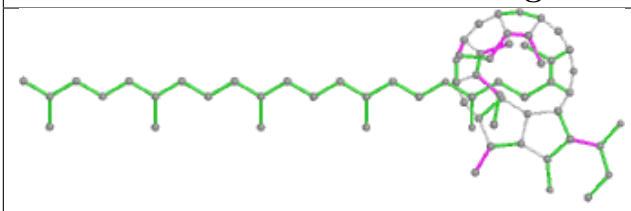


Rings

Ligand PHO d 404



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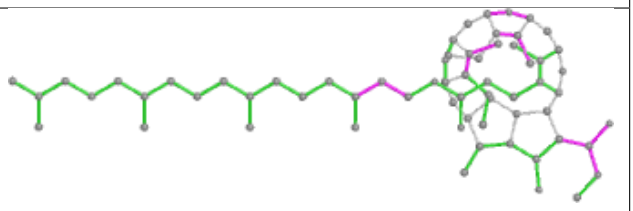

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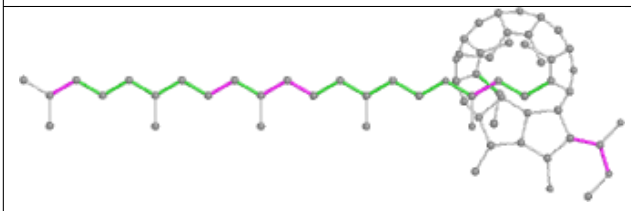

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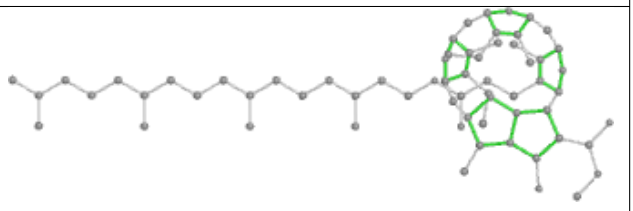
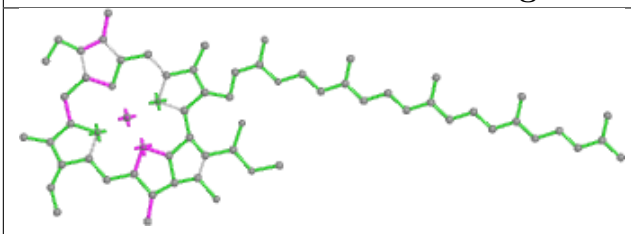


Rings

Ligand CLA 38 310



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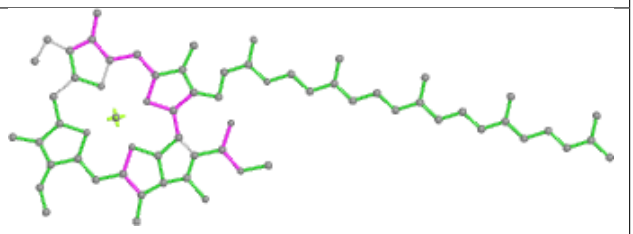

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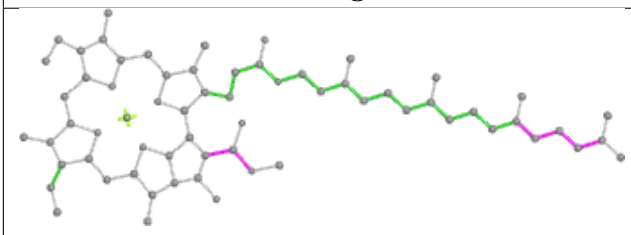

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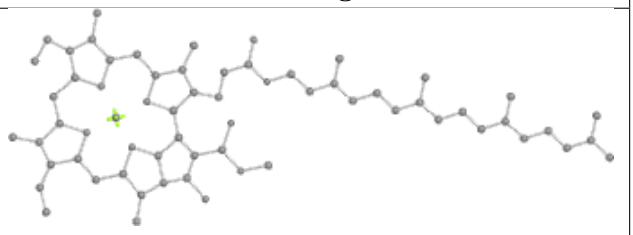
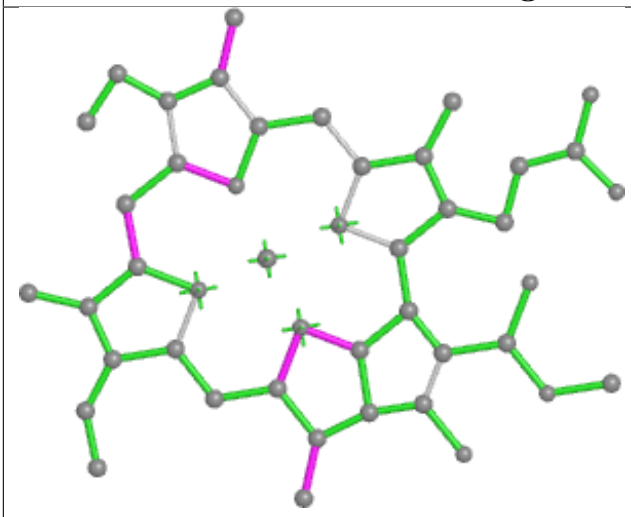


Rings

Ligand CLA 41 305



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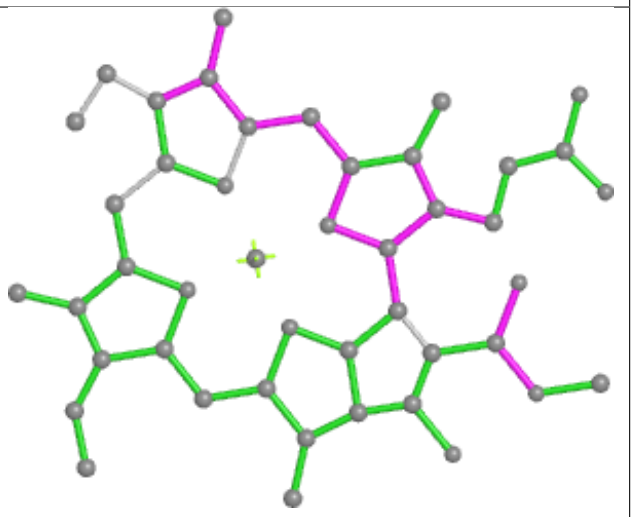

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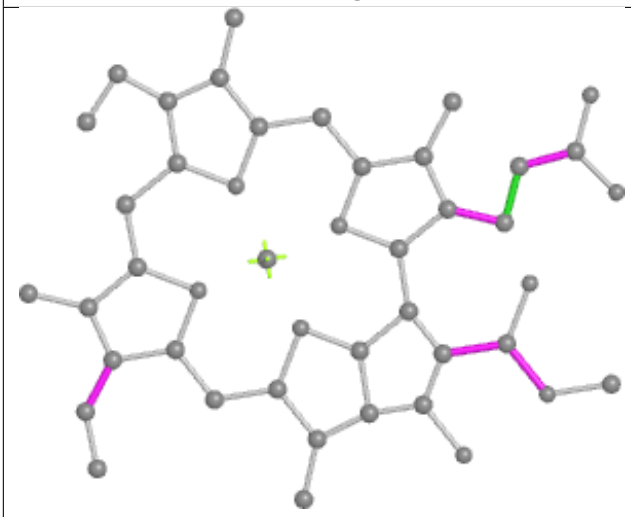

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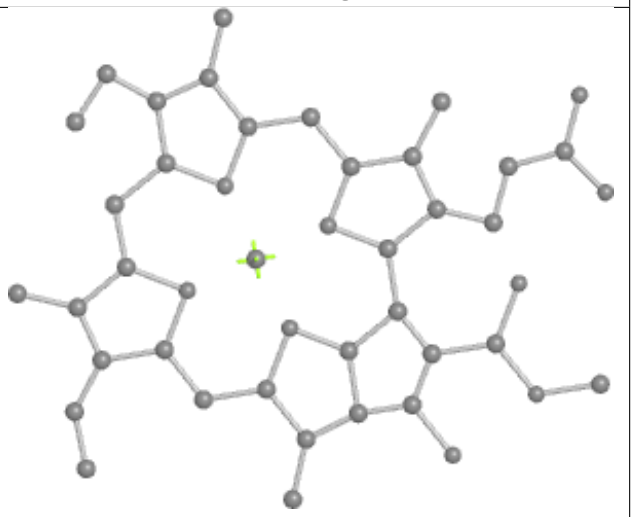
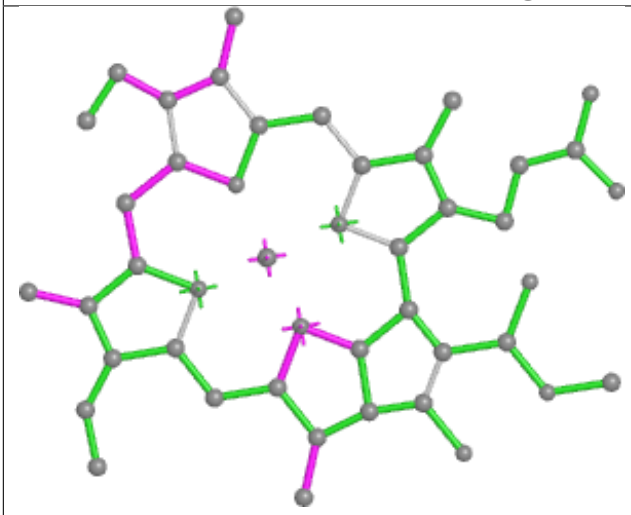


Rings

Ligand CLA 19 306



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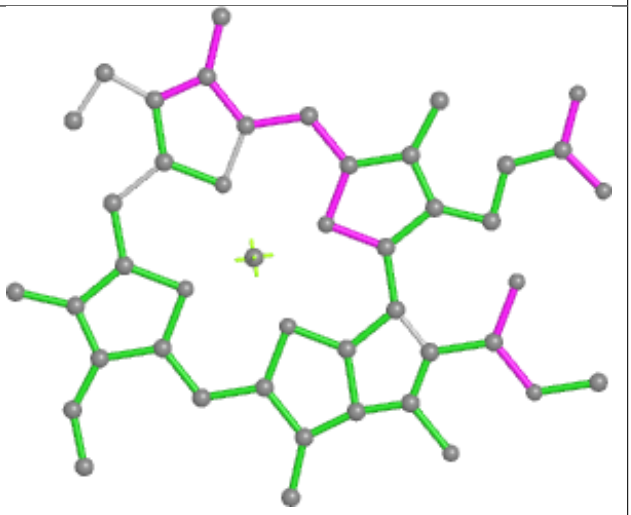

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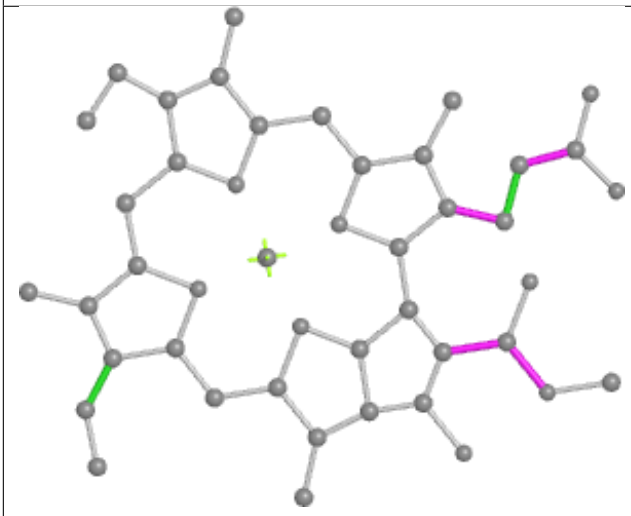

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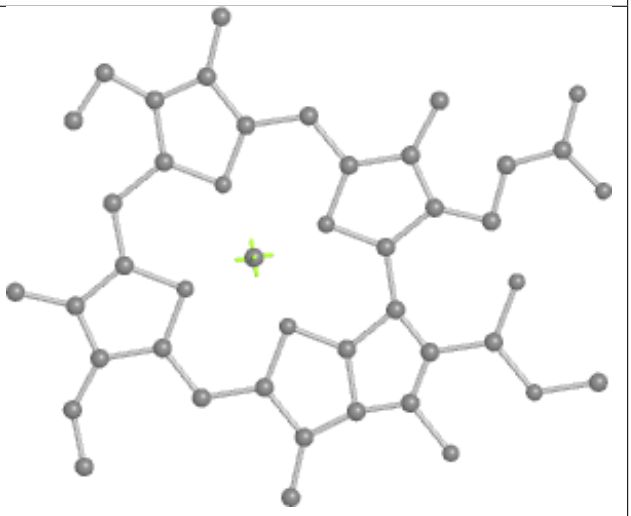
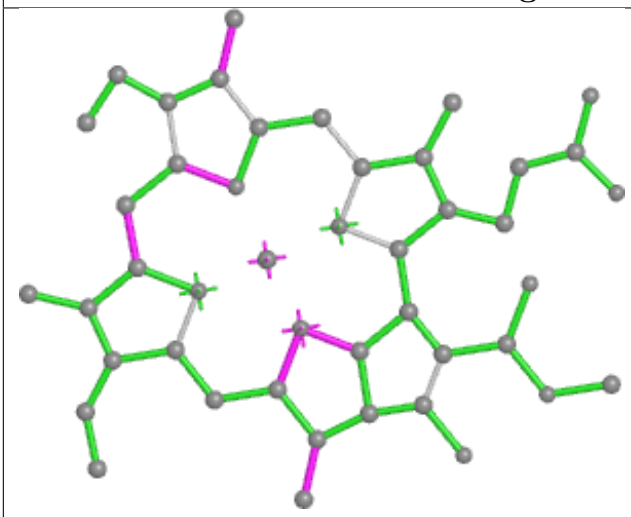


Rings

Ligand CLA 37 306



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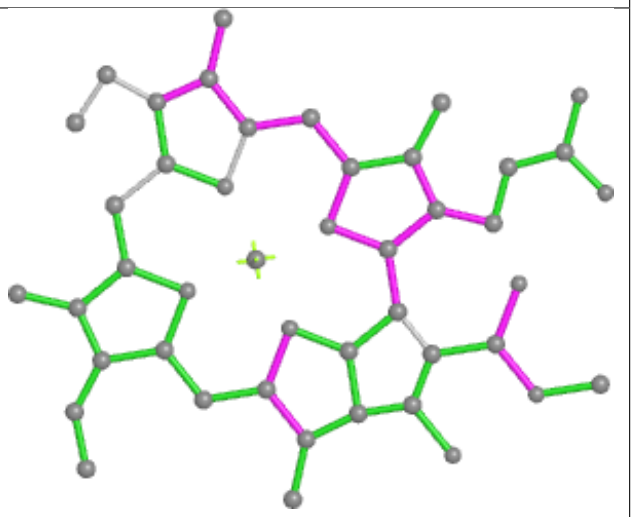

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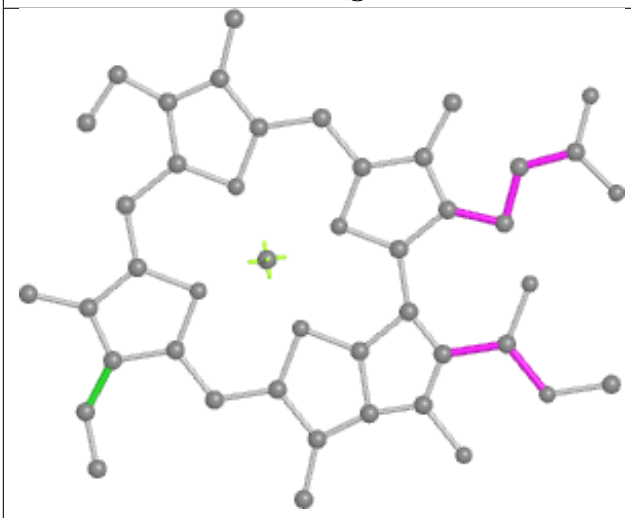

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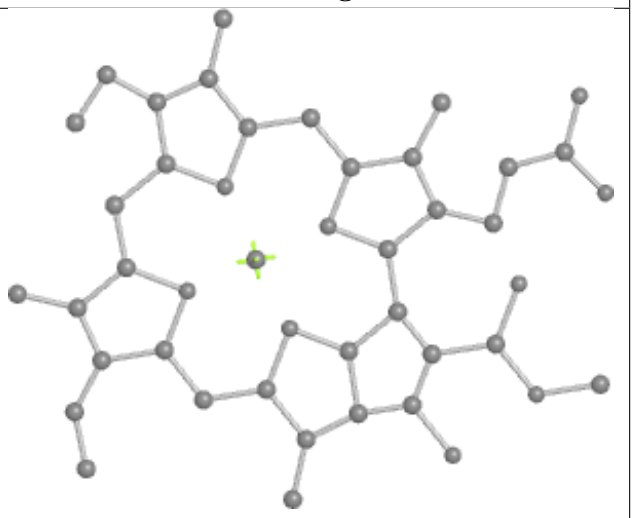
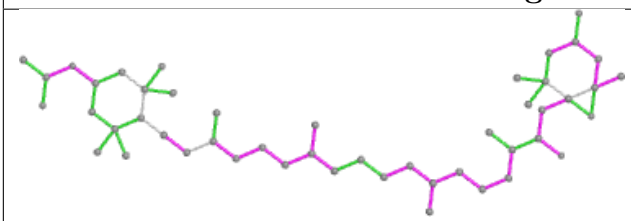


Rings

Ligand A86 38 313



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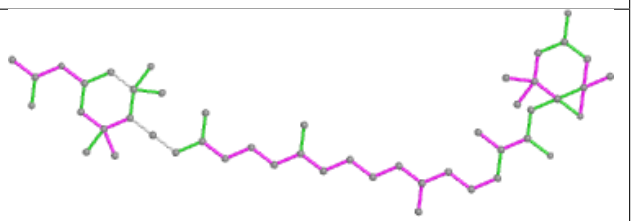
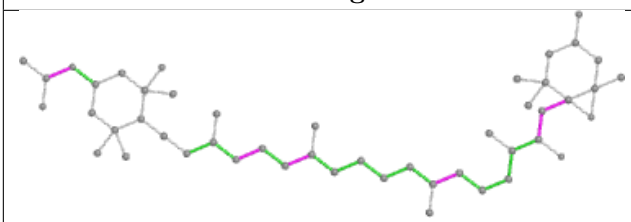
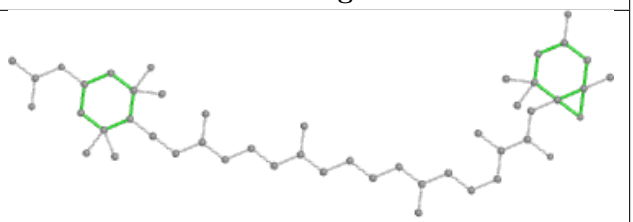


Bond angles

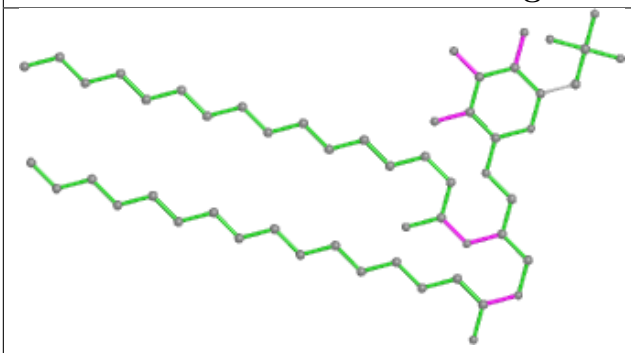


Torsions



Rings

Ligand SQD A 406



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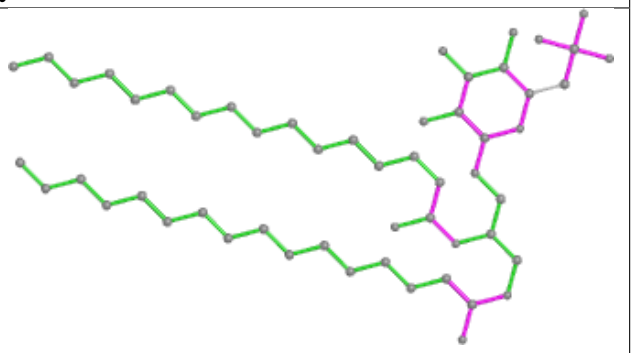
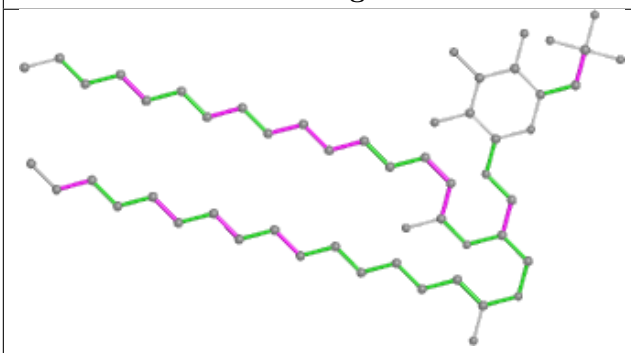
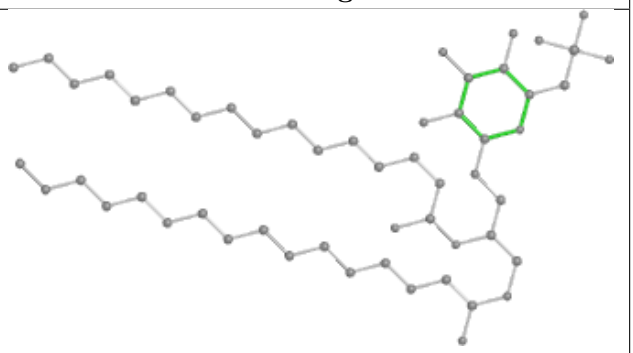


Bond angles

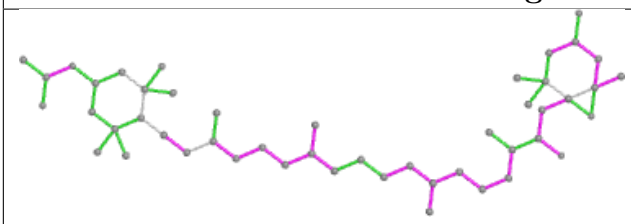


Torsions



Rings

Ligand A86 14 313



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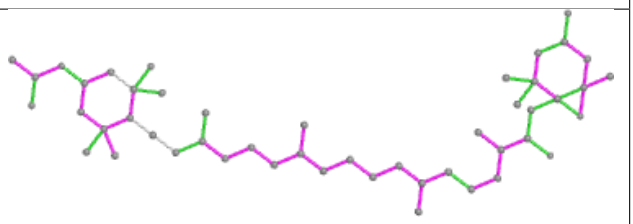
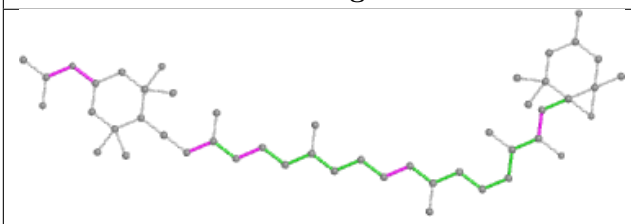
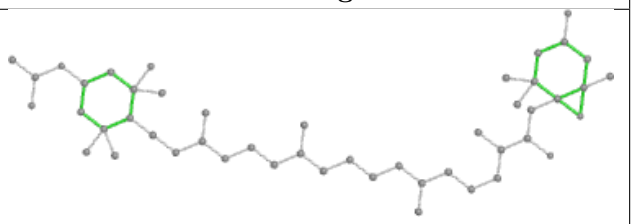


Bond angles

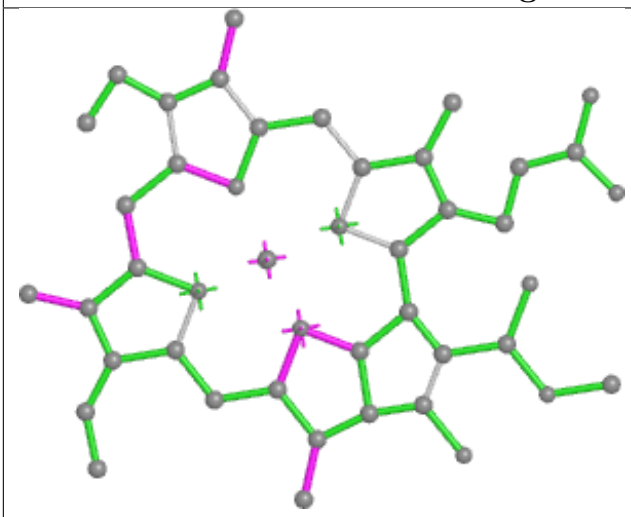


Torsions



Rings

Ligand CLA 16 303



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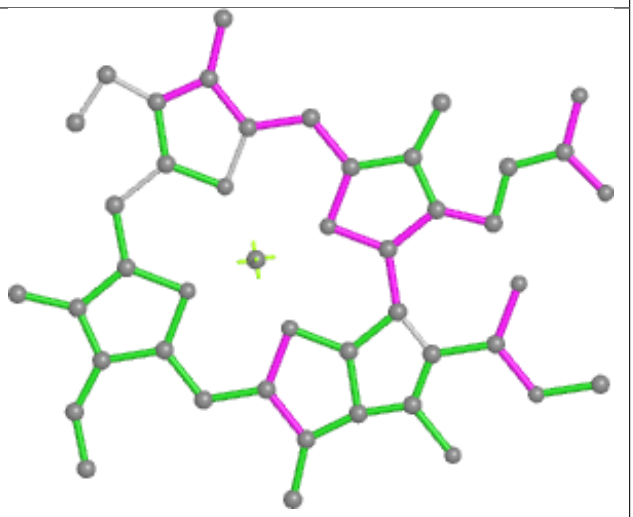
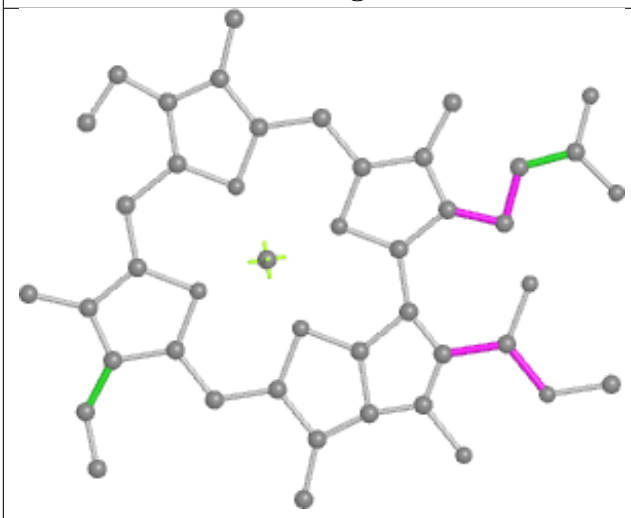
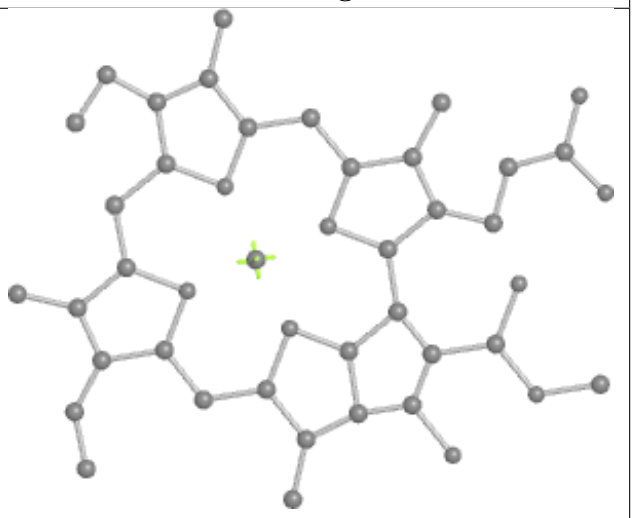


Bond angles

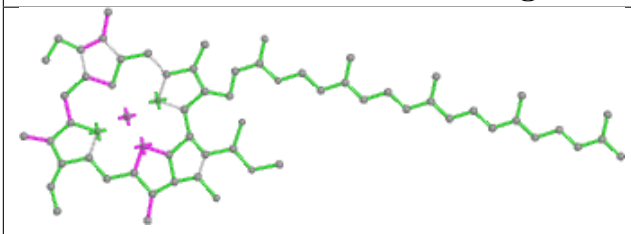


Torsions



Rings

Ligand CLA 12 312



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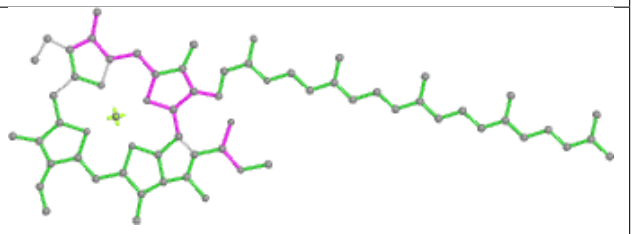

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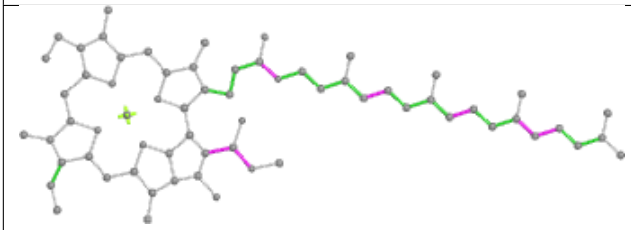

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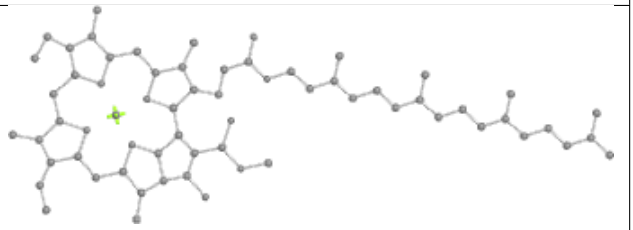
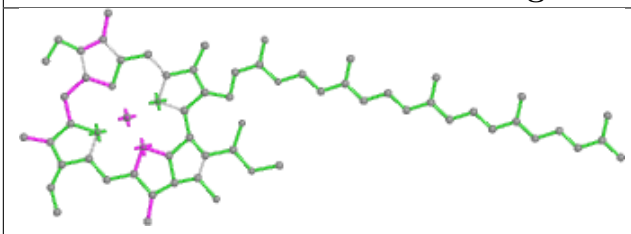


Rings

Ligand CLA b 614



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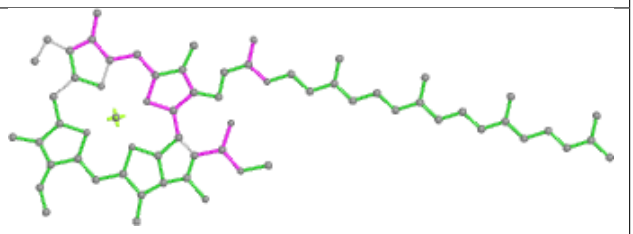

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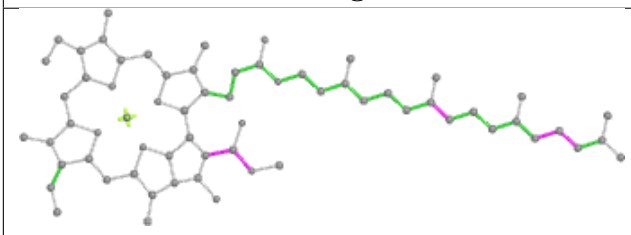

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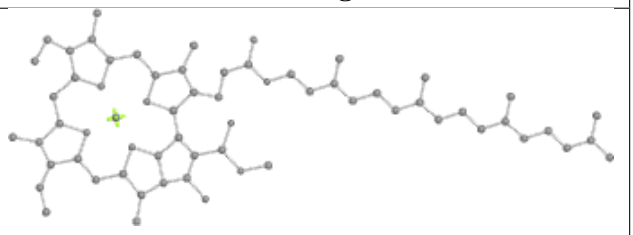
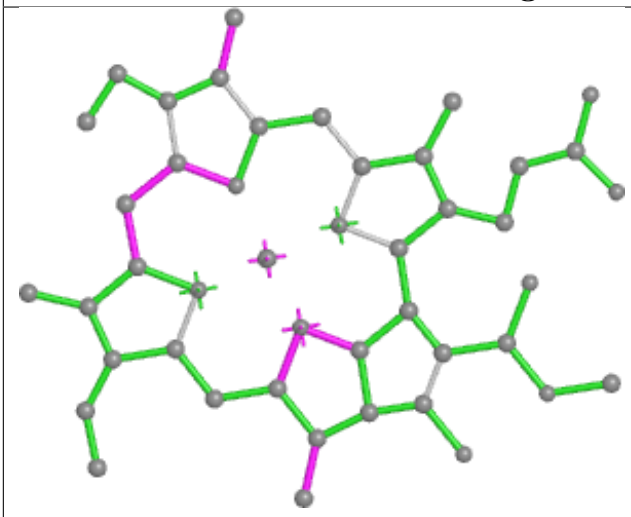


Rings

Ligand CLA 38 304



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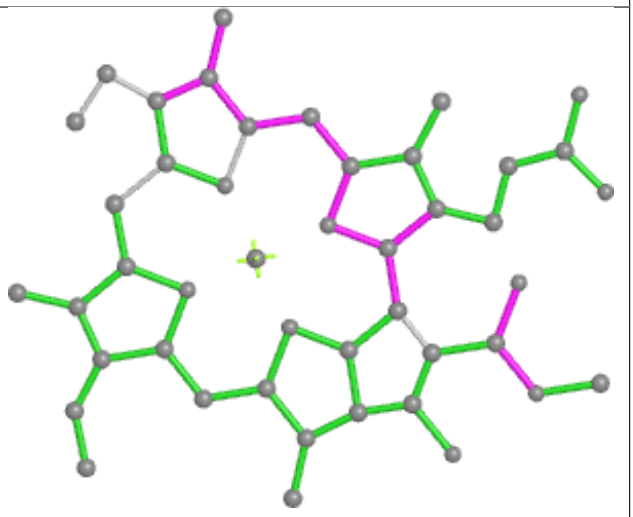

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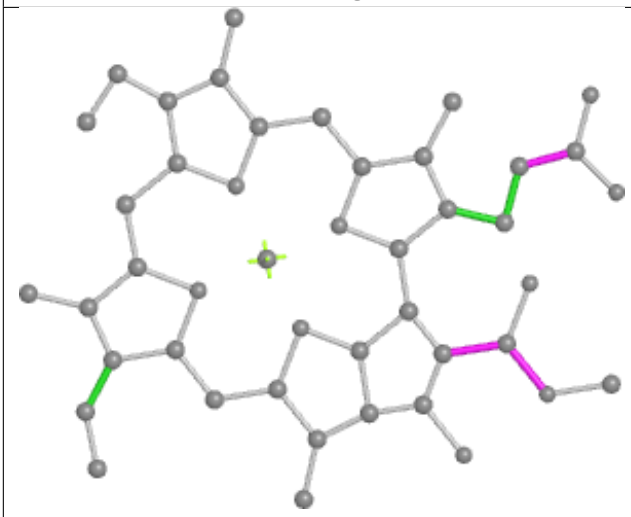

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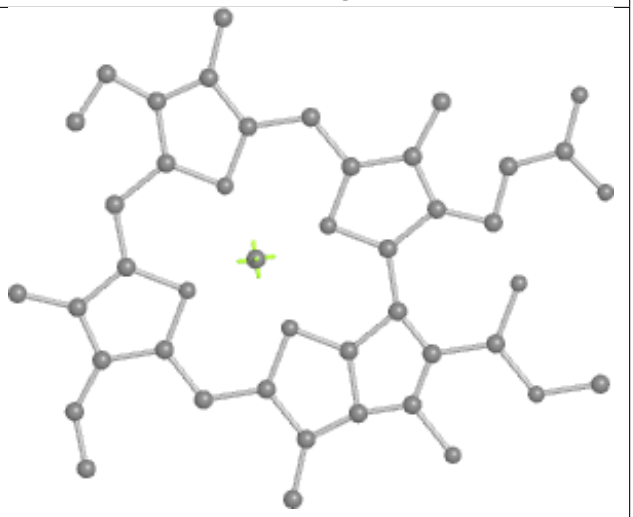
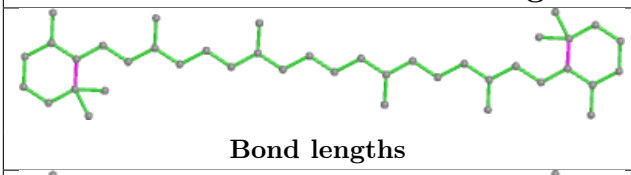


Rings

Ligand BCR a 404



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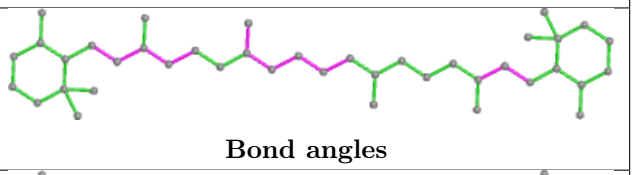

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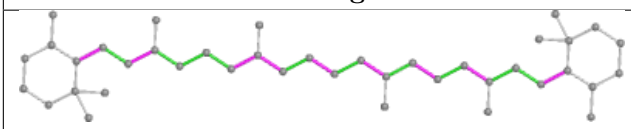

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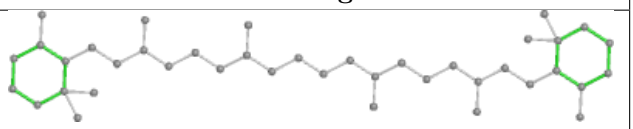

Rings

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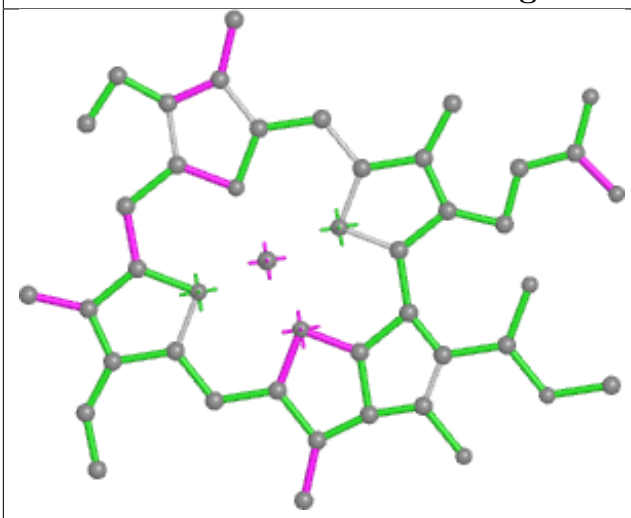

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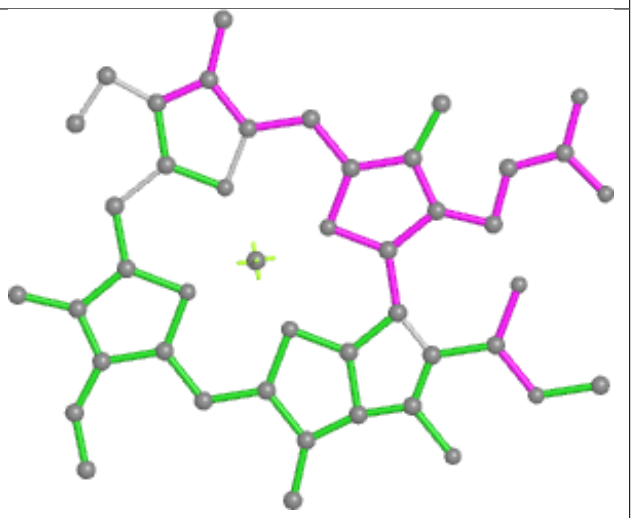

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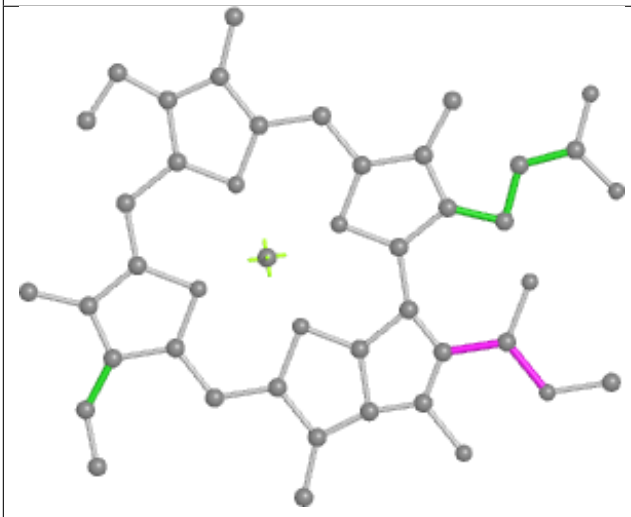

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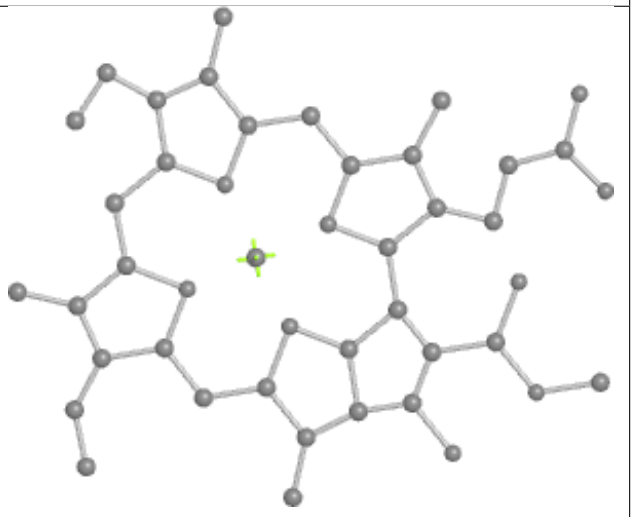
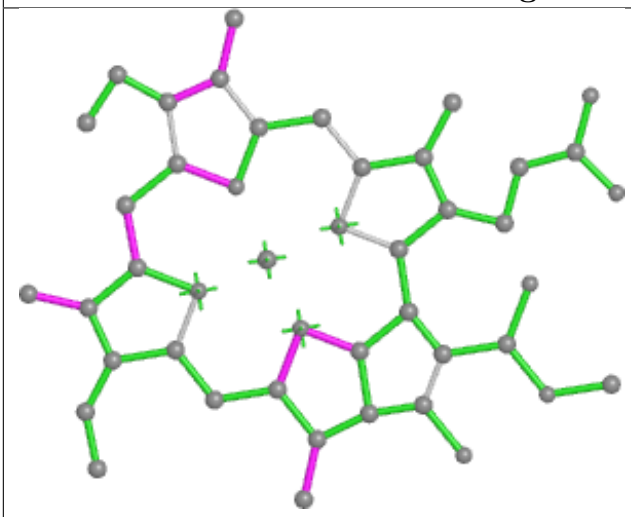


Rings

Ligand CLA 15 302



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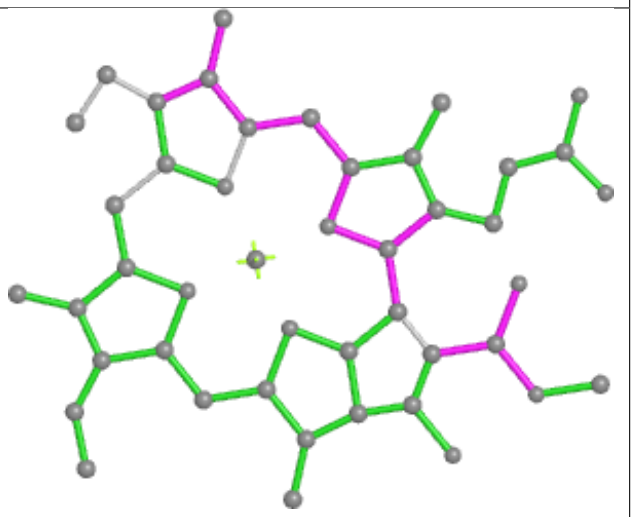

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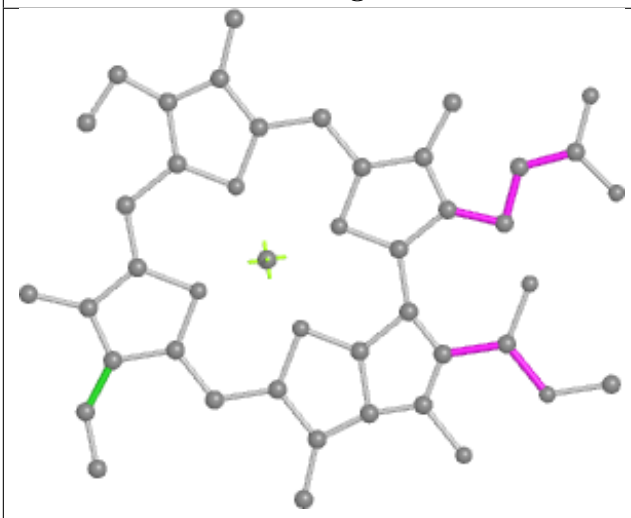

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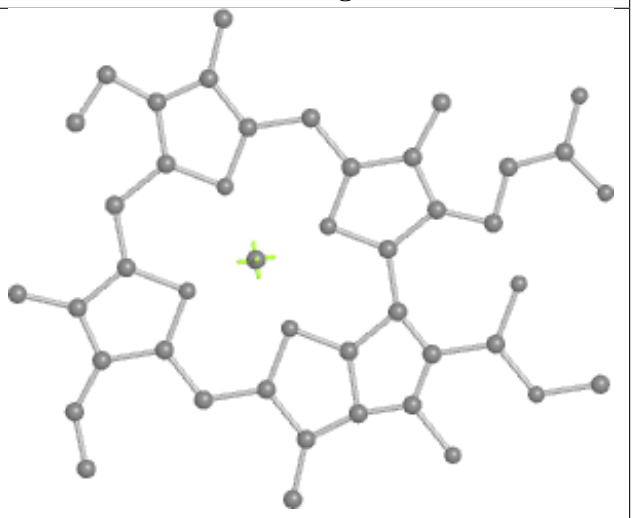
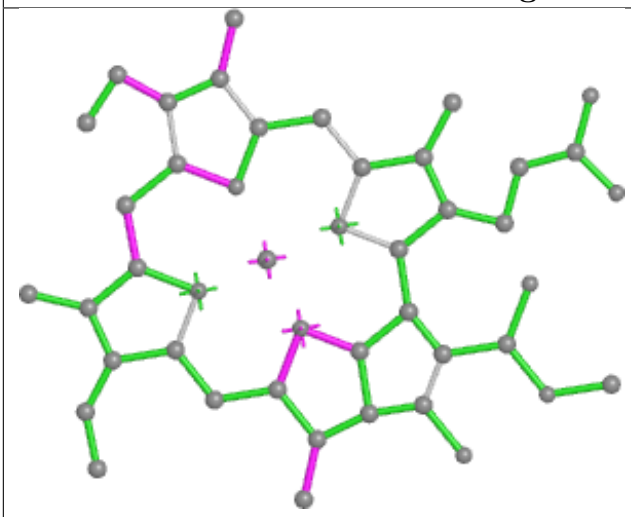


Rings

Ligand CLA 35 309



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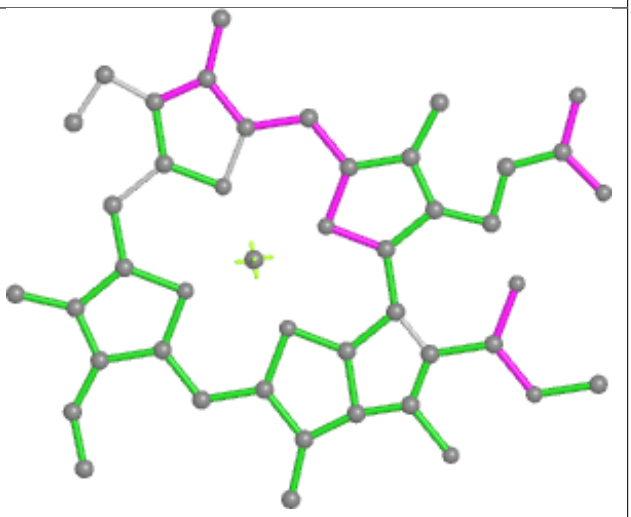

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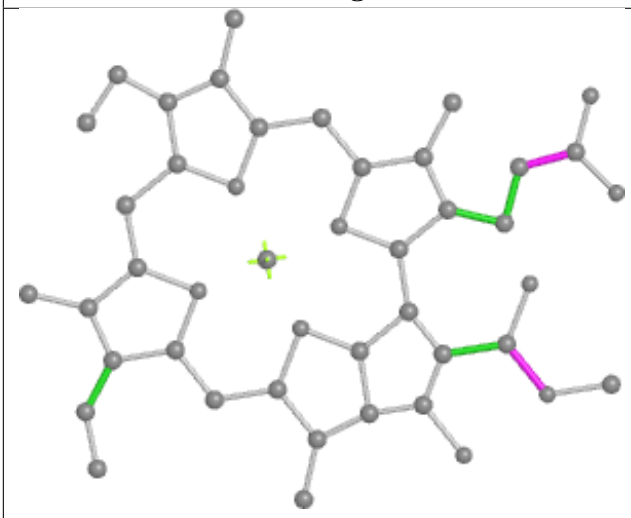

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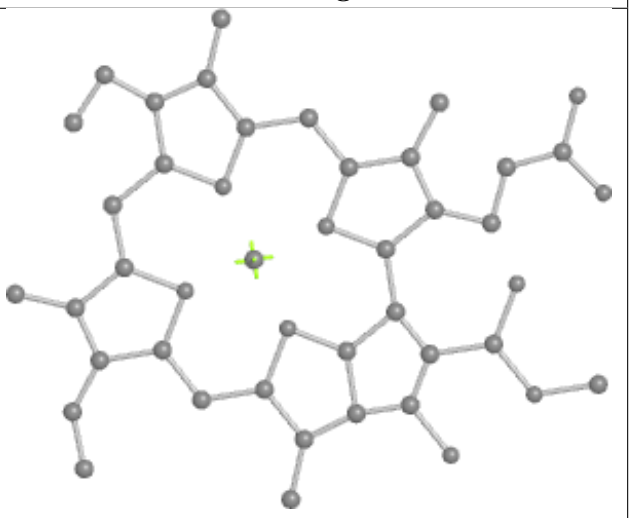
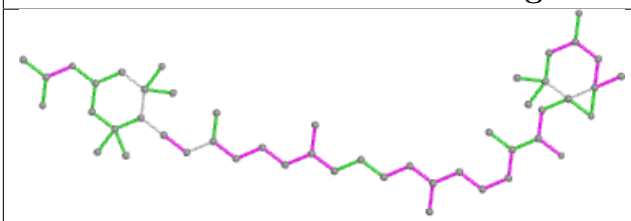


Rings

Ligand A86 19 310



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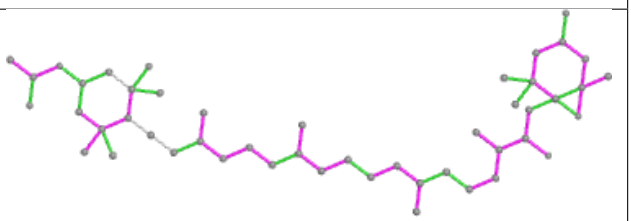

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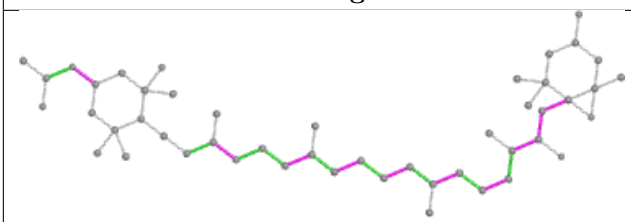

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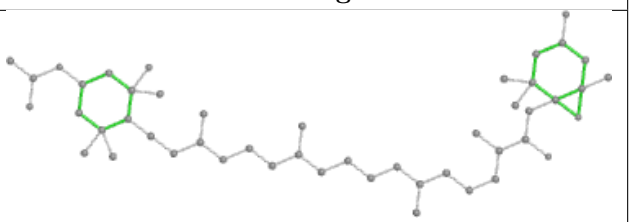

Rings

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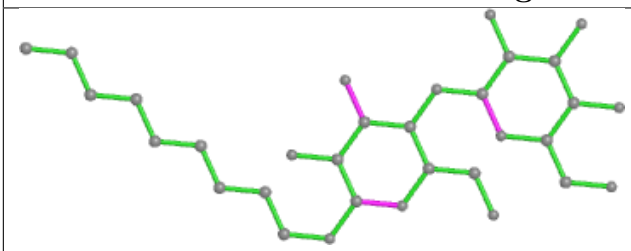

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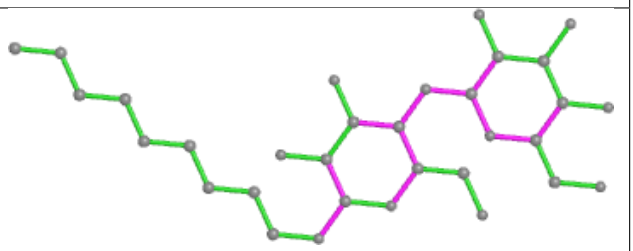

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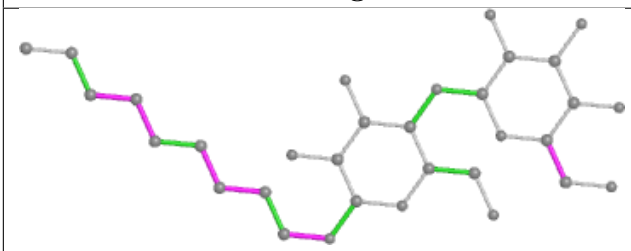

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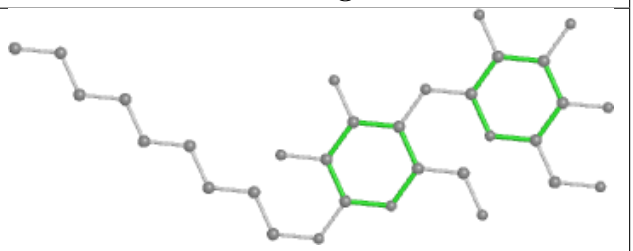
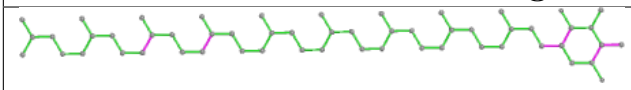


Rings

Ligand PL9 D 404



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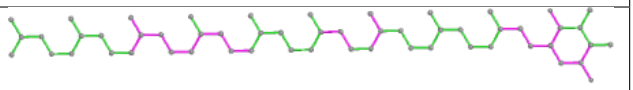

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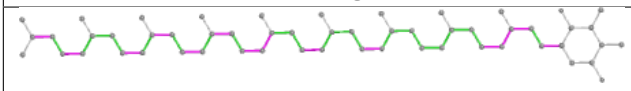

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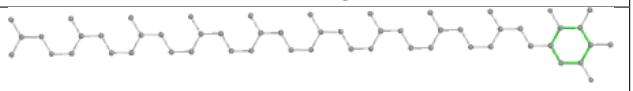
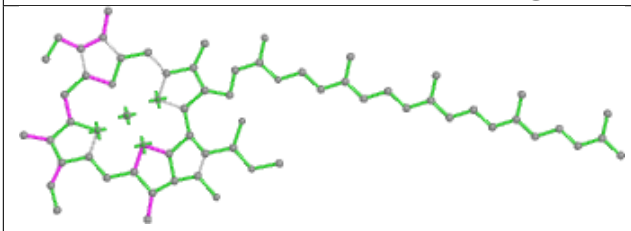


Rings

Ligand CLA b 605



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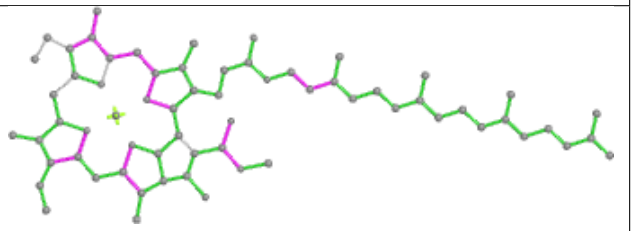
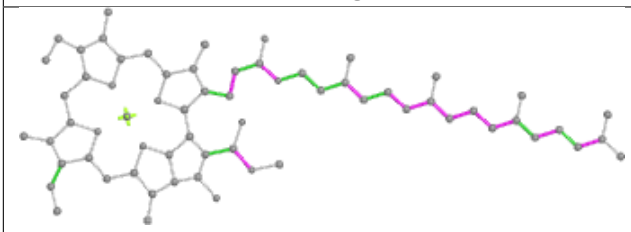


Bond angles



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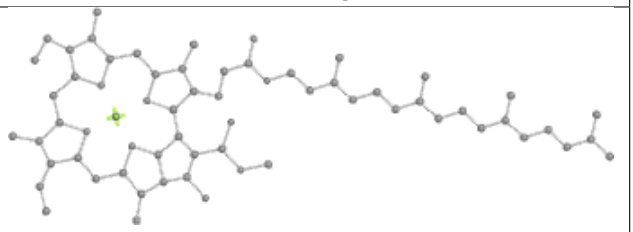
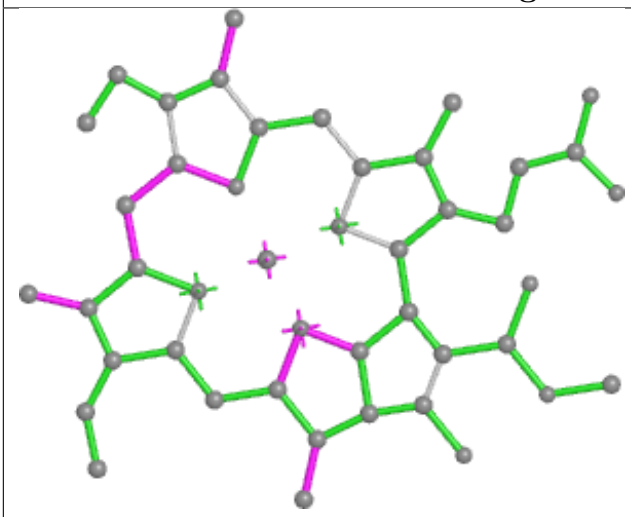


Rings

Ligand CLA 33 306



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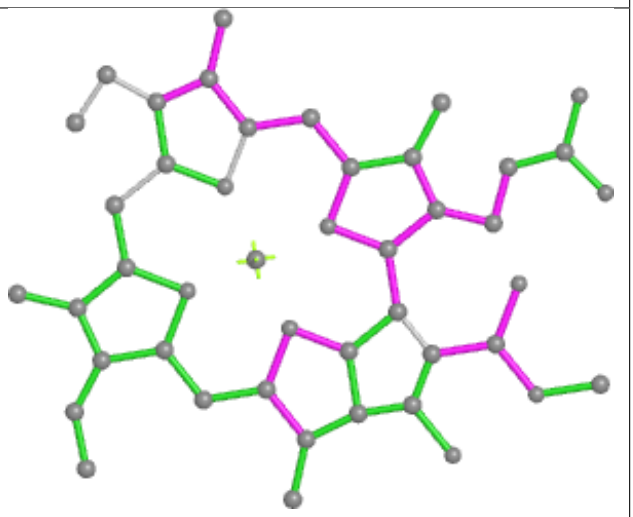

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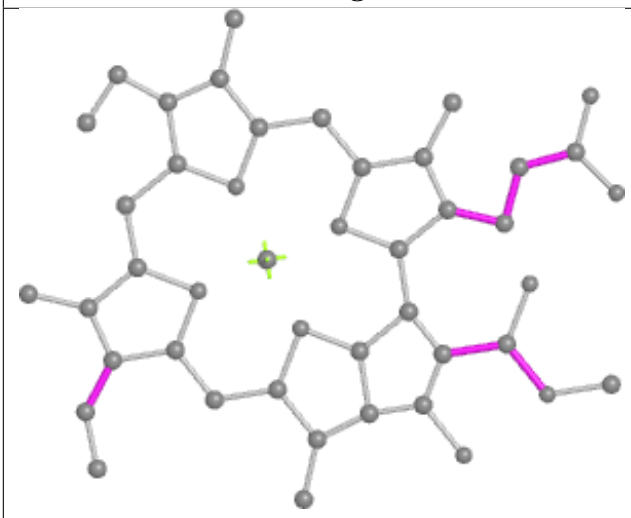

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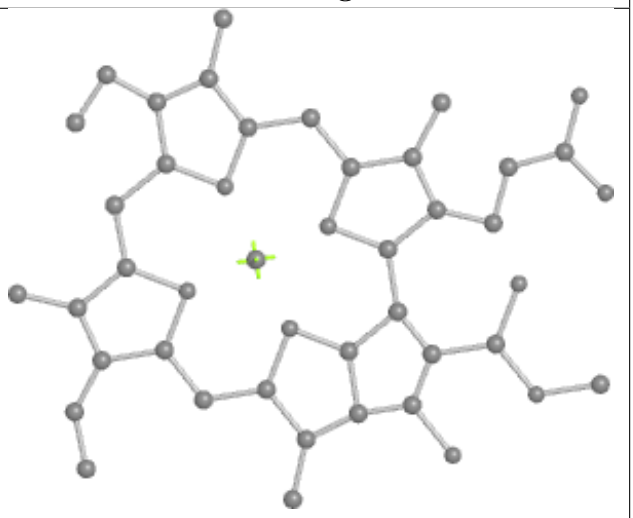
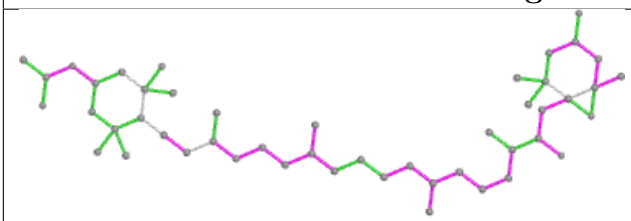


Rings

Ligand A86 18 315



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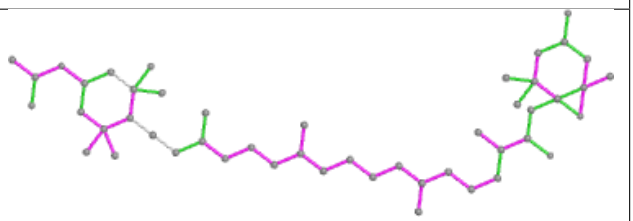
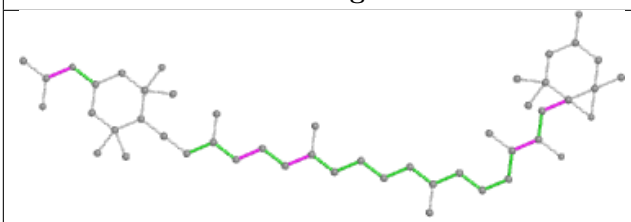


Bond angles



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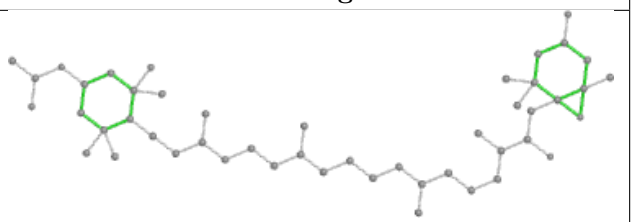
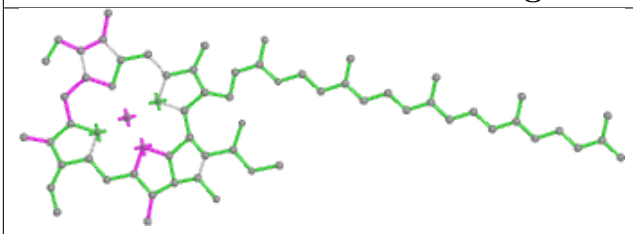


Rings

Ligand CLA C 504



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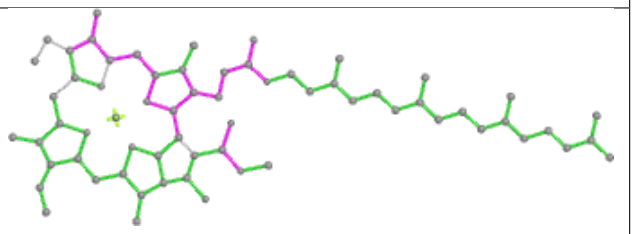
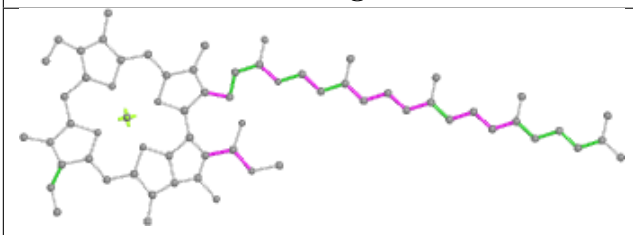
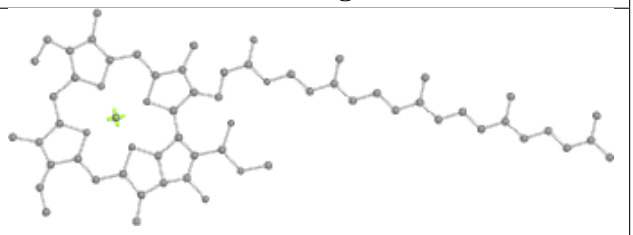


Bond angles

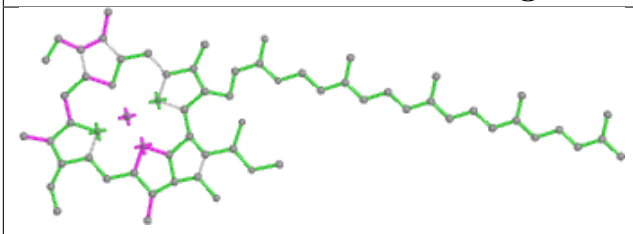


Torsions



Rings

Ligand CLA 12 311



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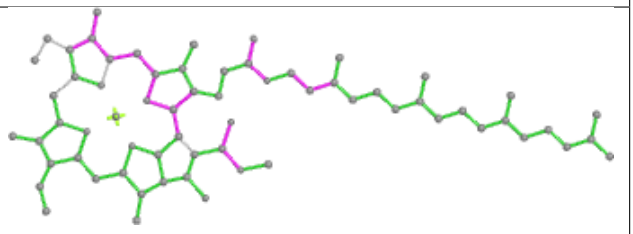

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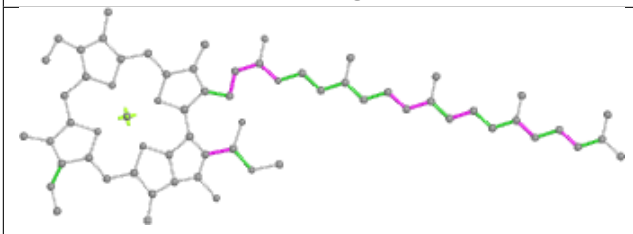

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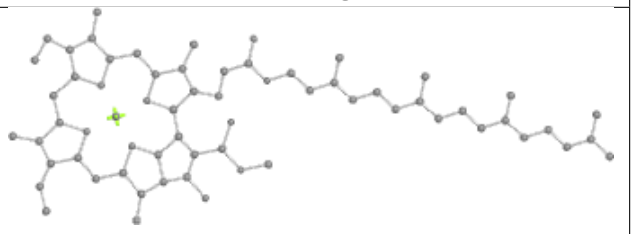
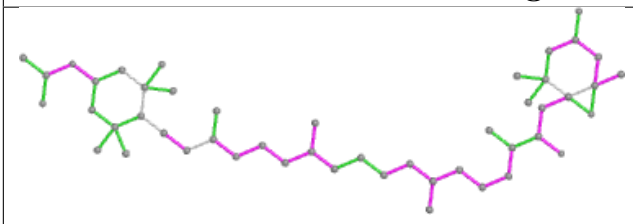


Rings

Ligand A86 33 317



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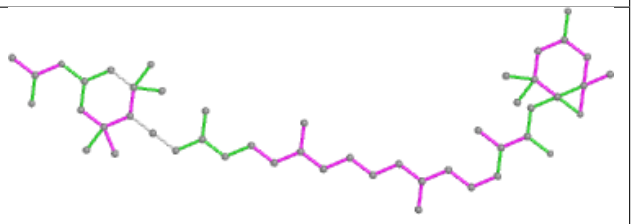

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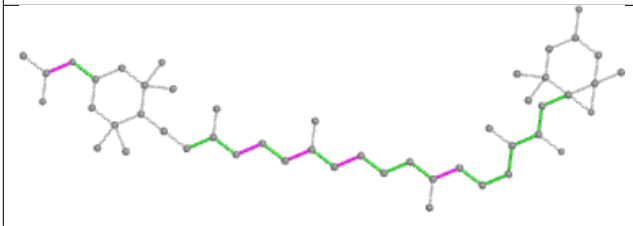

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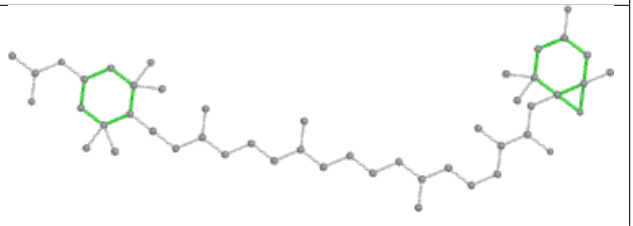
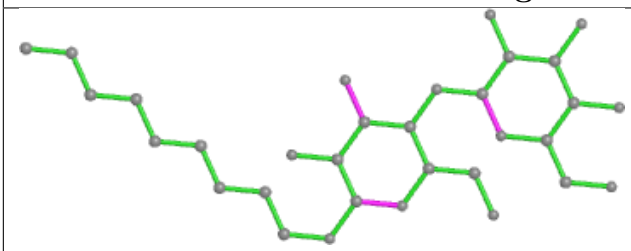


Rings

Ligand LMU 32 302



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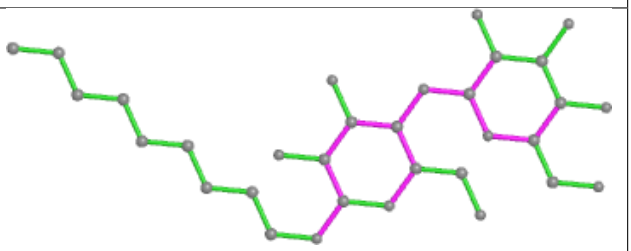

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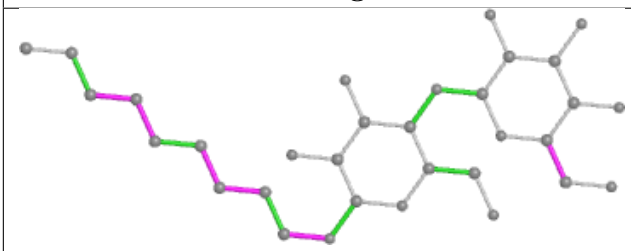

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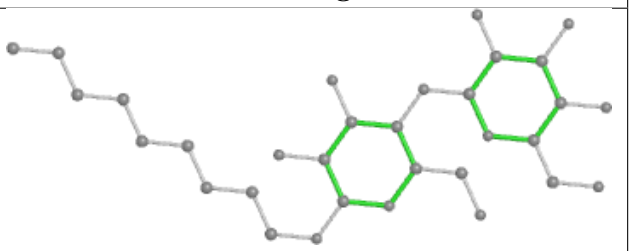
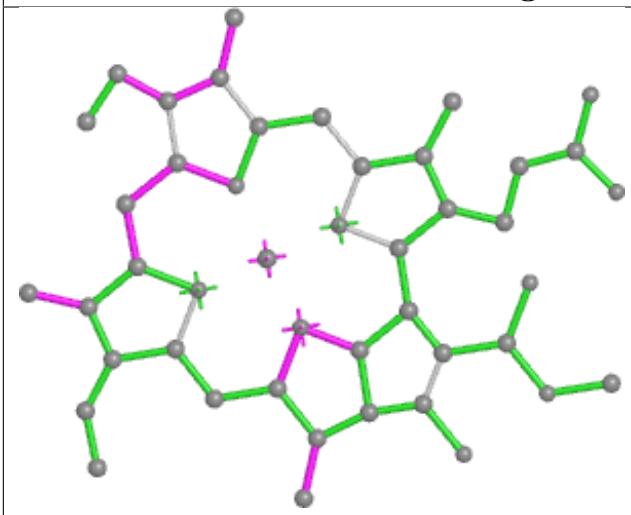


Rings

Ligand CLA 32 306



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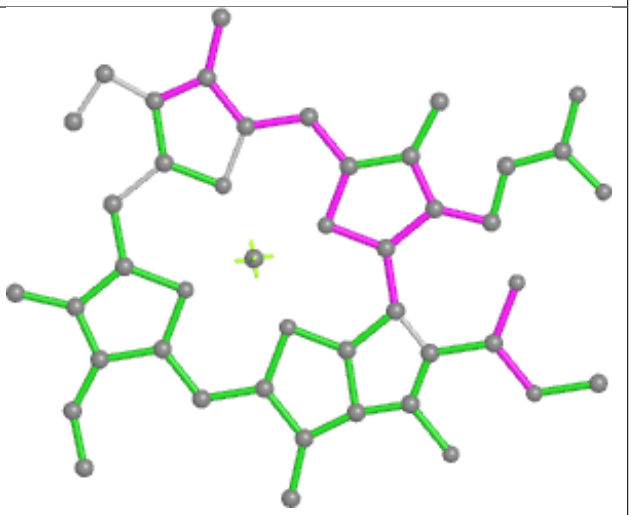

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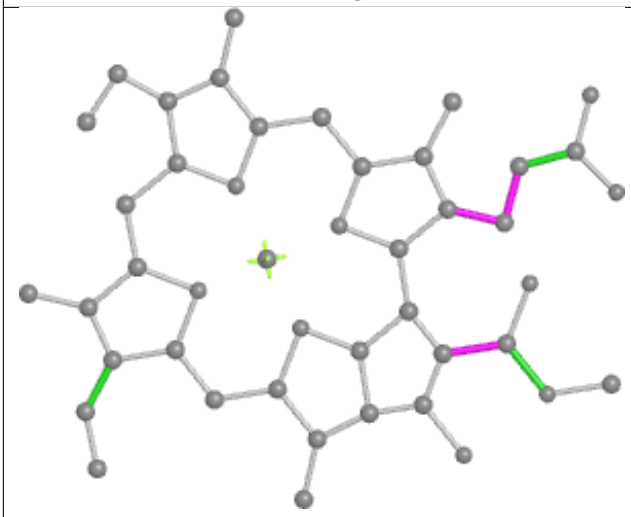

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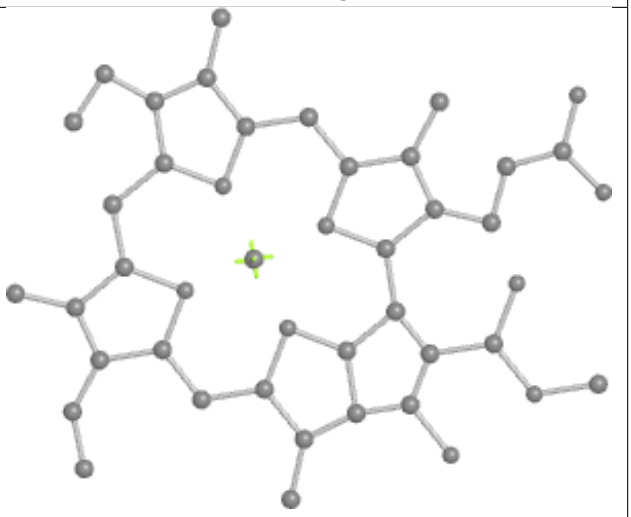
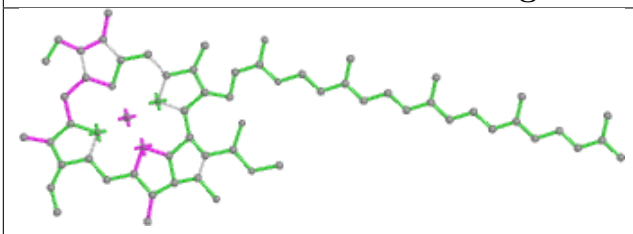


Rings

Ligand CLA 38 301



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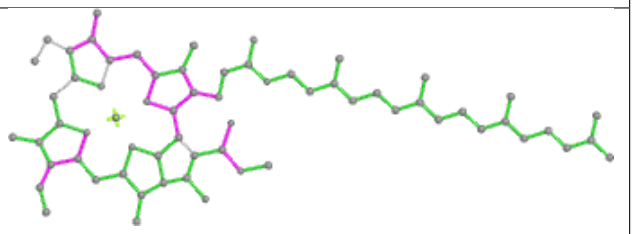

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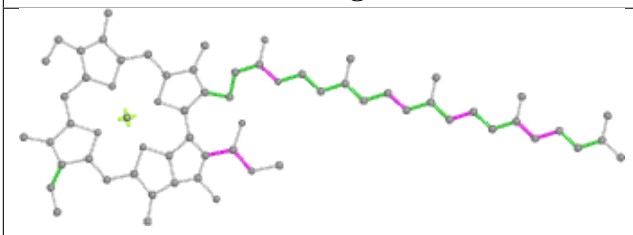

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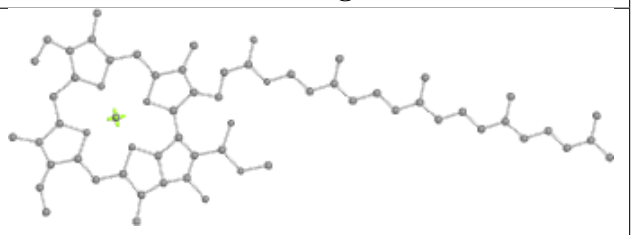
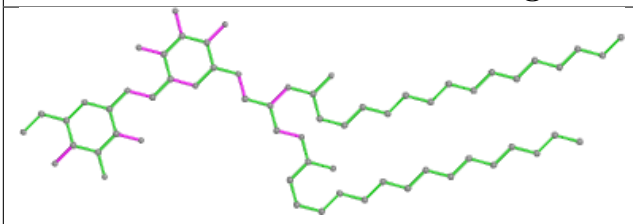


Rings

Ligand DGD J 101



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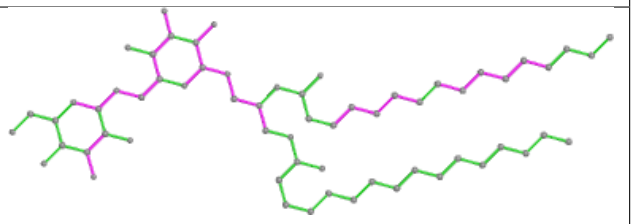
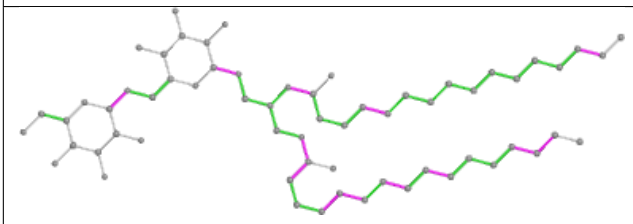


Bond angles



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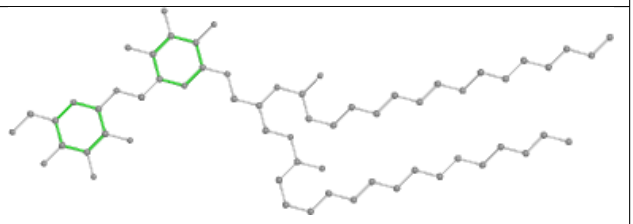
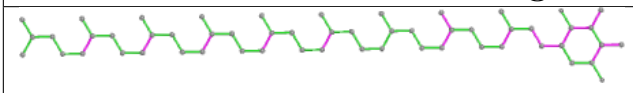


Rings

Ligand PL9 D 407



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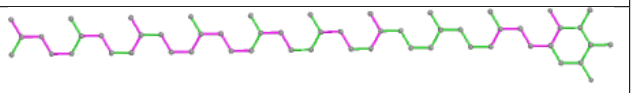

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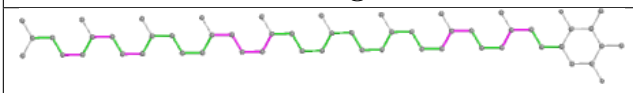

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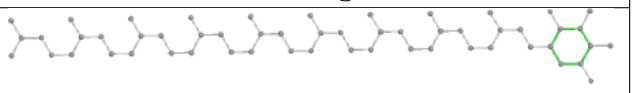
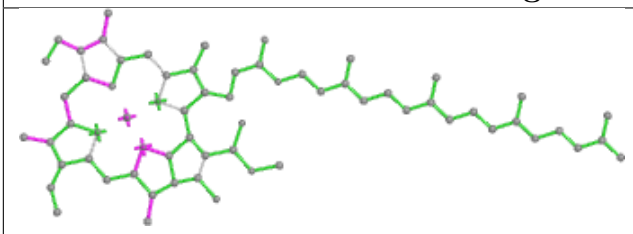


Rings

Ligand CLA D 402



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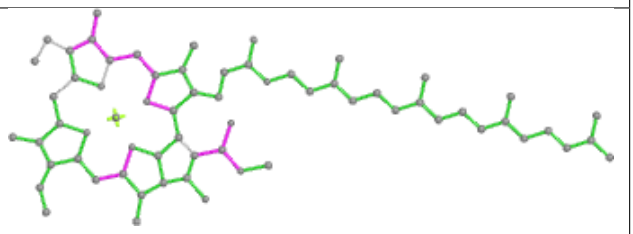

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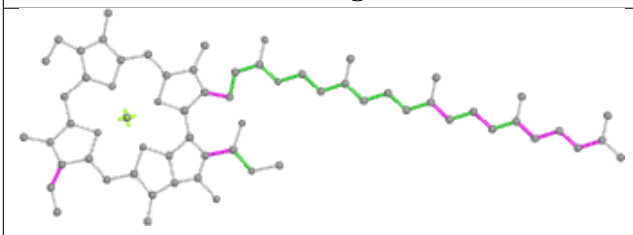

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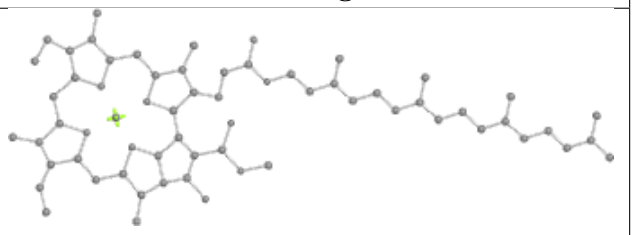
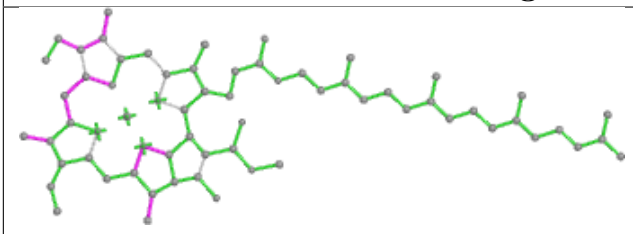


Rings

Ligand CLA 36 302



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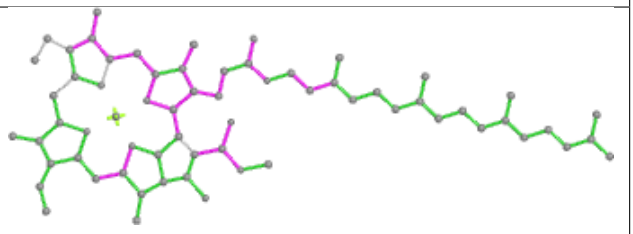

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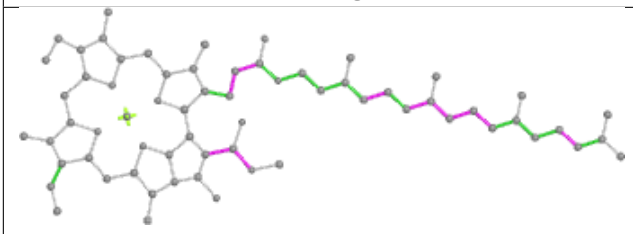

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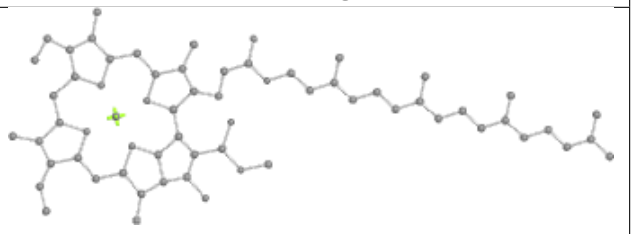
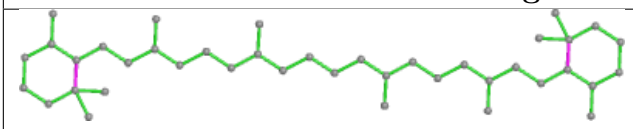


Rings

Ligand BCR B 618



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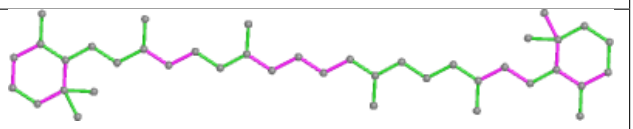

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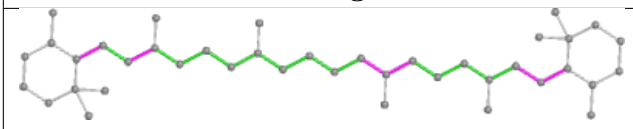
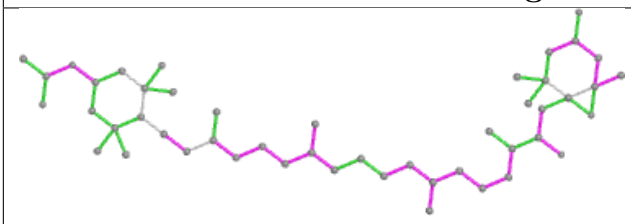


Torsions

Rings

Ligand A86 20 201



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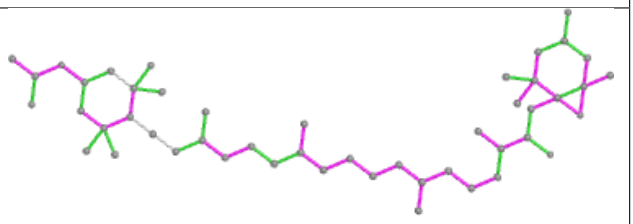

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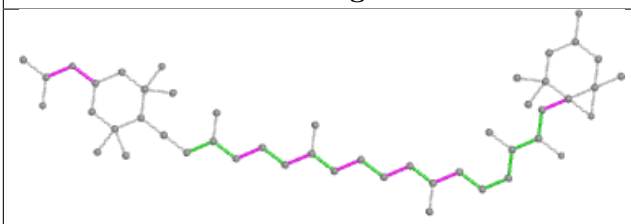

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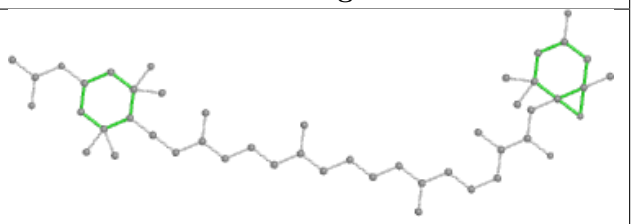
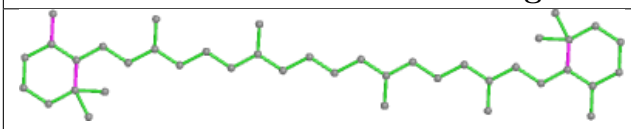


Rings

Ligand BCR Z 101



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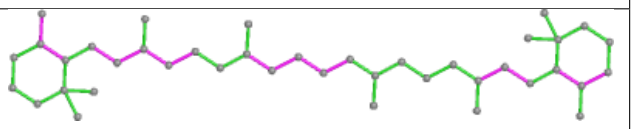
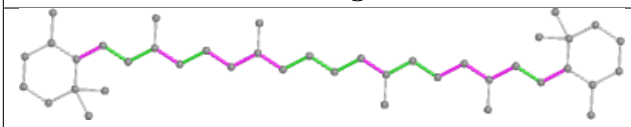


Bond angles



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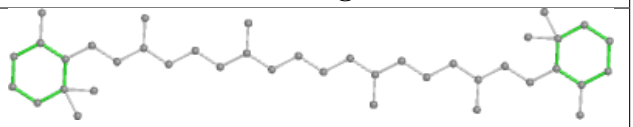
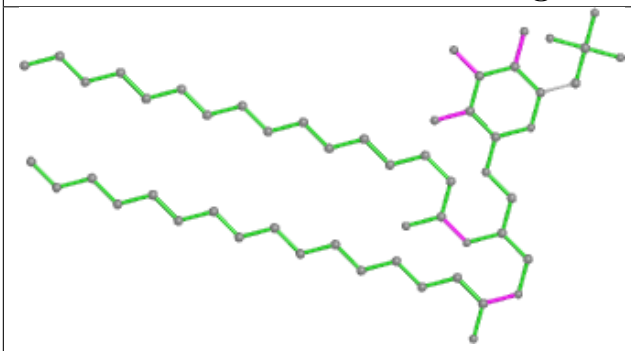


Rings

Ligand SQD l 101



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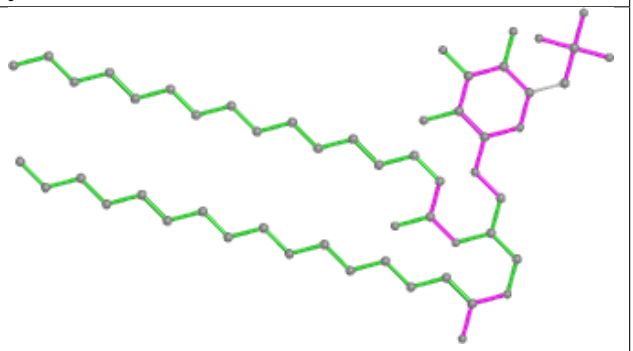
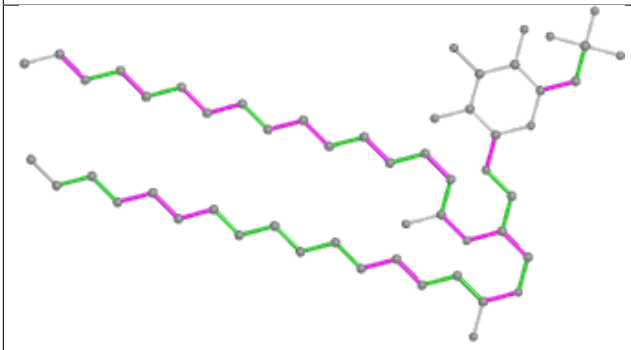


Bond angles



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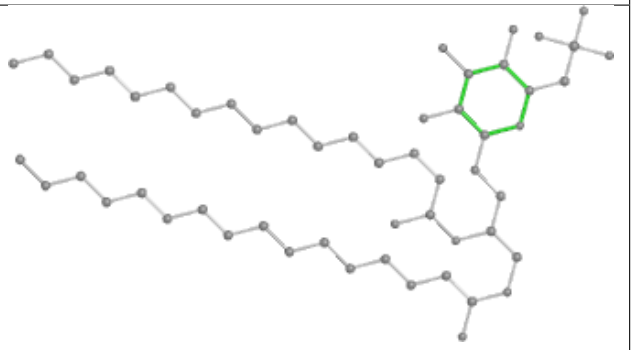
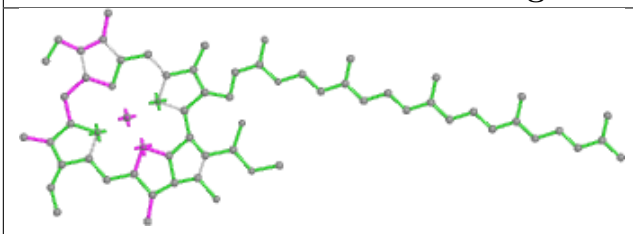


Rings

Ligand CLA b 601



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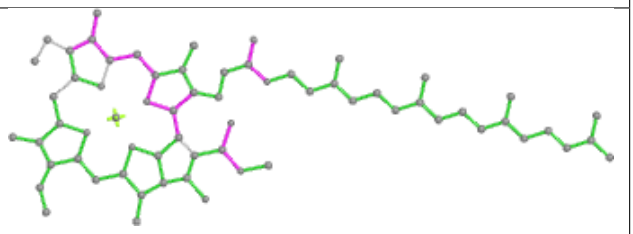
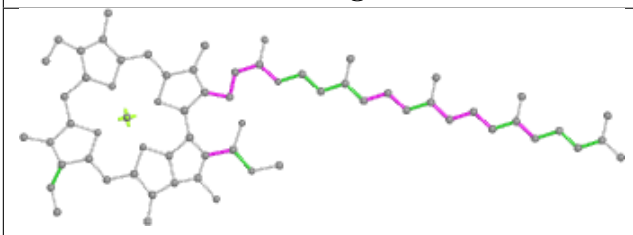
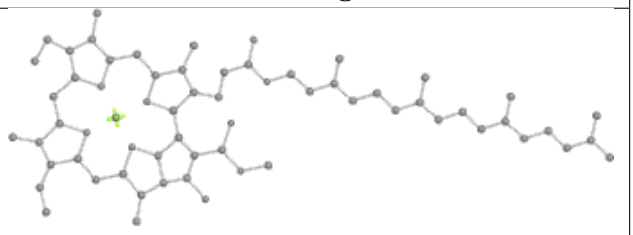


Bond angles

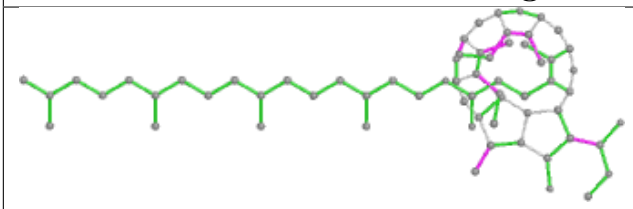


Torsions



Rings

Ligand PHO D 403



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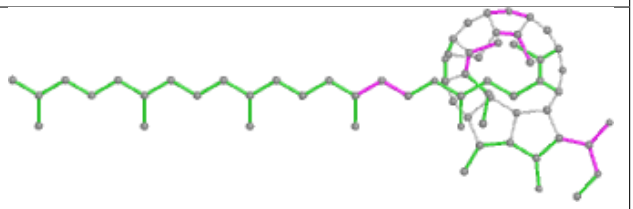

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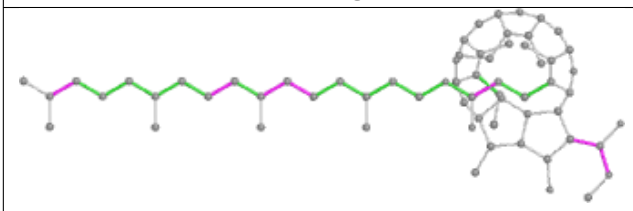

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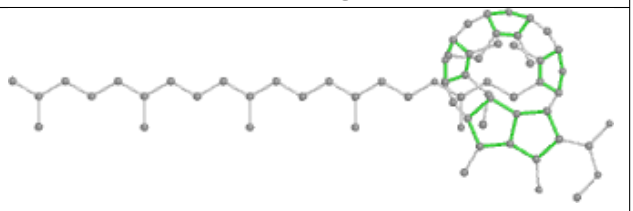
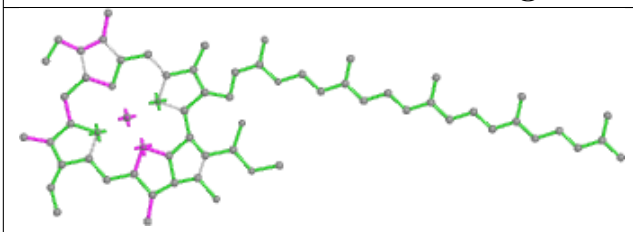


Rings

Ligand CLA 13 308



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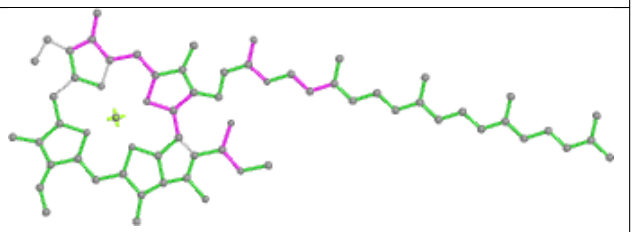

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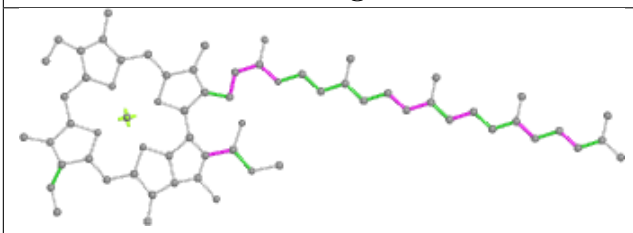

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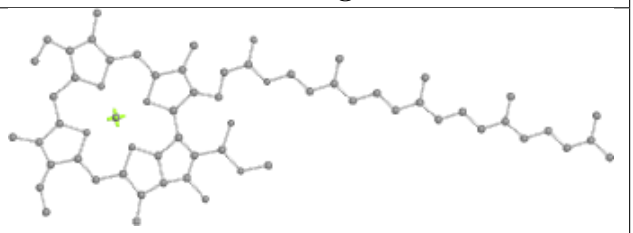
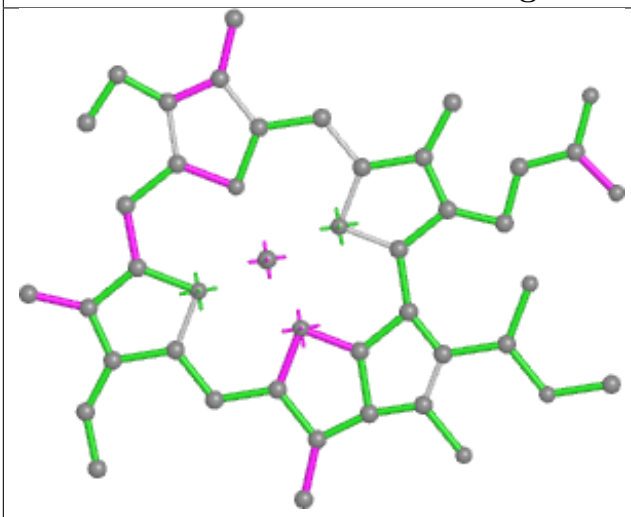


Rings

Ligand CLA 37 309



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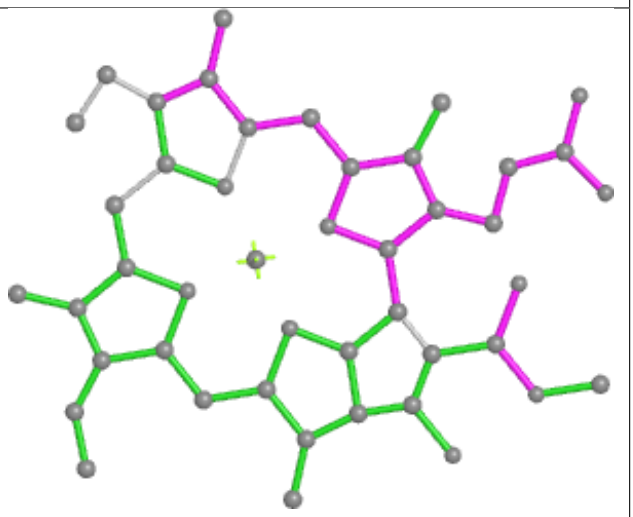

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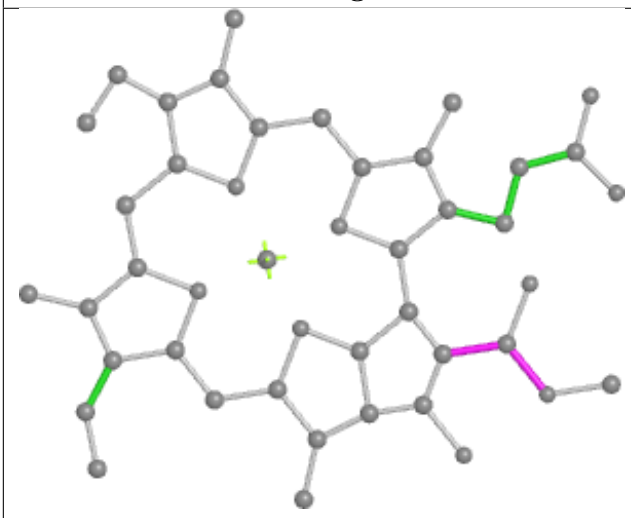

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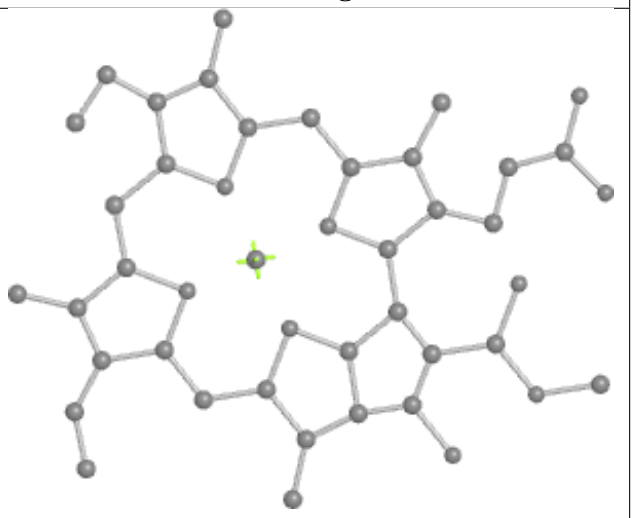
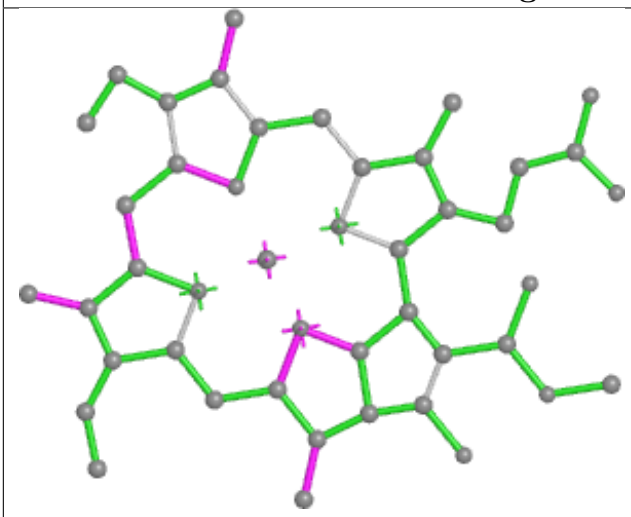


Rings

Ligand CLA 12 308



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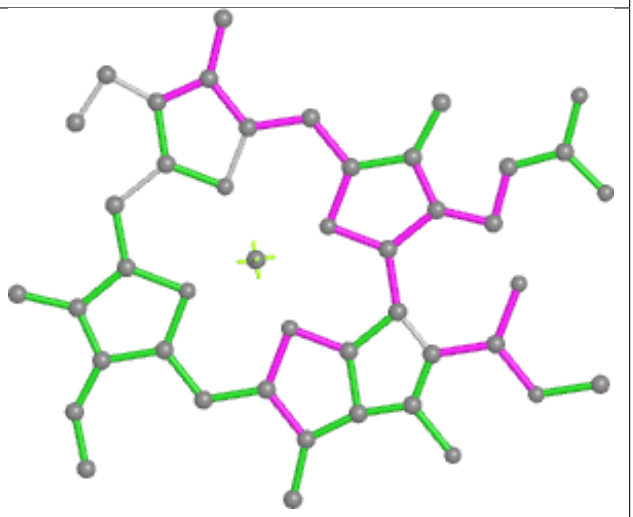

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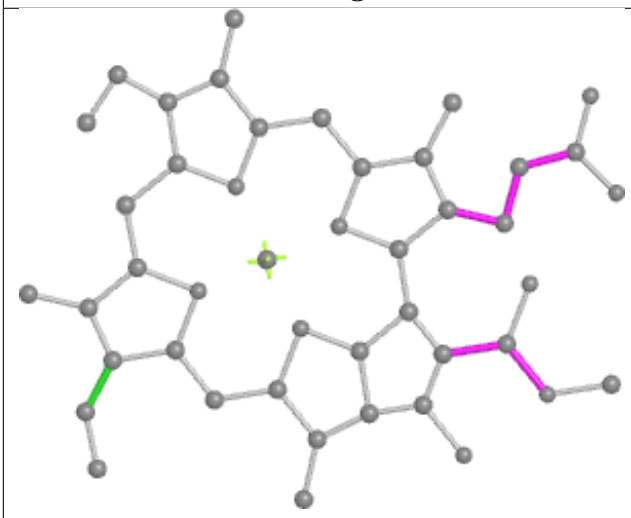

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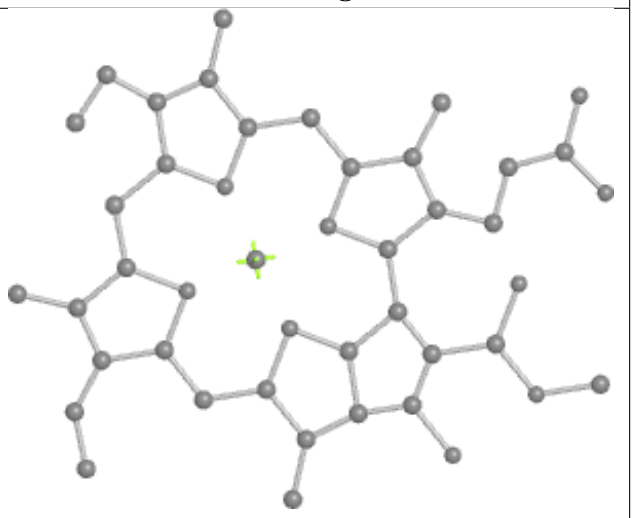

Rings

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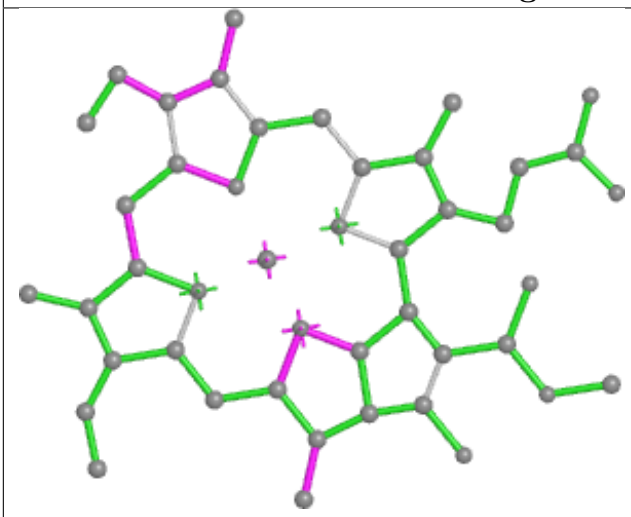

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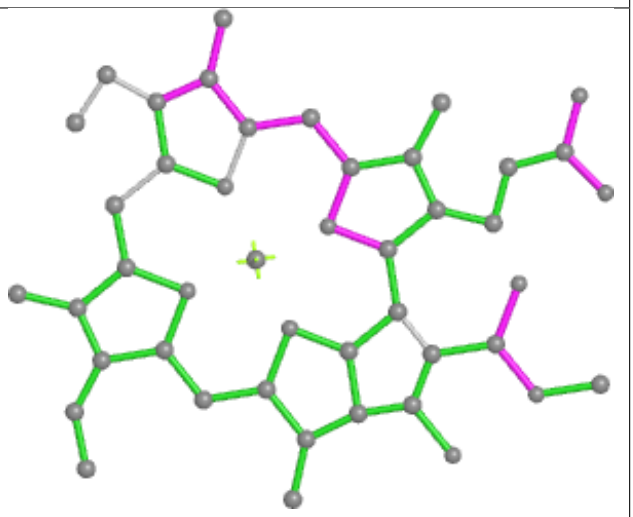

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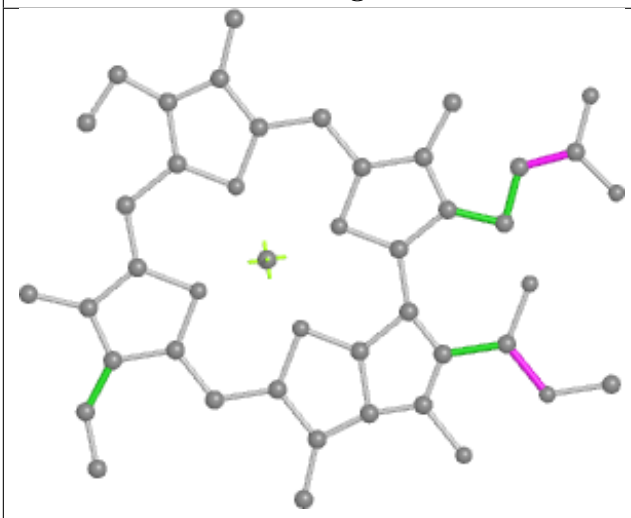

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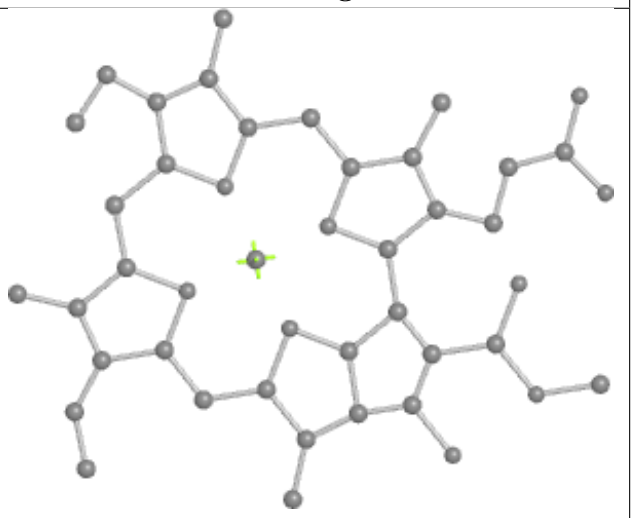
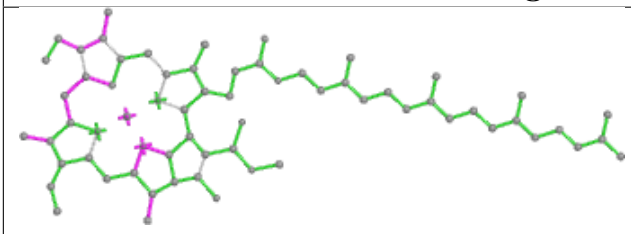


Rings

Ligand CLA B 607



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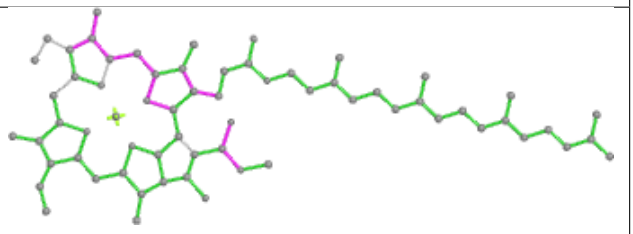

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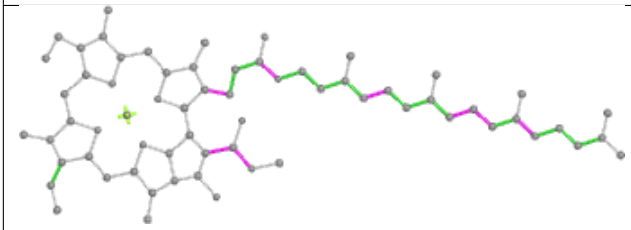

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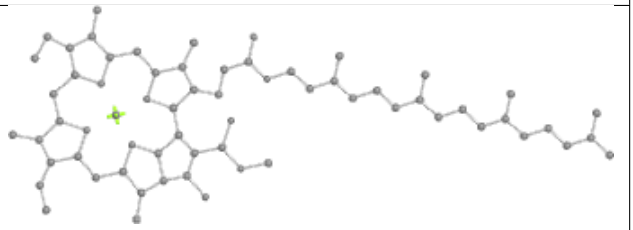

Rings

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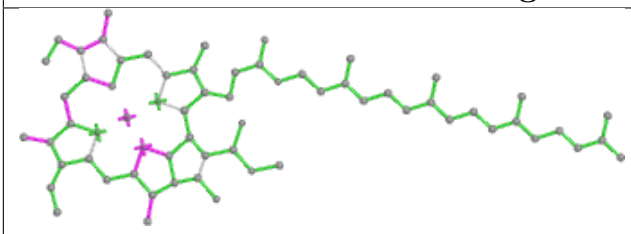

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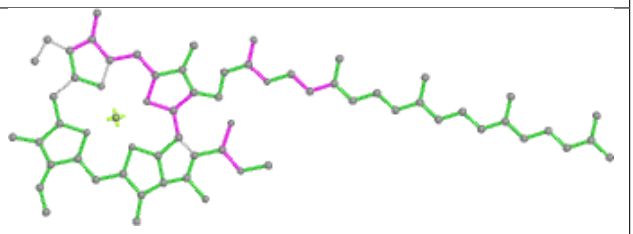

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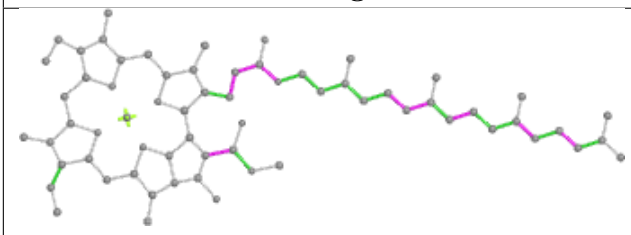

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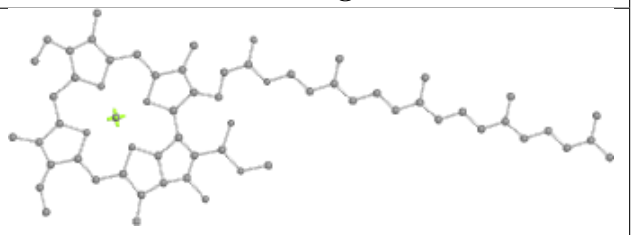

Rings

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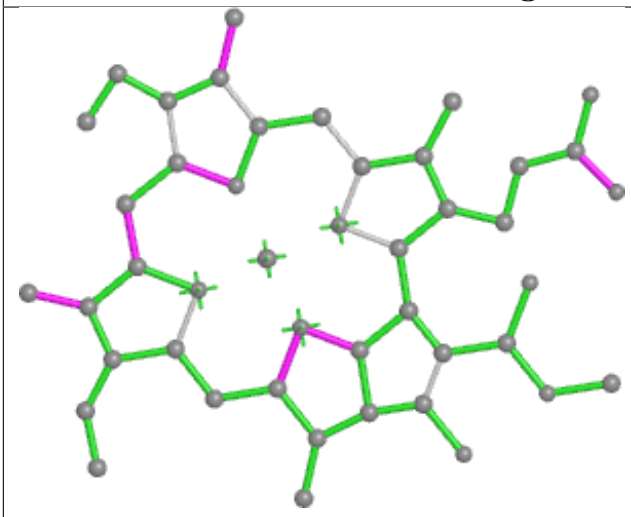

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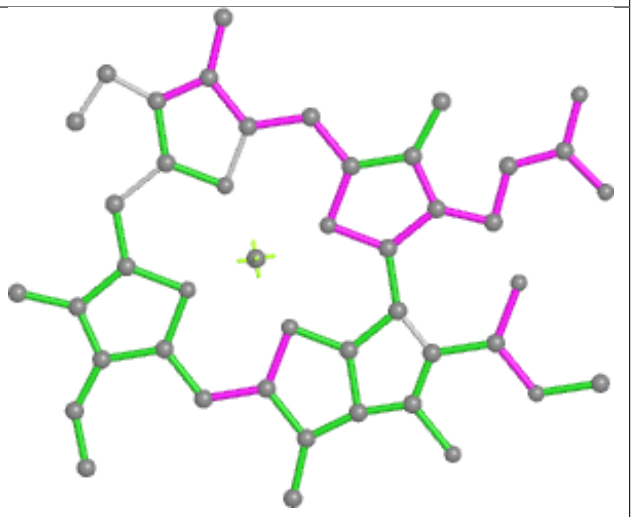

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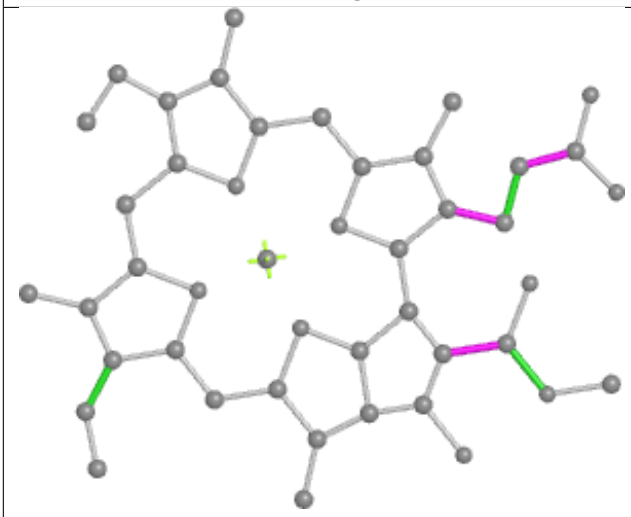

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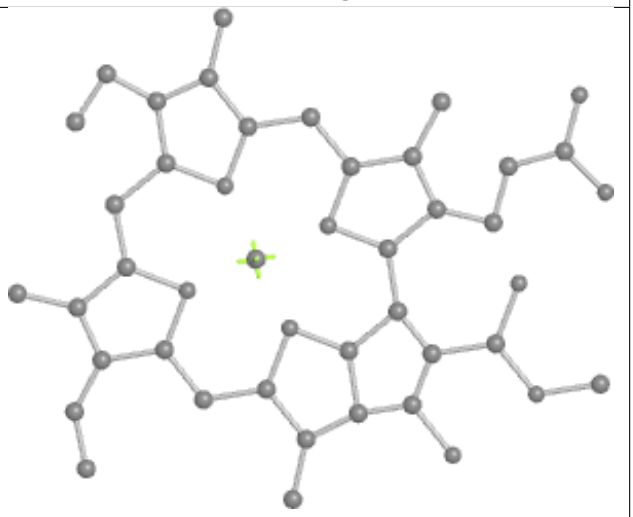

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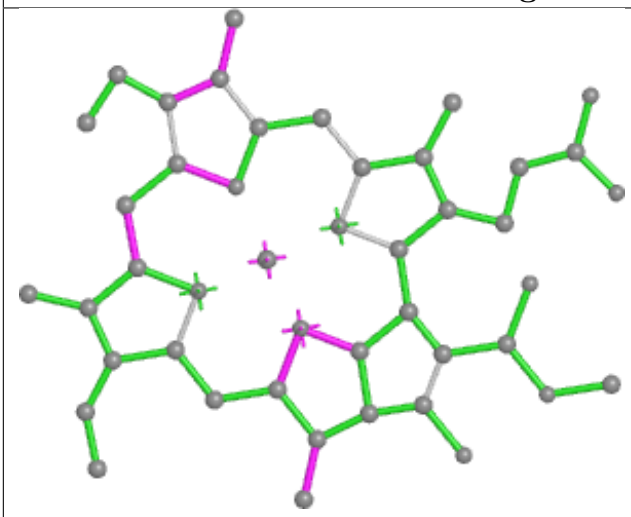

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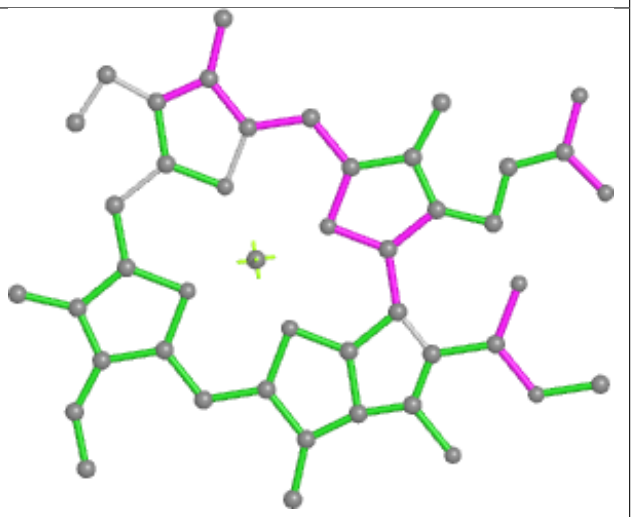

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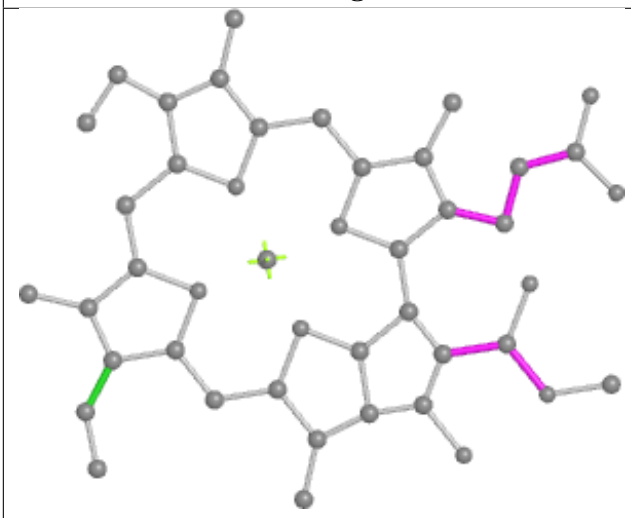

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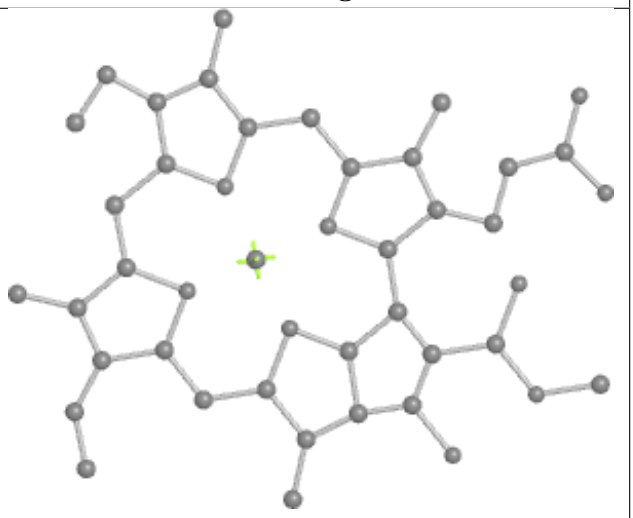
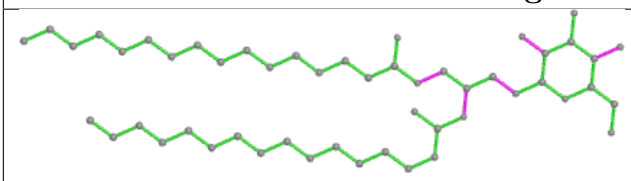


Rings

Ligand LMG c 519



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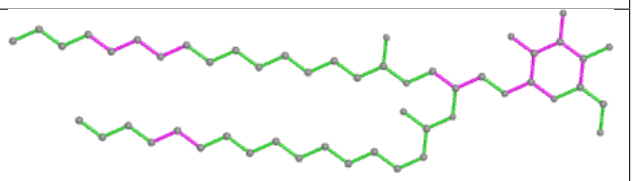

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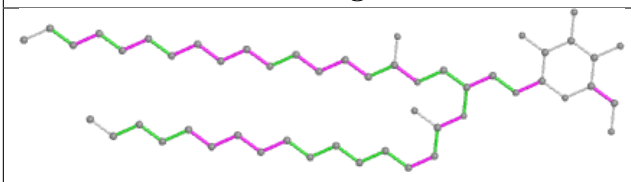

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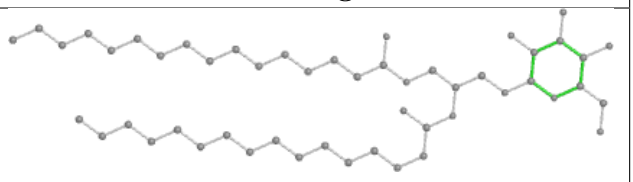

Rings

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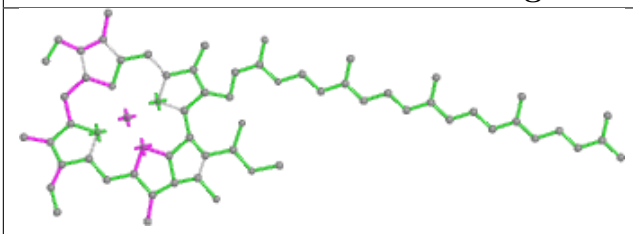

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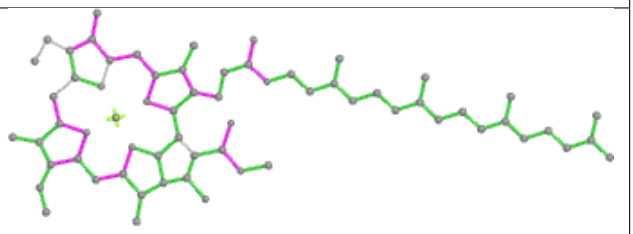

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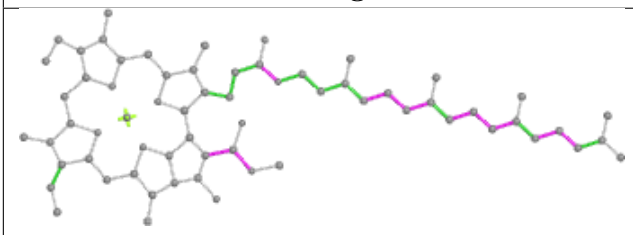

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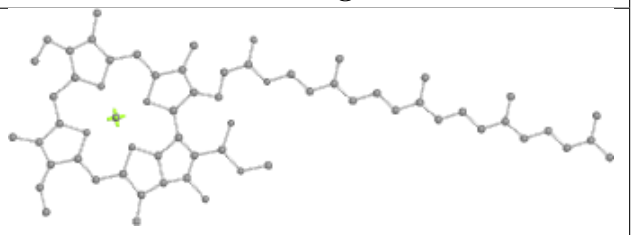

Rings

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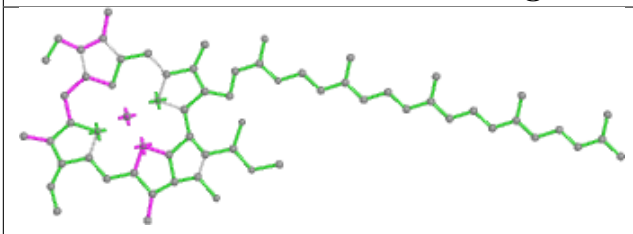

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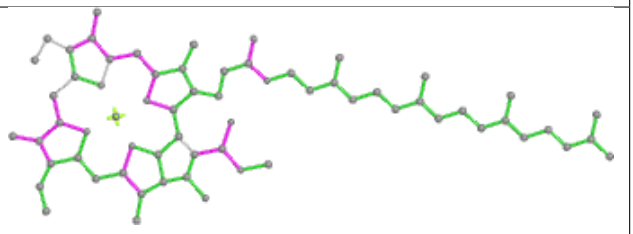

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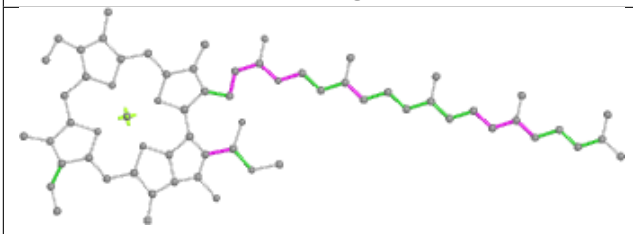

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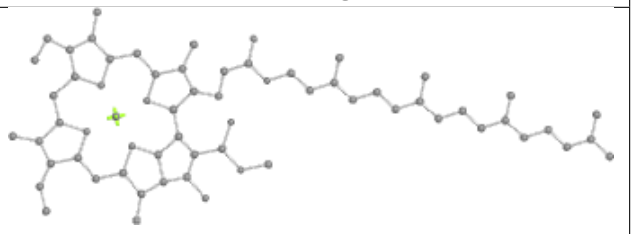
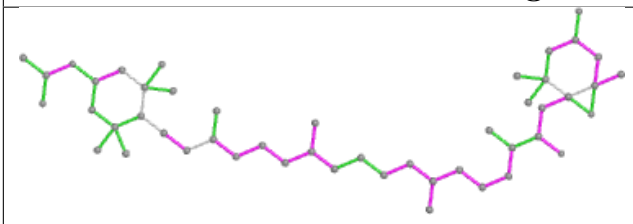


Rings

Ligand A86 20 212



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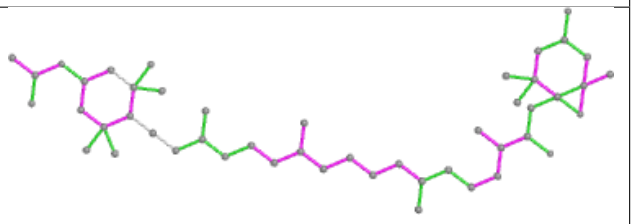
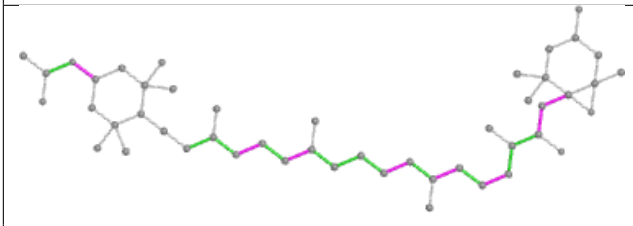


Bond angles



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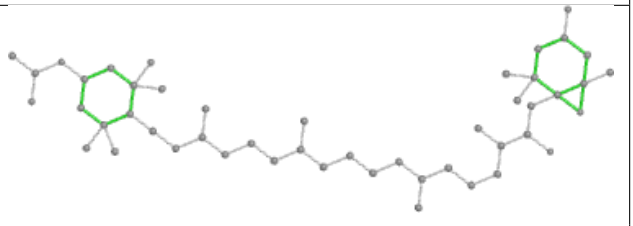
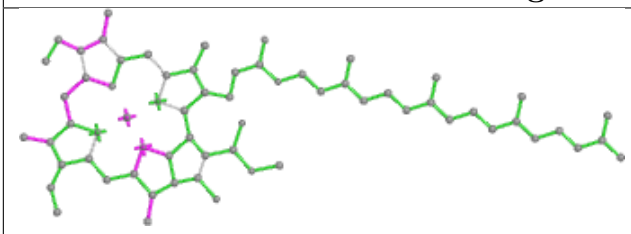


Rings

Ligand CLA b 607



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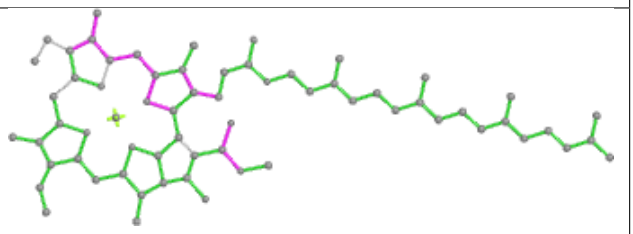
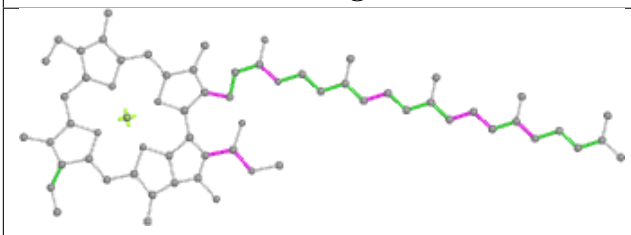
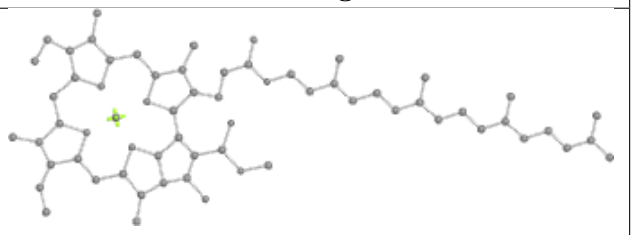


Bond angles

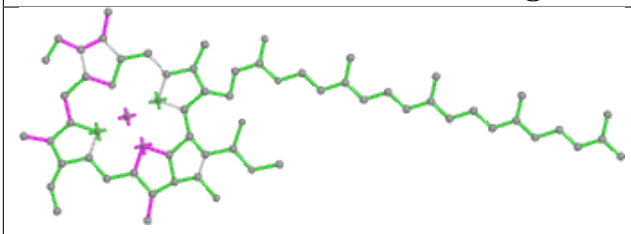


Torsions



Rings

Ligand CLA C 512



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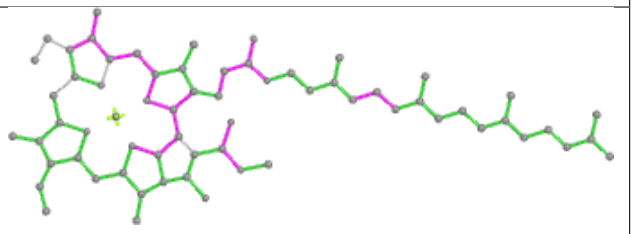

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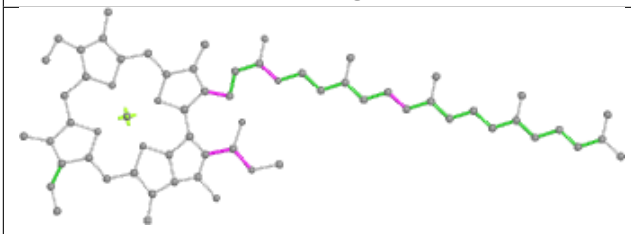

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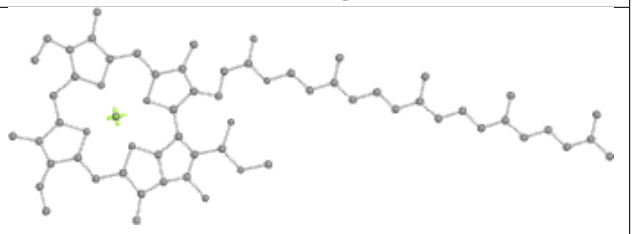
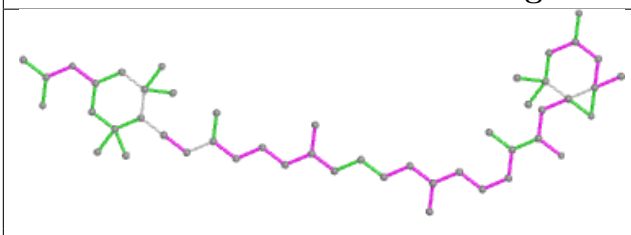


Rings

Ligand A86 37 315



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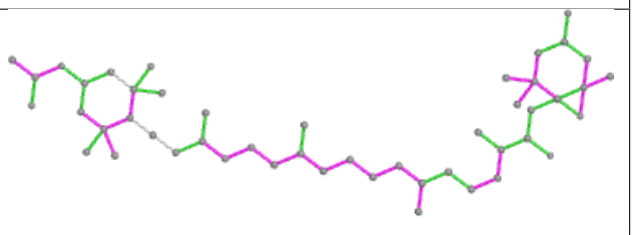

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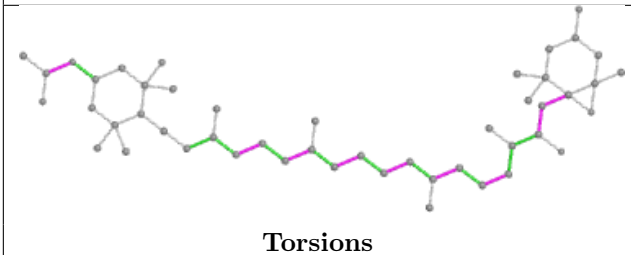

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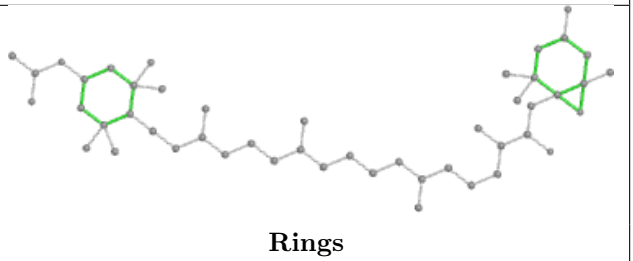
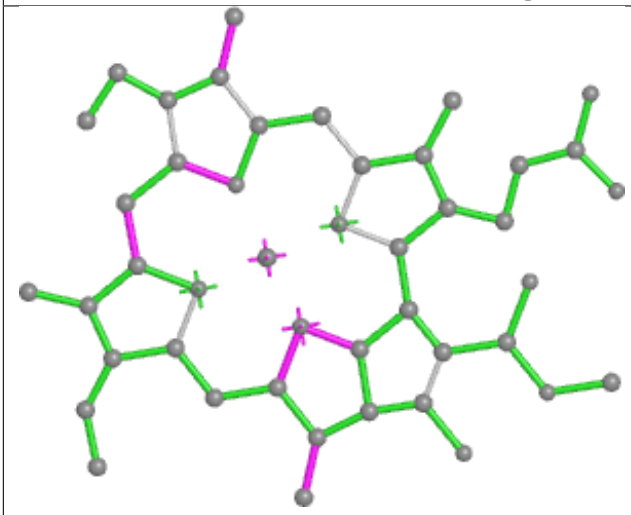


Rings

Ligand CLA 31 304



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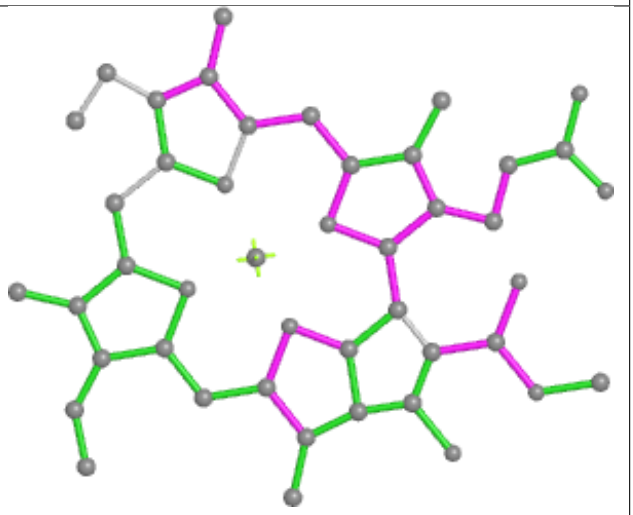

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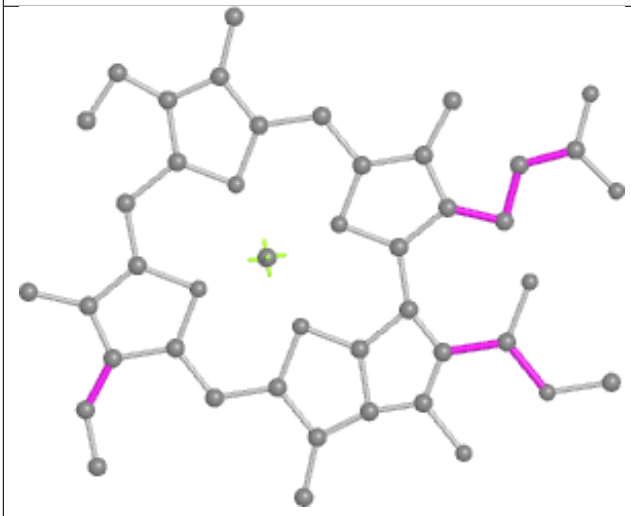

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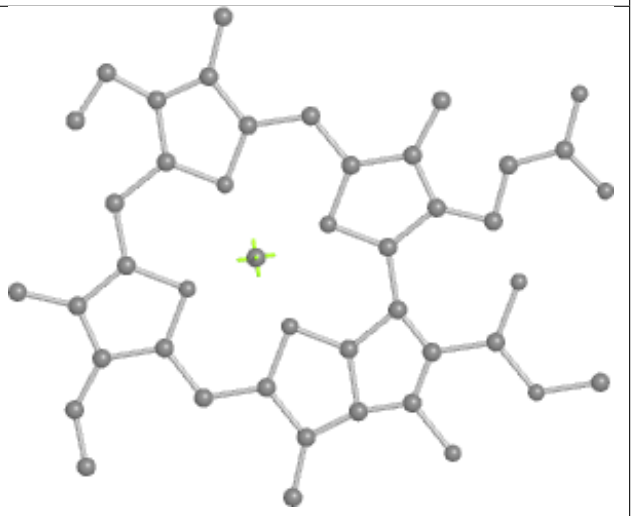

Rings

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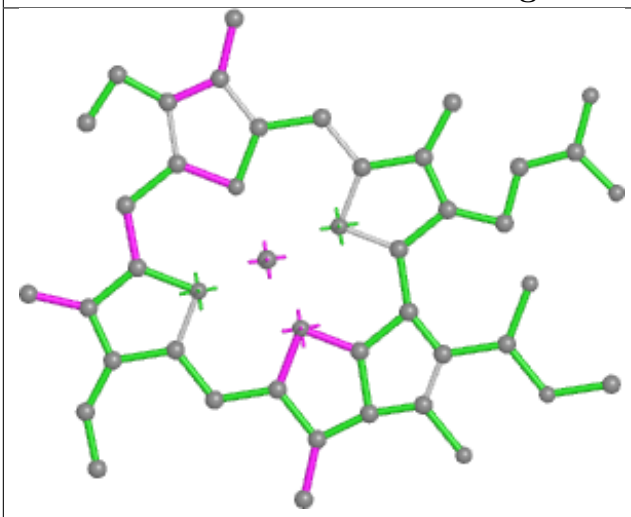

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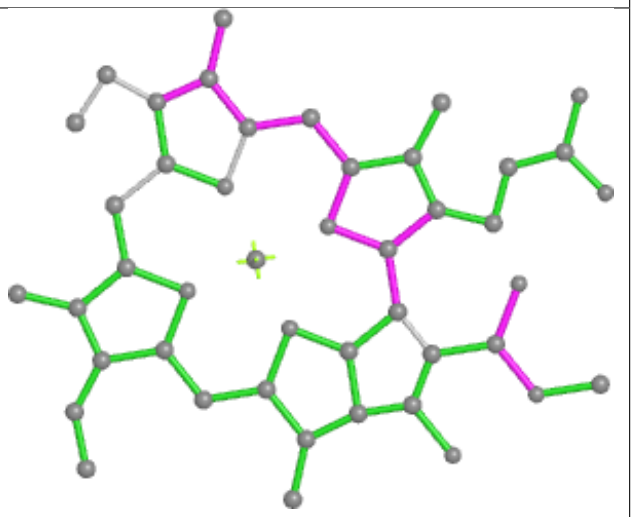

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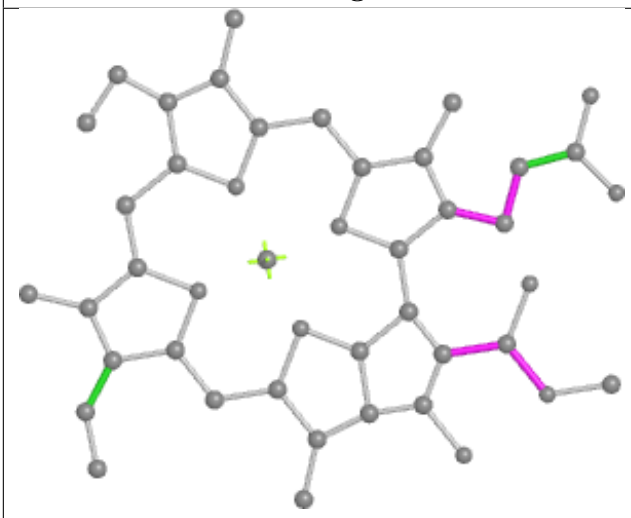

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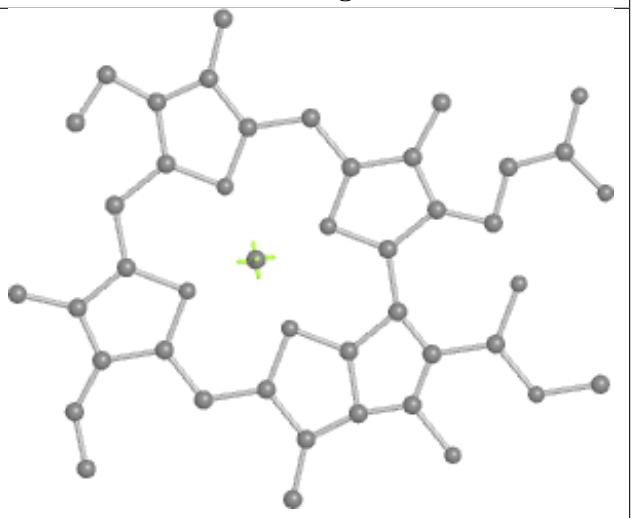
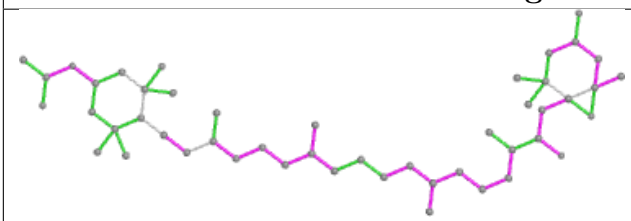


Rings

Ligand A86 40 211



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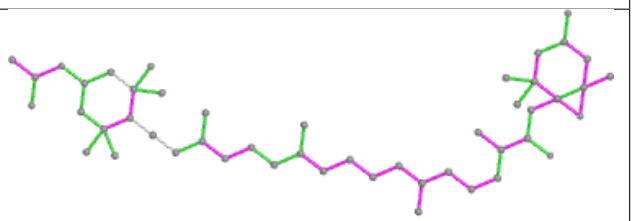

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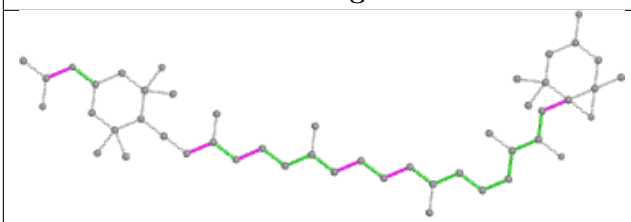

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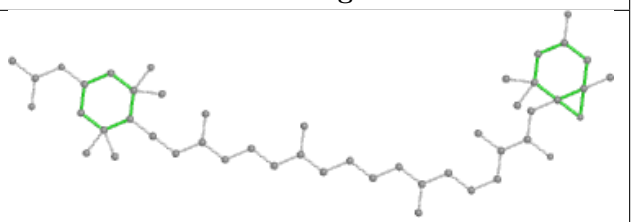

Rings

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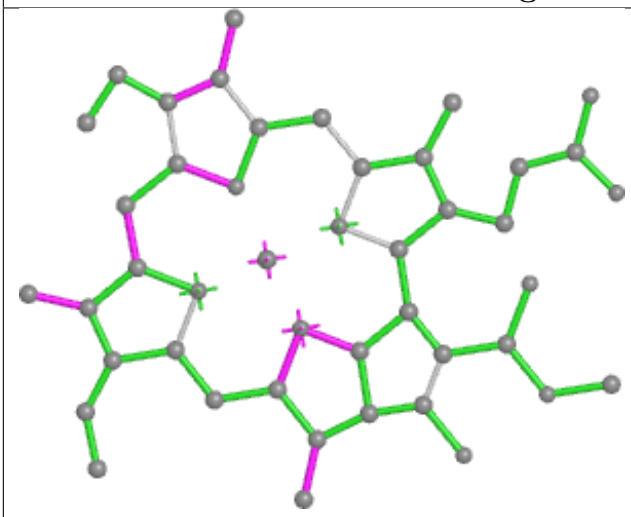

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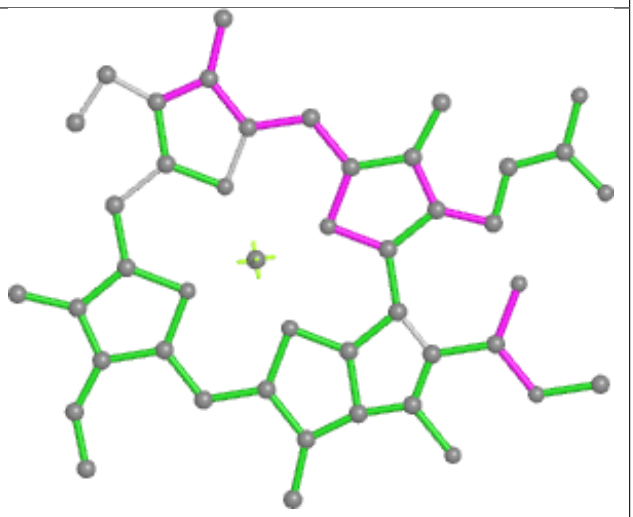

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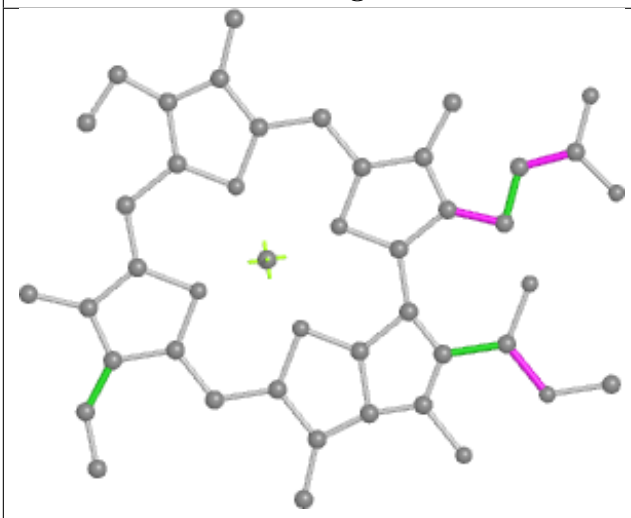

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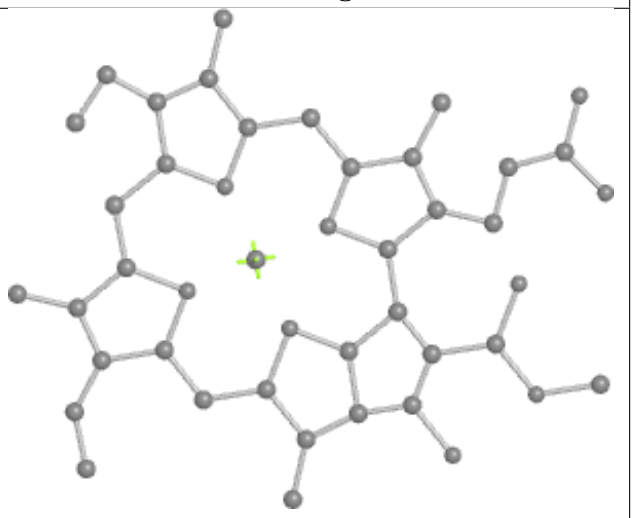
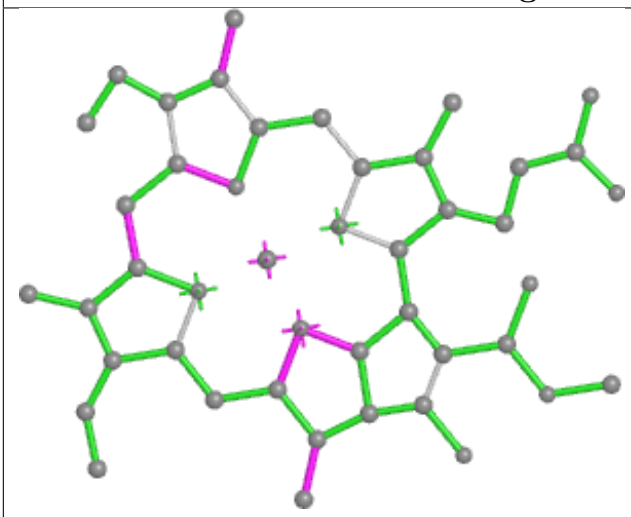


Rings

Ligand CLA 19 308



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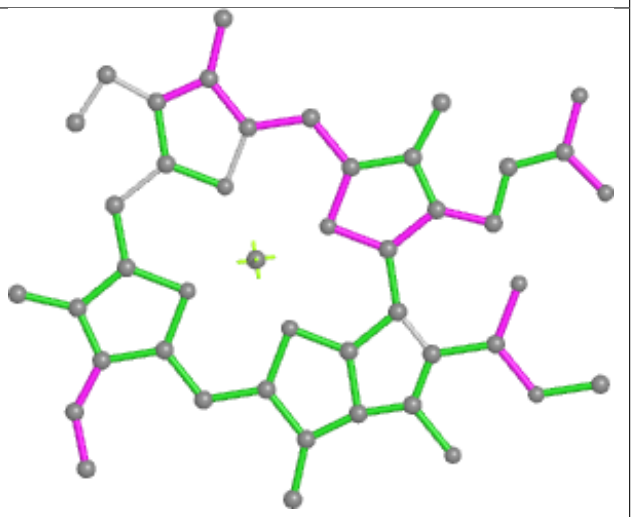

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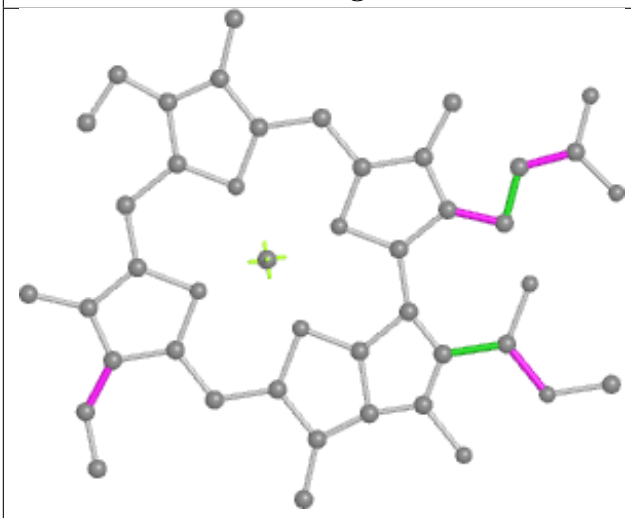

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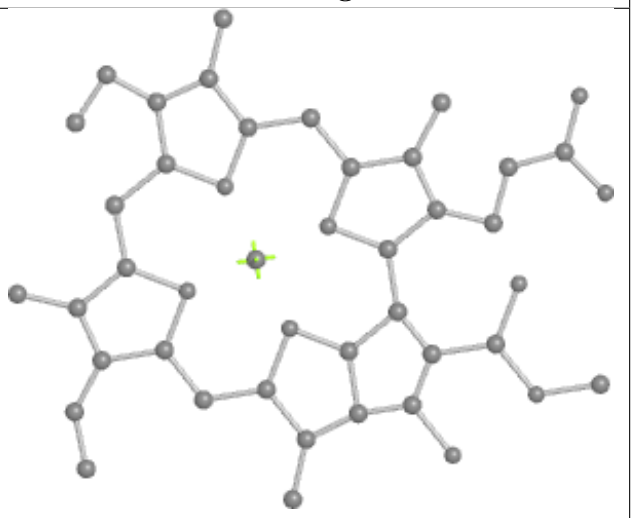
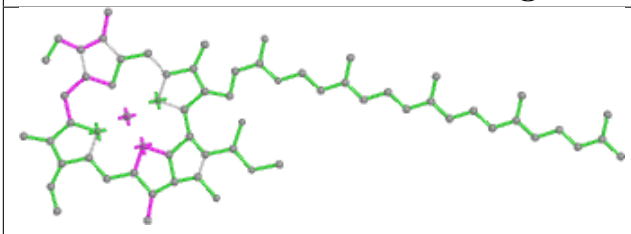


Rings

Ligand CLA 37 308



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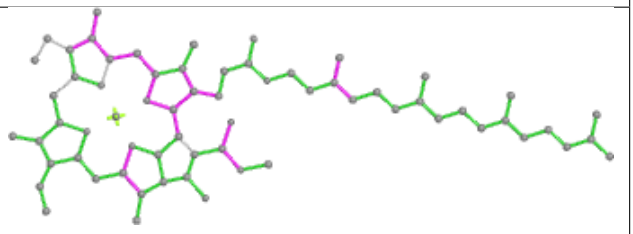

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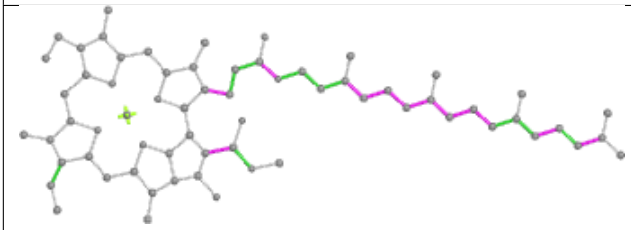

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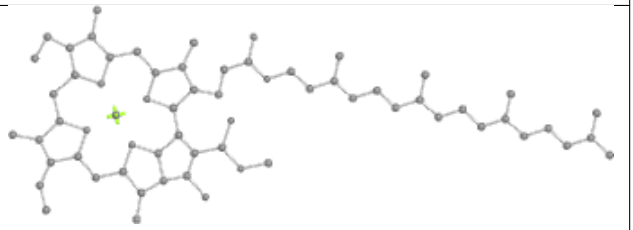
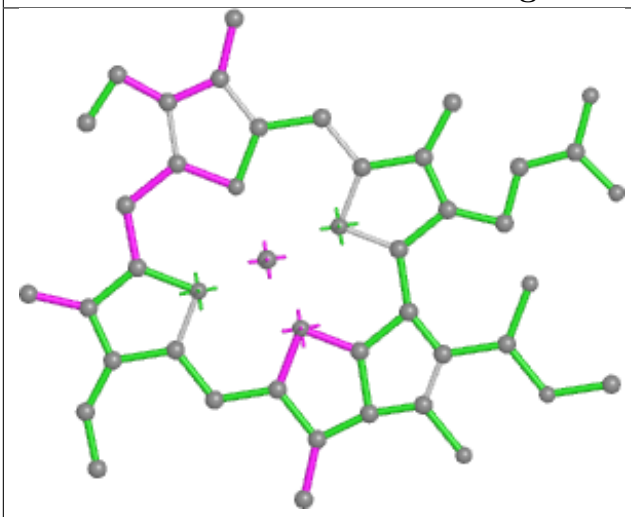


Rings

Ligand CLA 11 308



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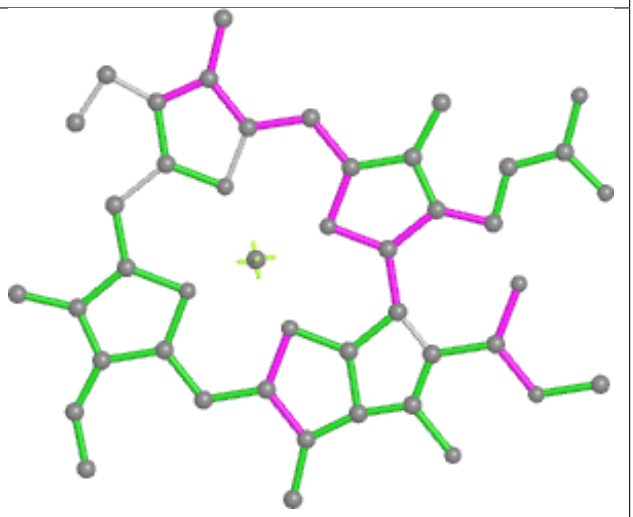

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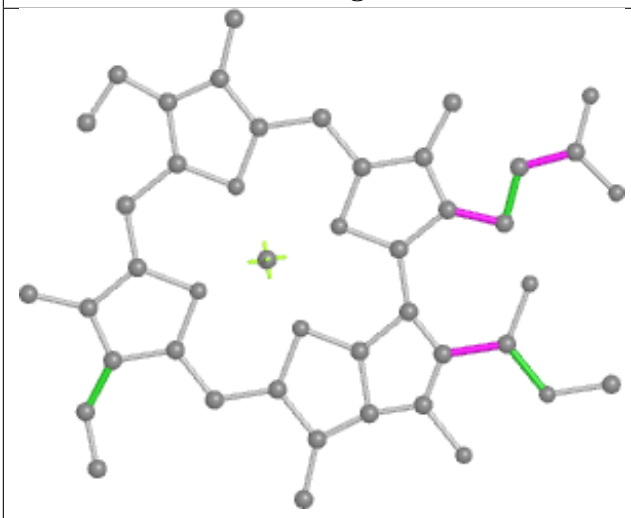

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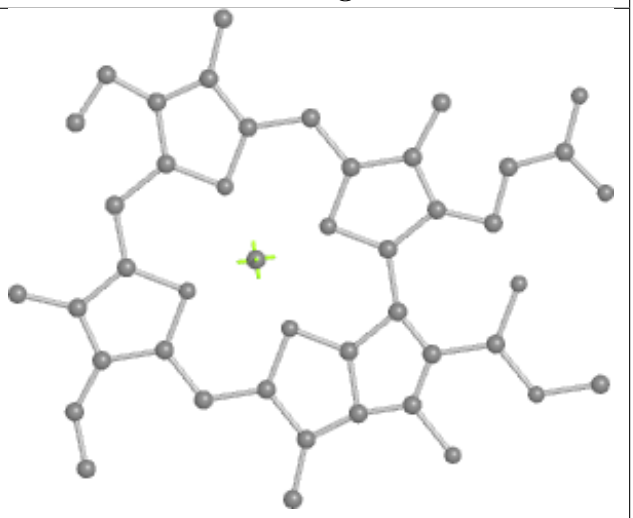
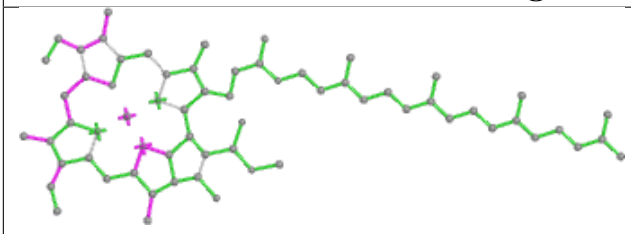


Rings

Ligand CLA b 611



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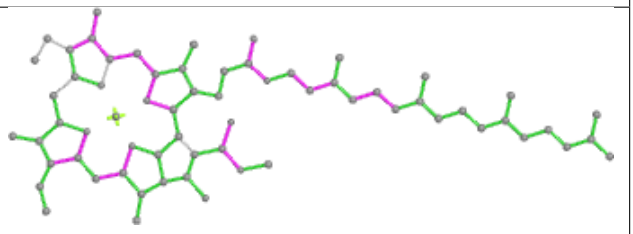

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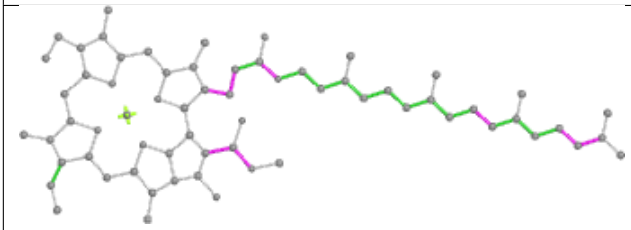

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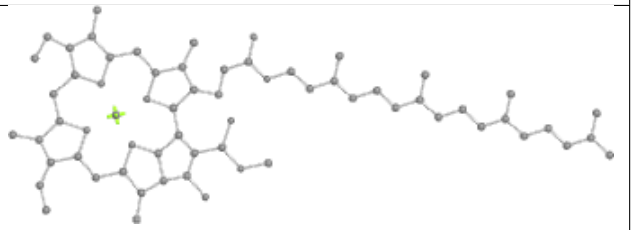
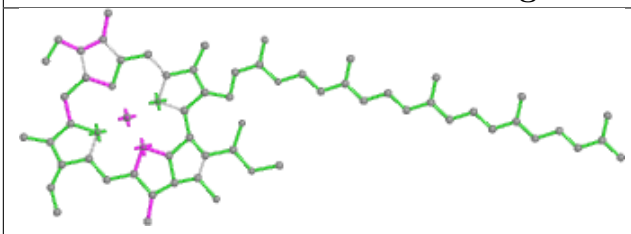


Rings

Ligand CLA 36 301



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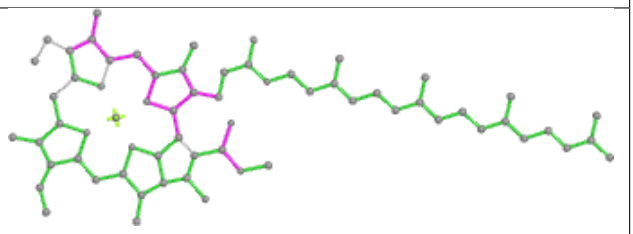

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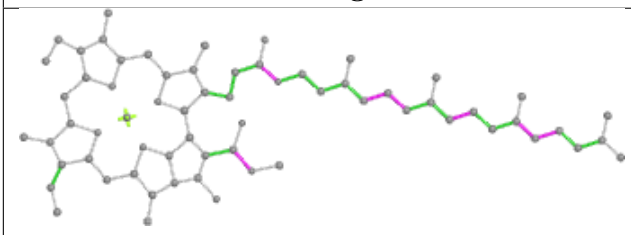

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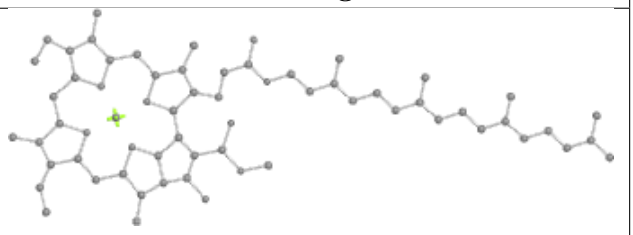
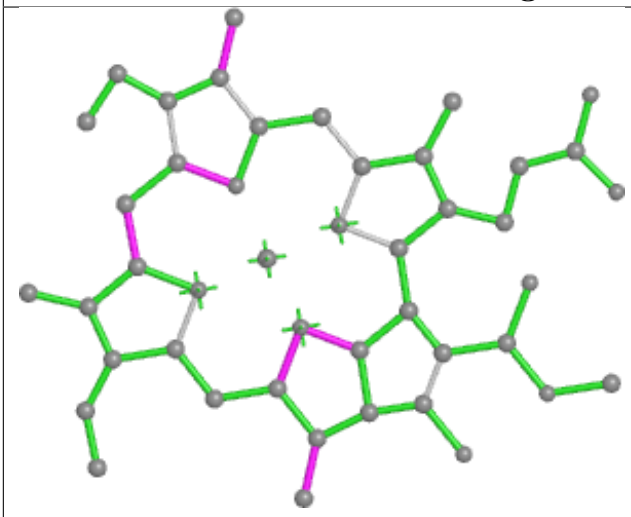


Rings

Ligand CLA 41 308



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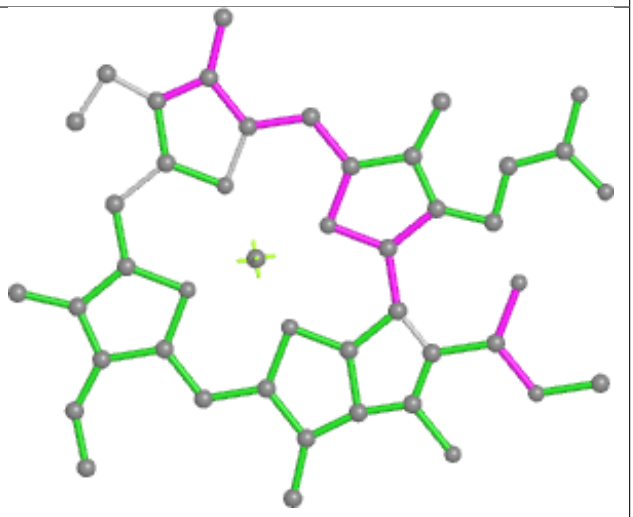

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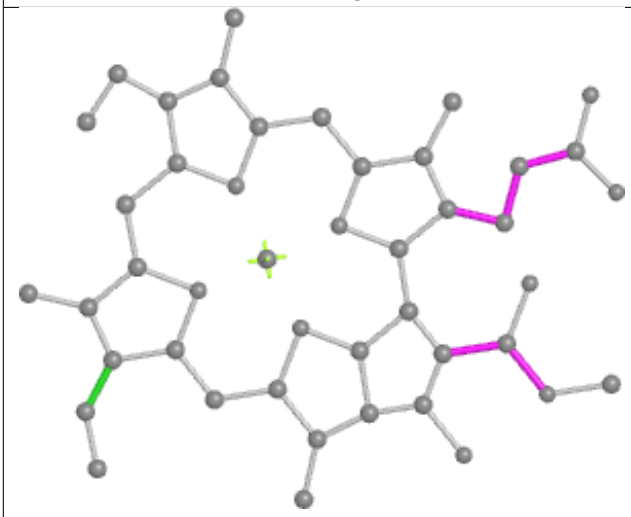

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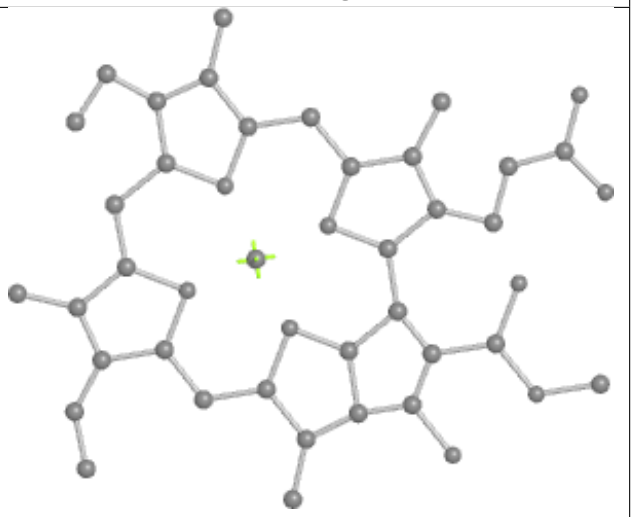
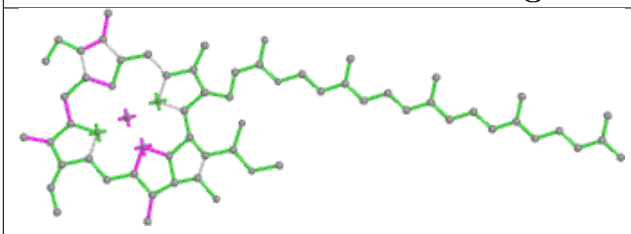


Rings

Ligand CLA C 521



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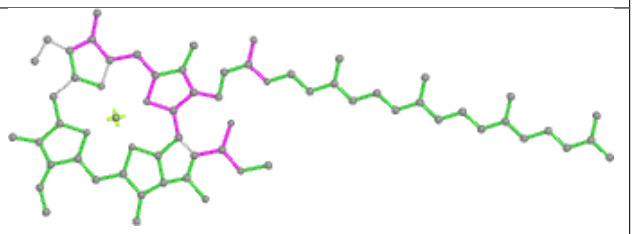
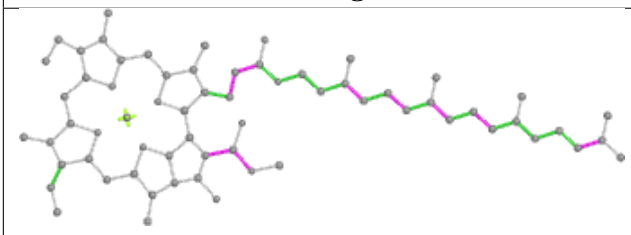


Bond angles



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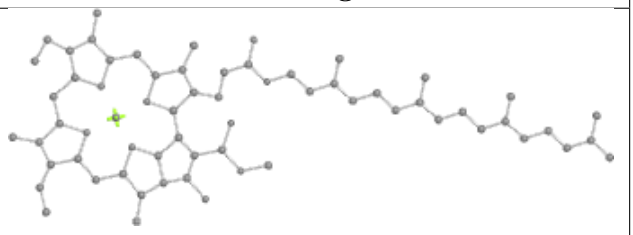
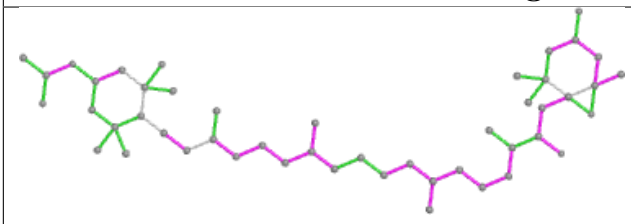


Rings

Ligand A86 40 212



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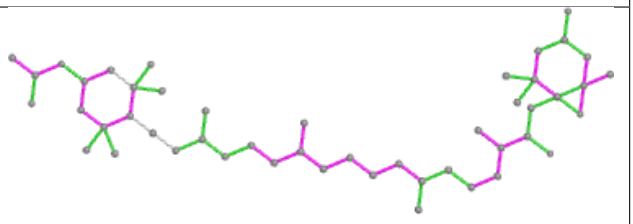
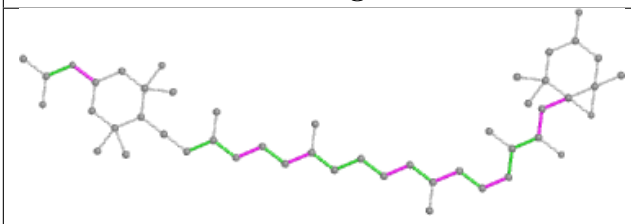
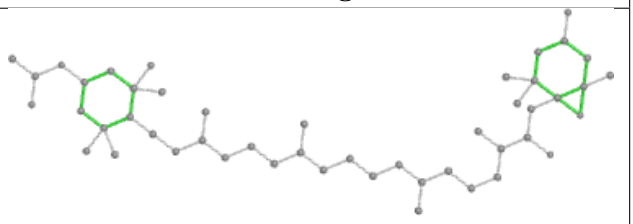


Bond angles

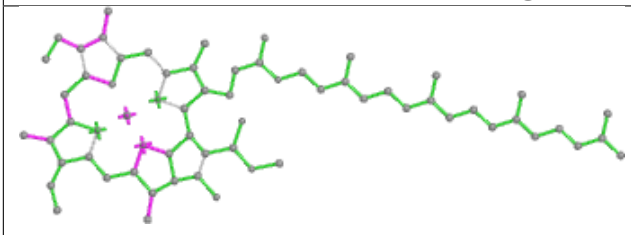


Torsions



Rings

Ligand CLA 19 301



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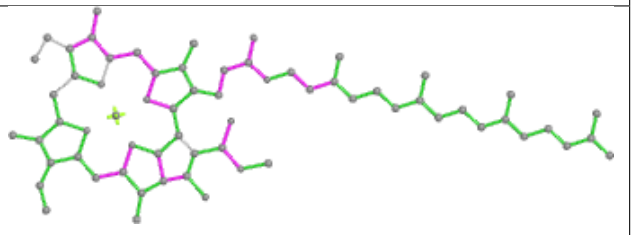

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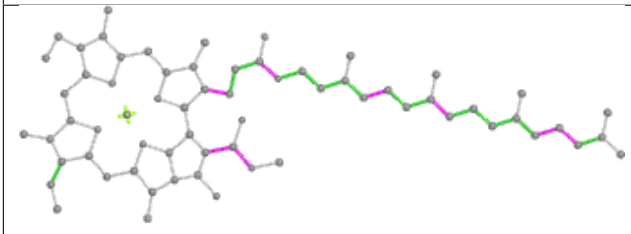

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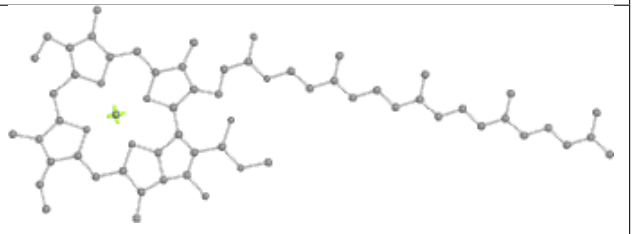
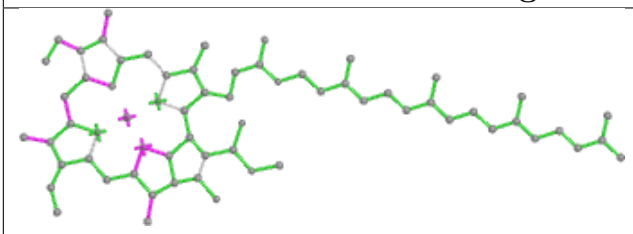


Rings

Ligand CLA 35 301



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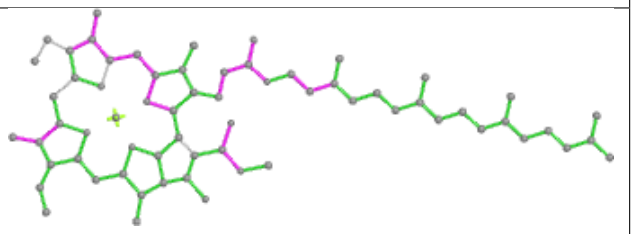

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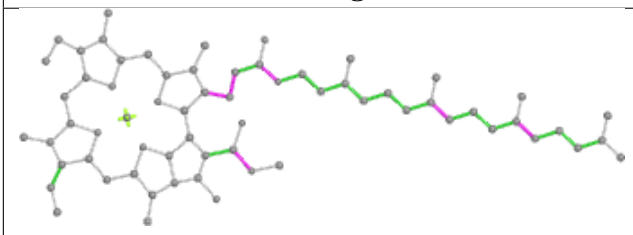

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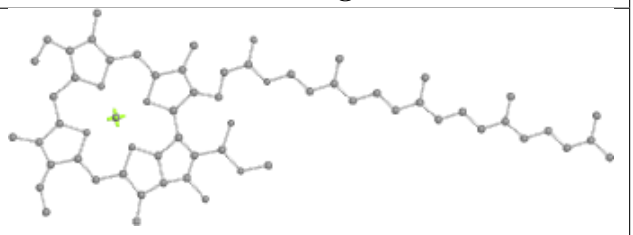
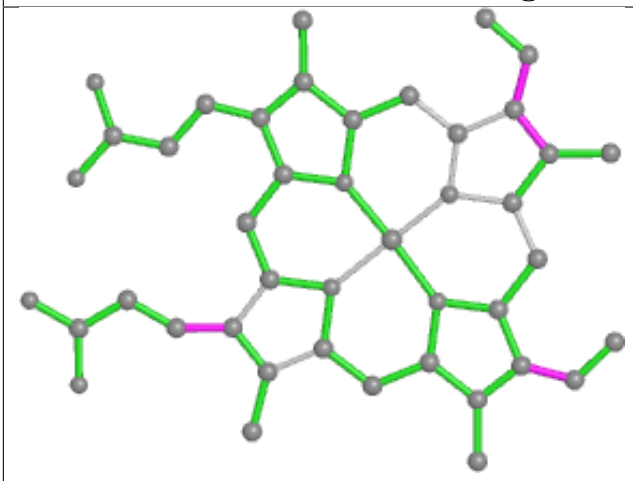


Rings

Ligand HEM E 101



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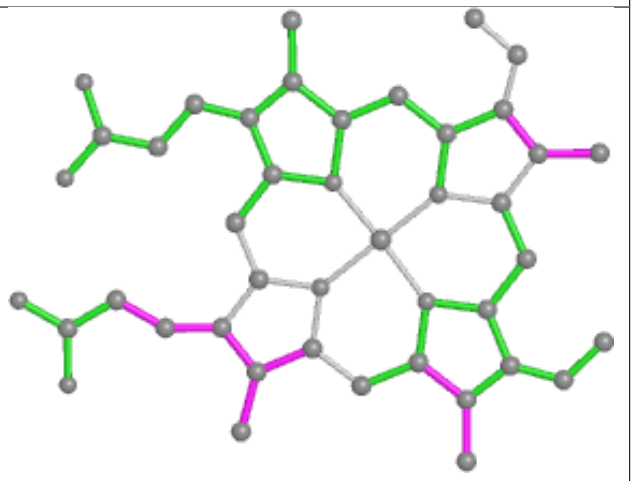

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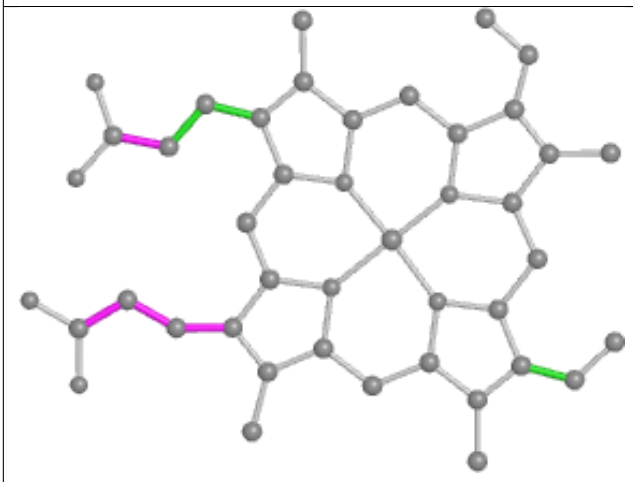

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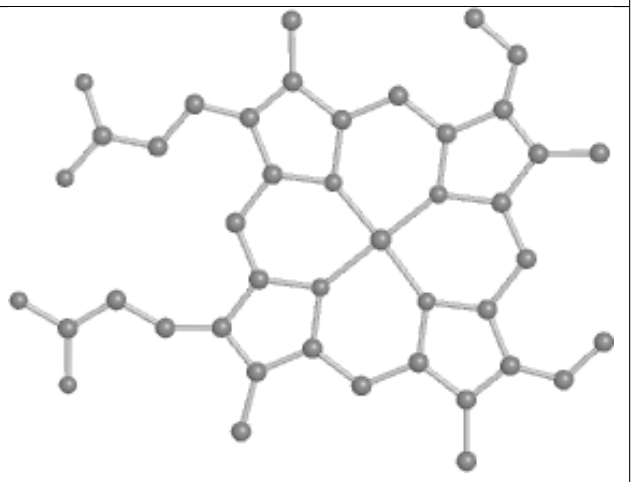
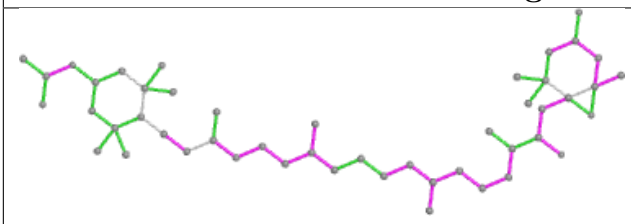


Rings

Ligand A86 33 314



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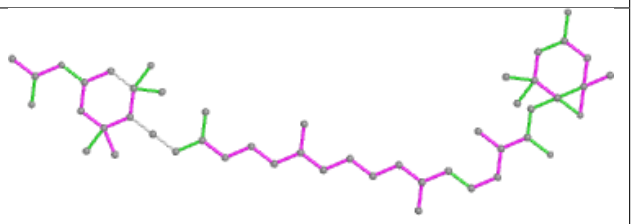

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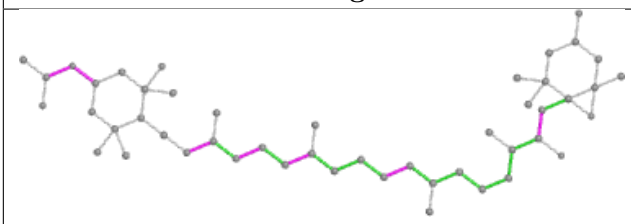

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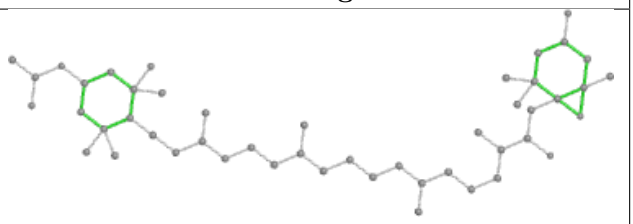
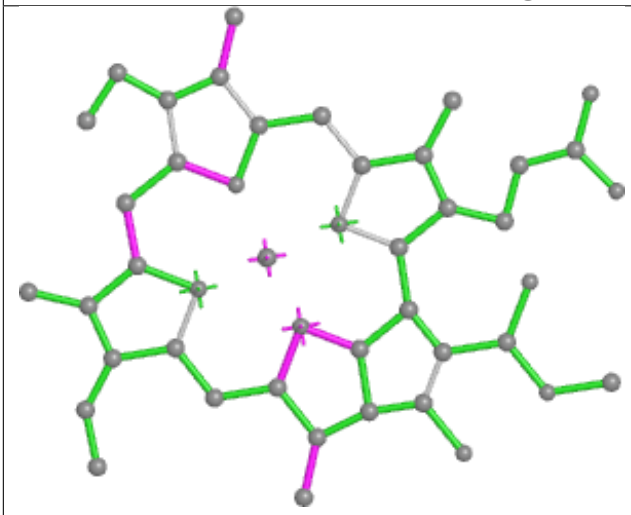


Rings

Ligand CLA 38 306



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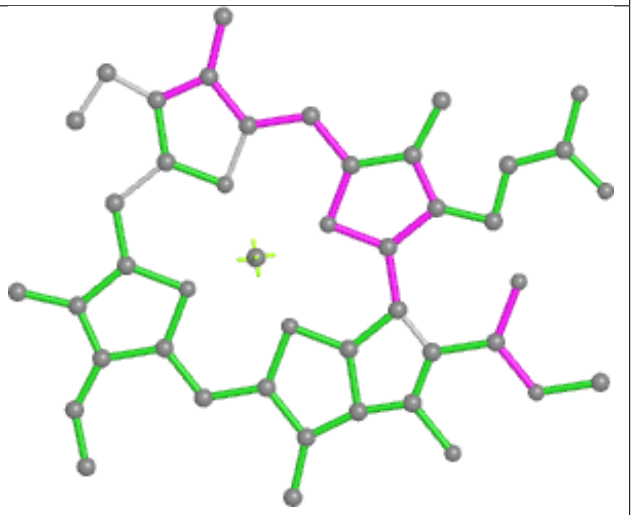

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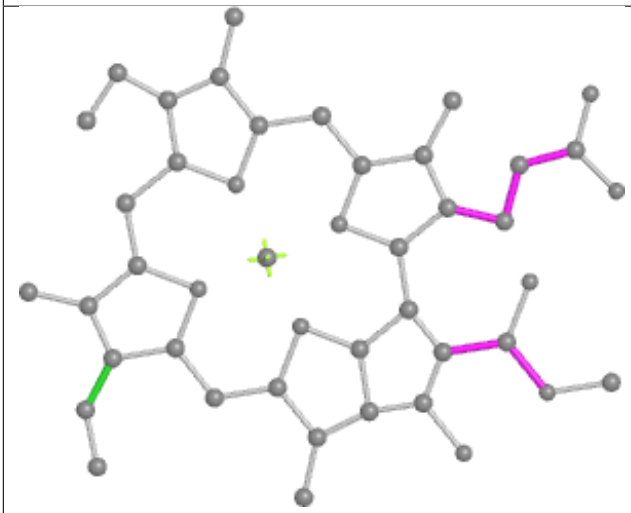

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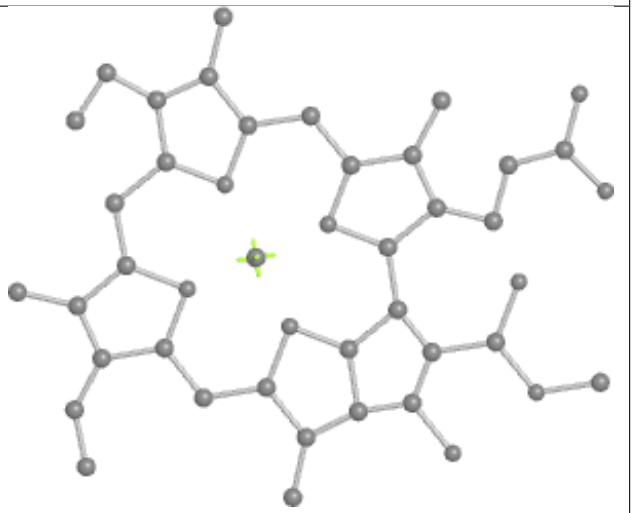
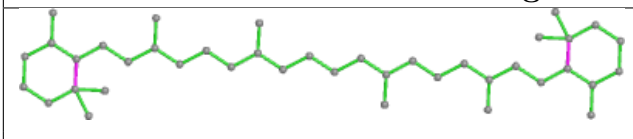


Rings

Ligand BCR B 616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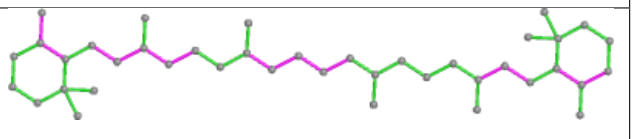
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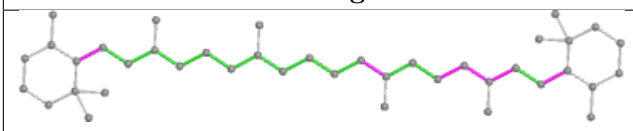
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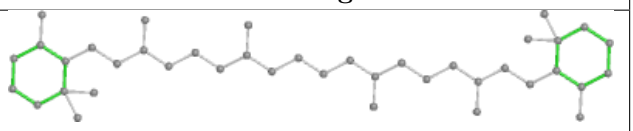
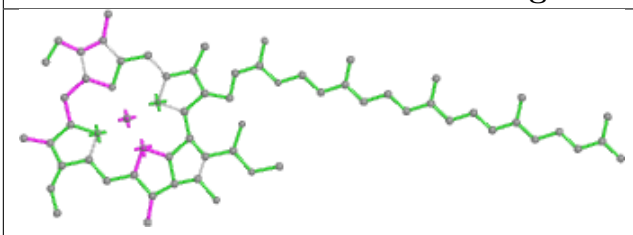

Rings

Ligand CLA c 506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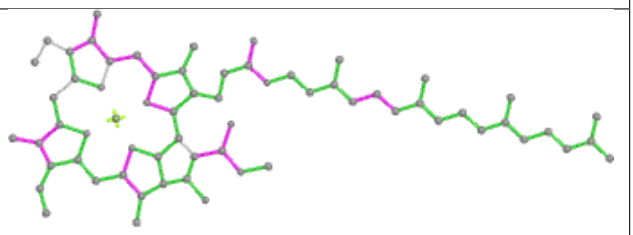
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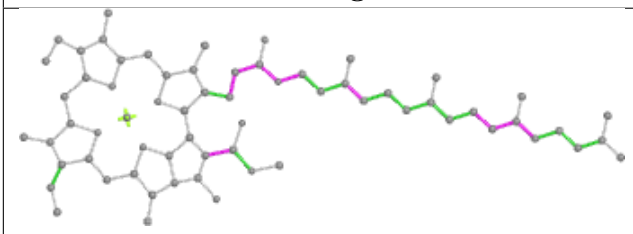
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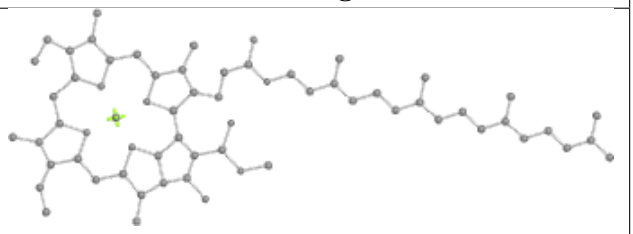
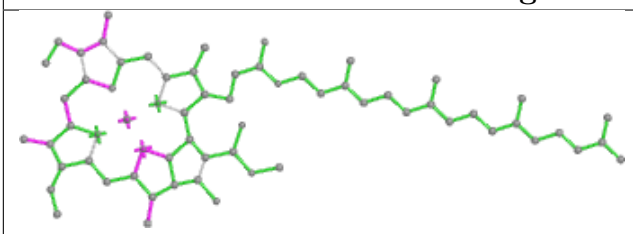

Rings

Ligand CLA 31 301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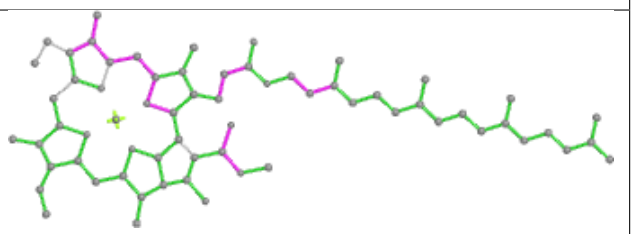
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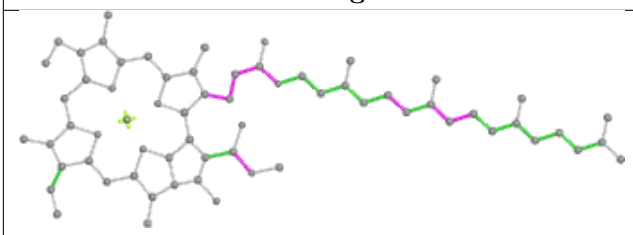
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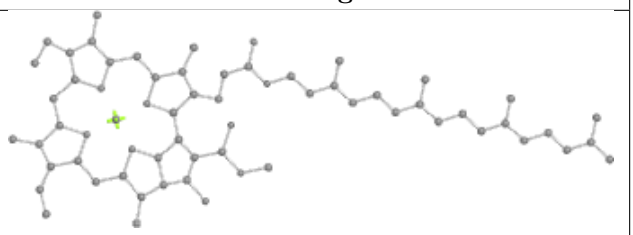
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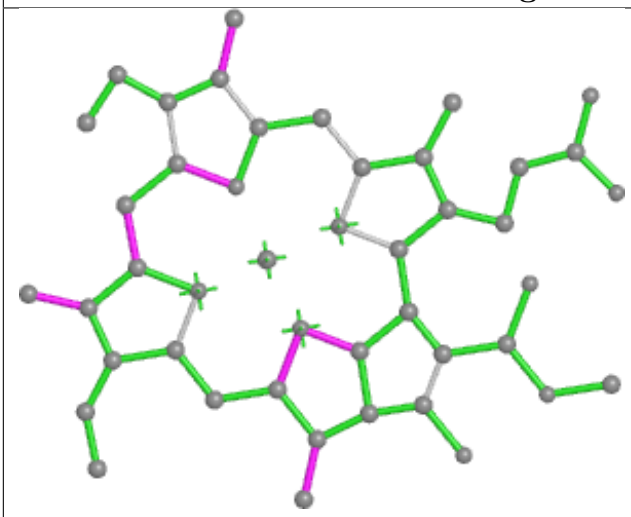

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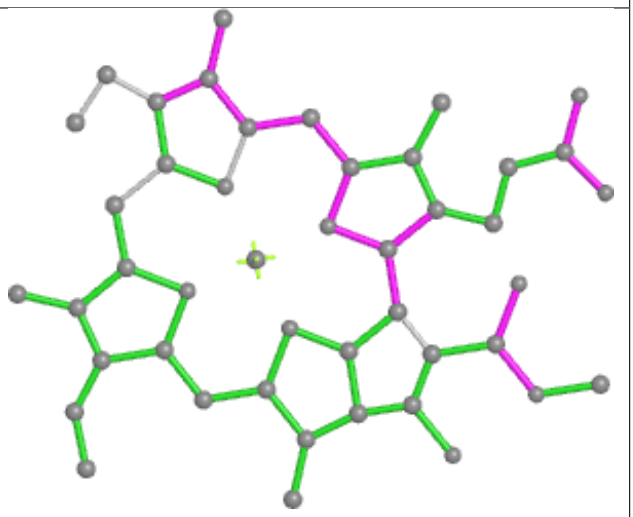

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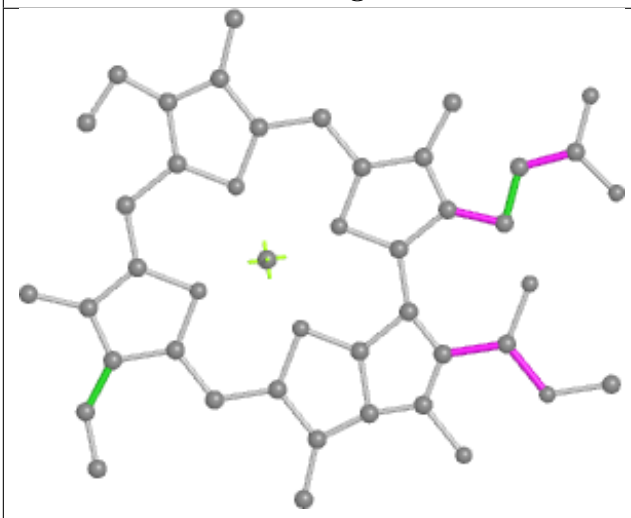

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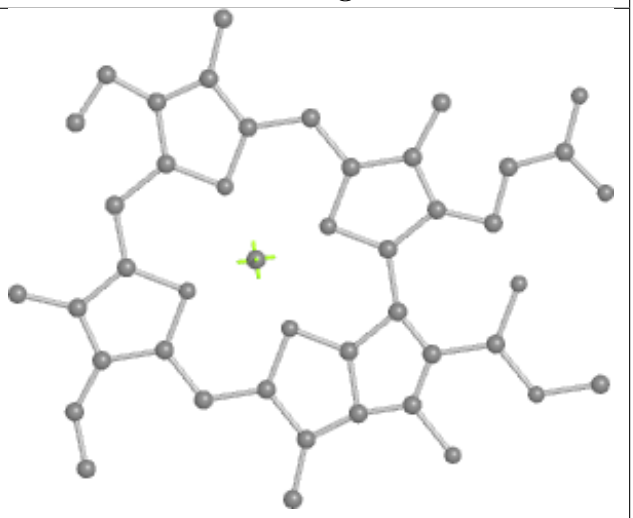
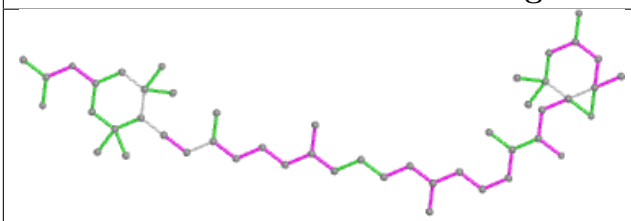


Rings

Ligand A86 32 314



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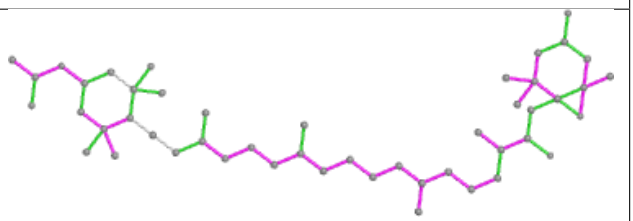

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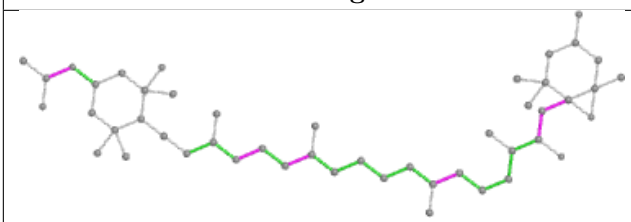

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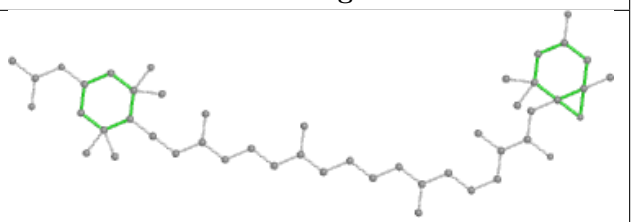

Rings

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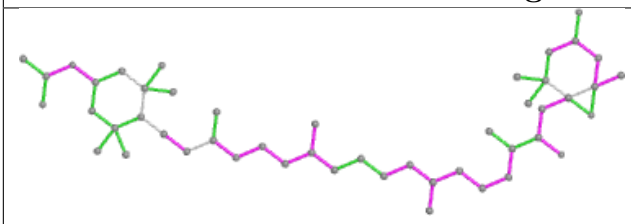

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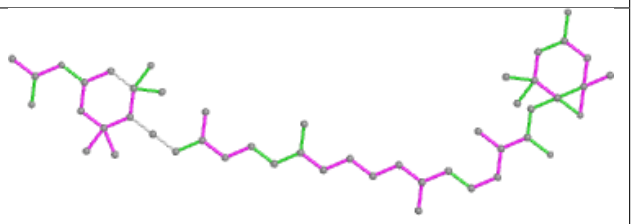

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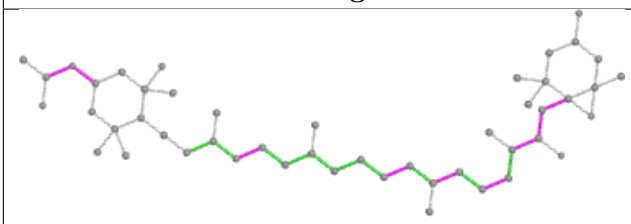

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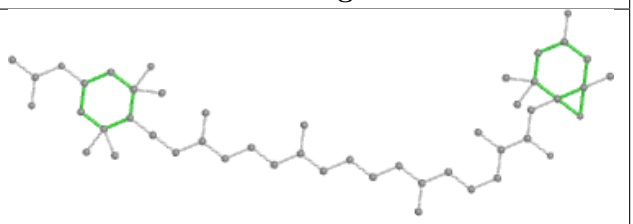
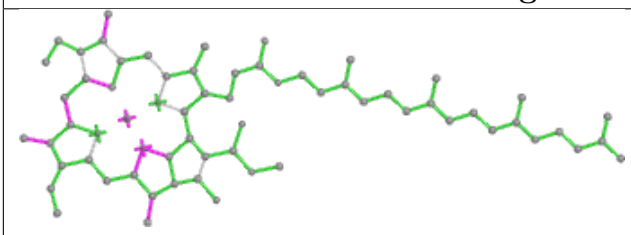


Rings

Ligand CLA 18 309



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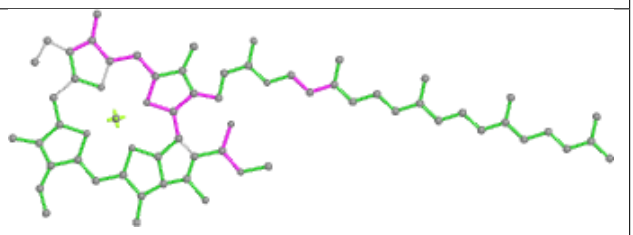

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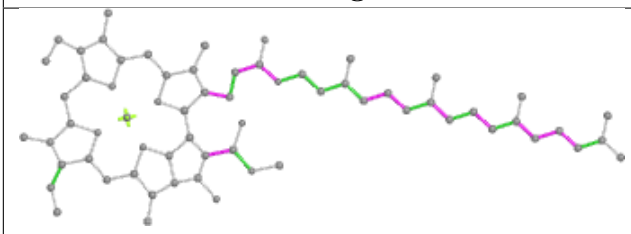

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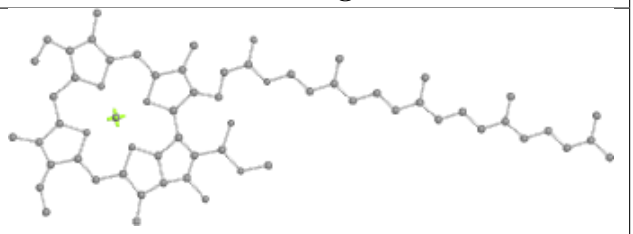
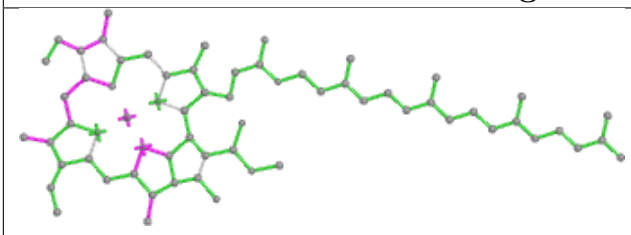


Rings

Ligand CLA 31 303



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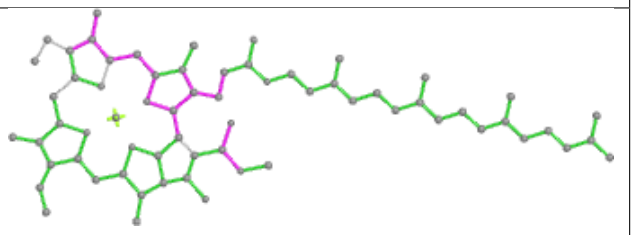
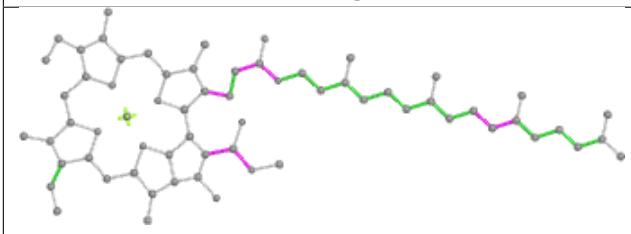


Bond angles



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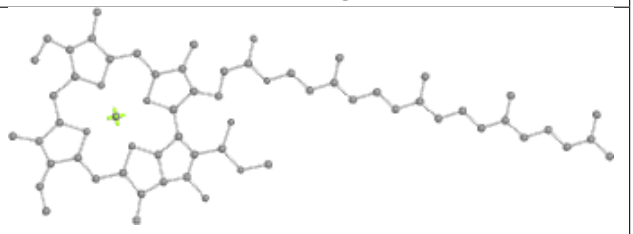

Rings

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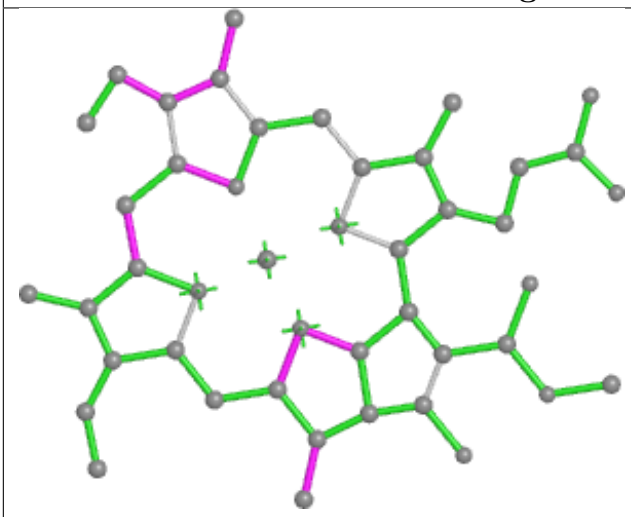

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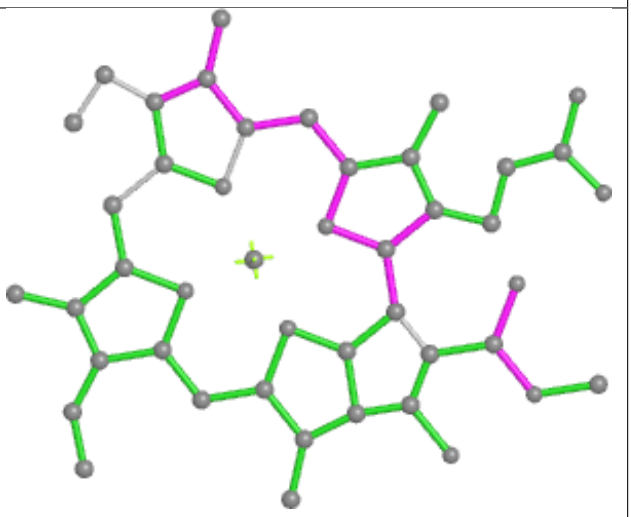
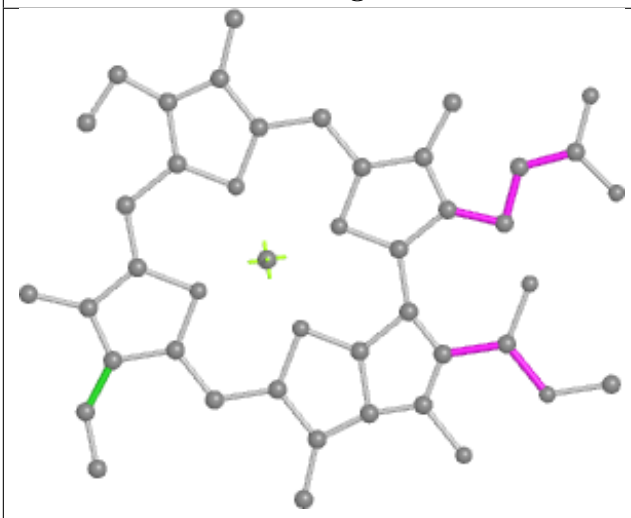
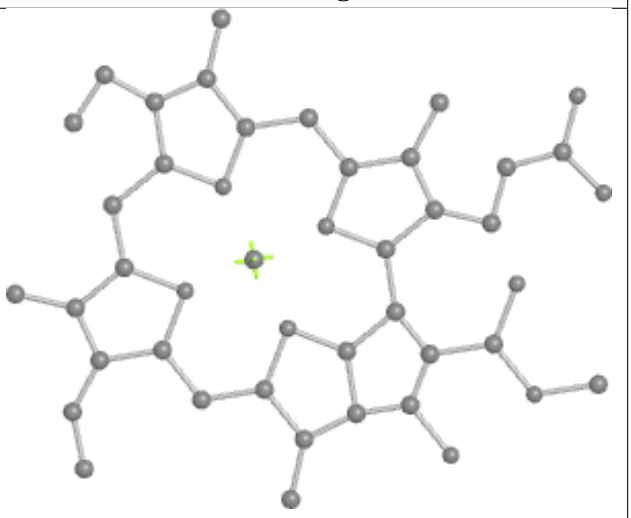


Bond angles

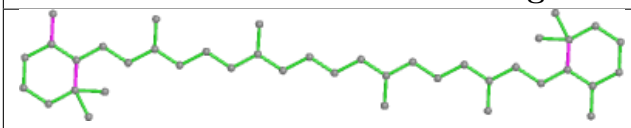


Torsions

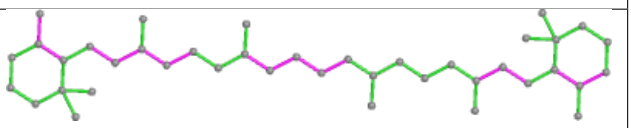


Rings

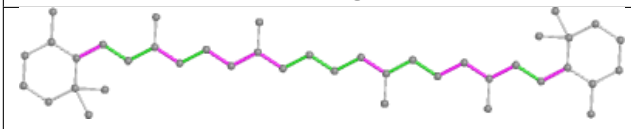
Ligand BCR c 515



Bond lengths



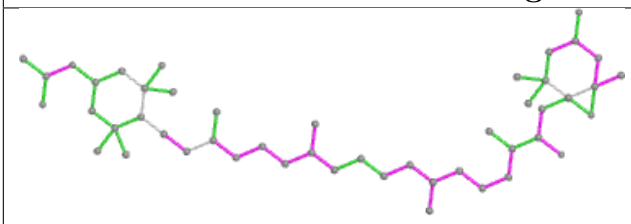
Bond angles



Torsions

Rings

Ligand A86 41 312



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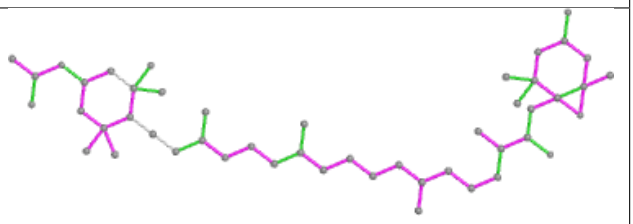

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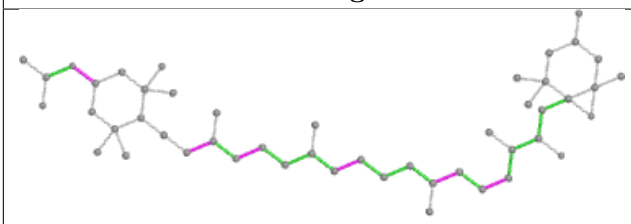

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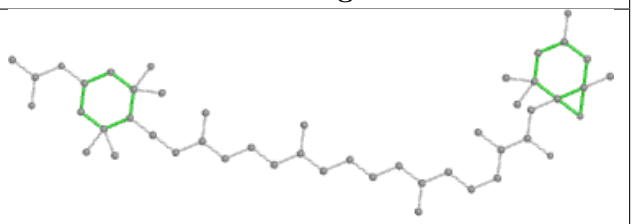
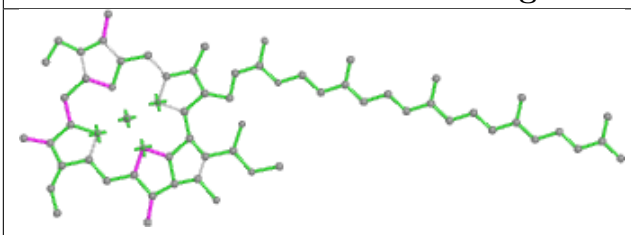


Rings

Ligand CLA 15 303



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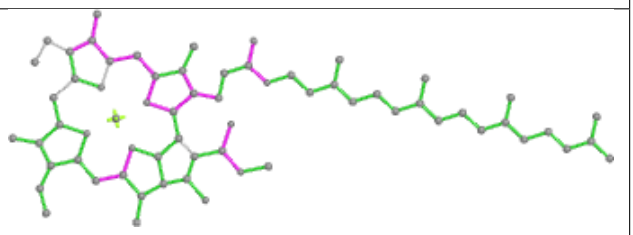

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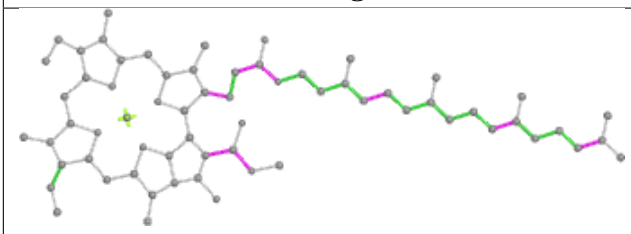

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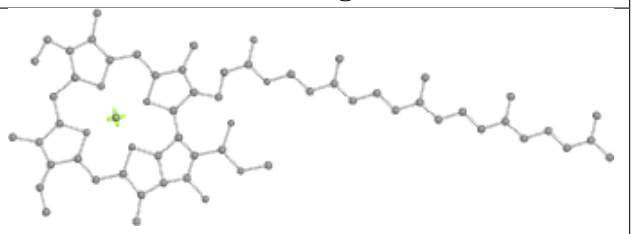
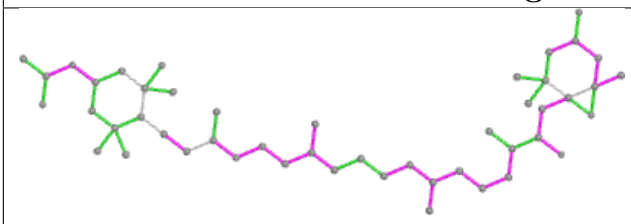


Rings

Ligand A86 36 311



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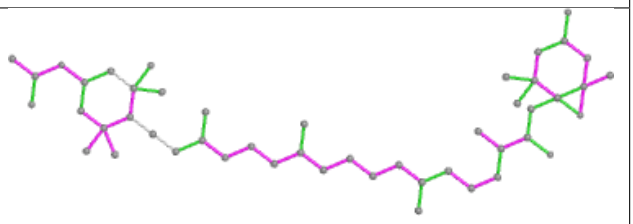

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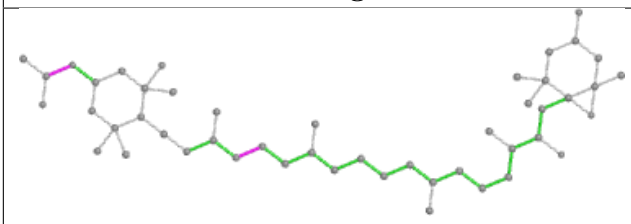

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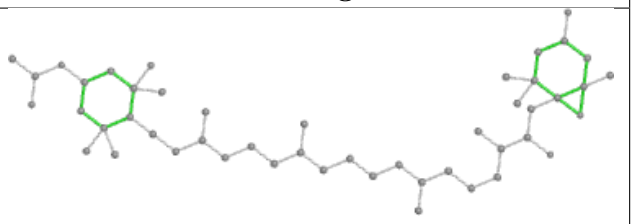
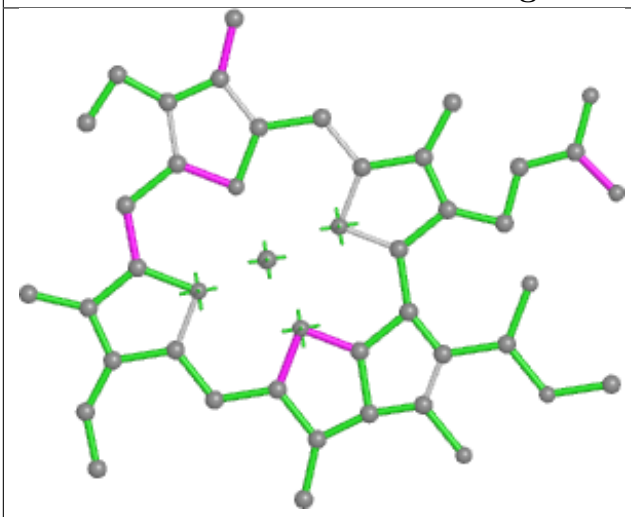


Rings

Ligand CLA 41 309



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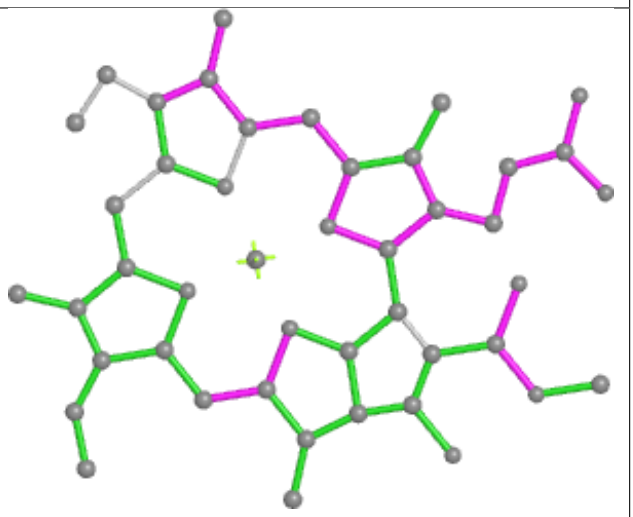

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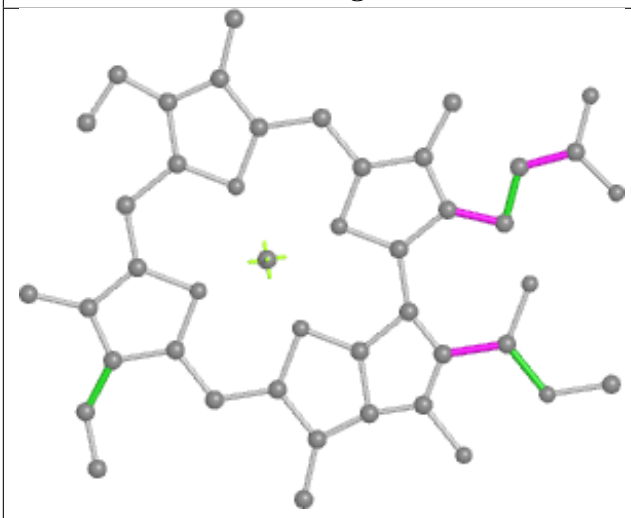

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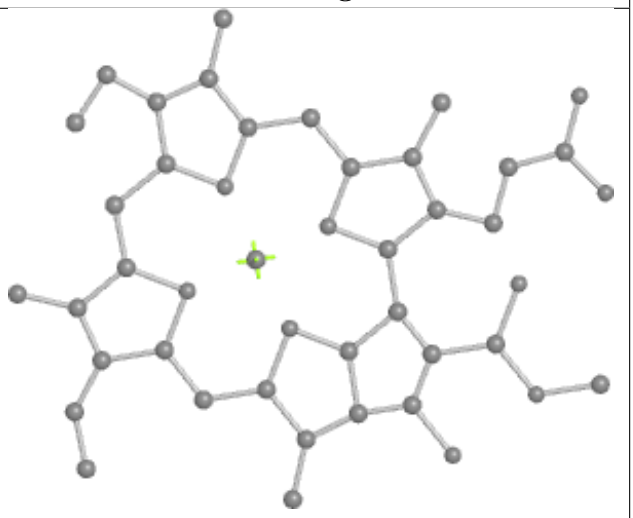
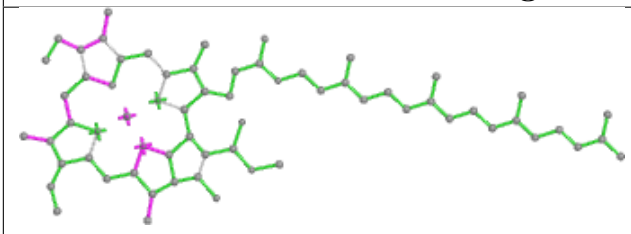


Rings

Ligand CLA 31 307



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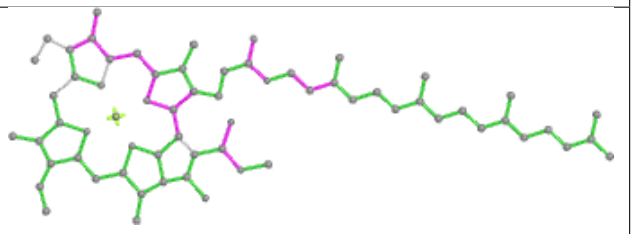

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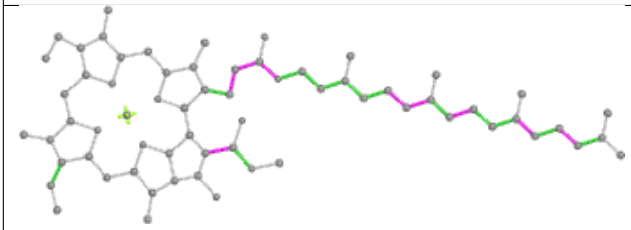

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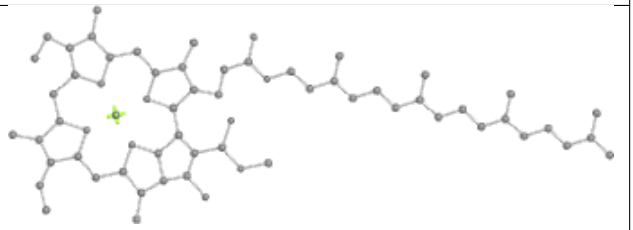
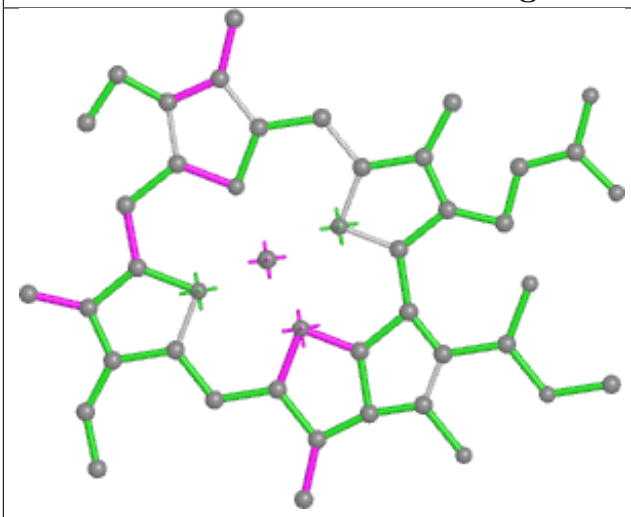


Rings

Ligand CLA 32 313



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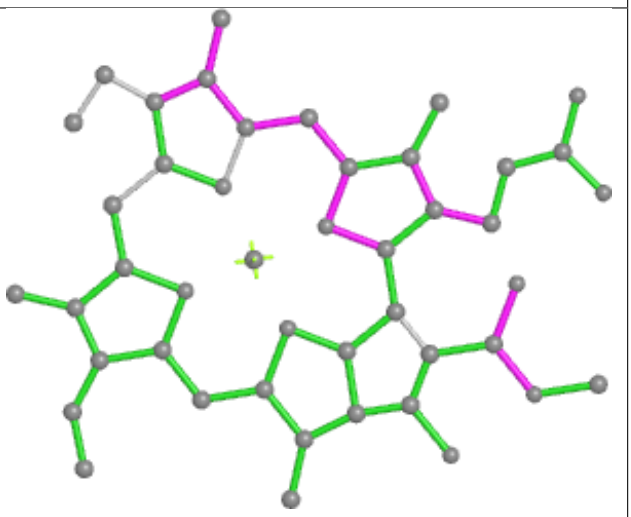

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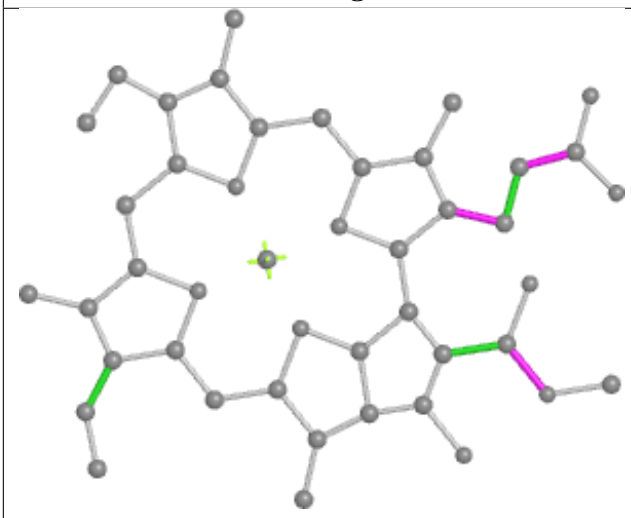

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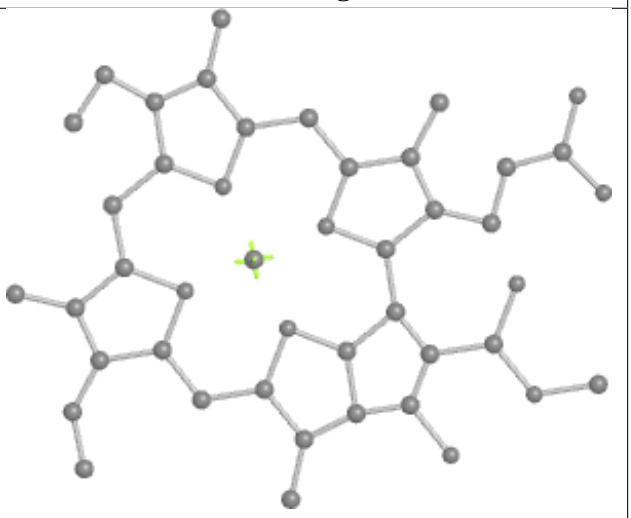
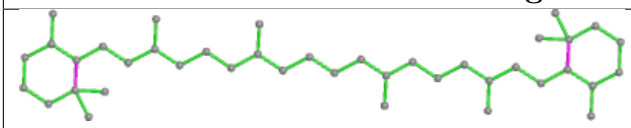


Rings

Ligand BCR b 616



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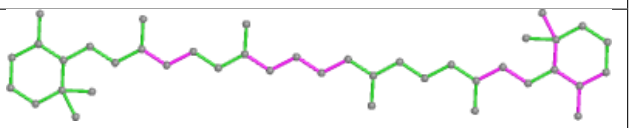

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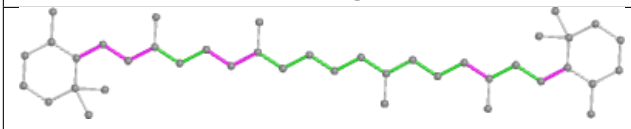
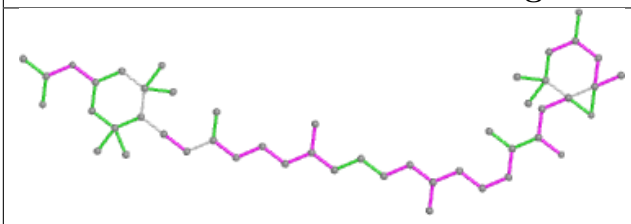


Torsions

Rings

Ligand A86 31 314



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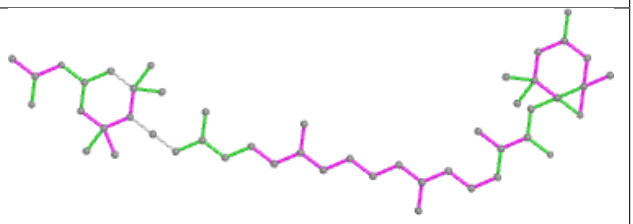

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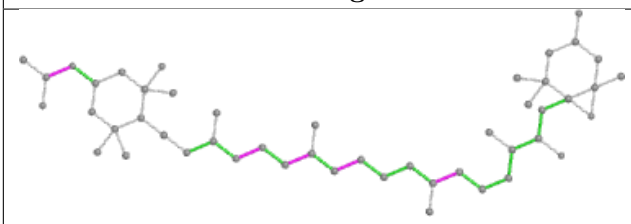

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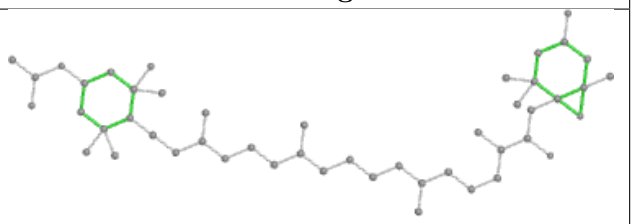
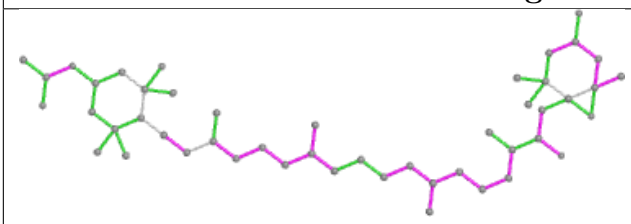


Rings

Ligand A86 19 311



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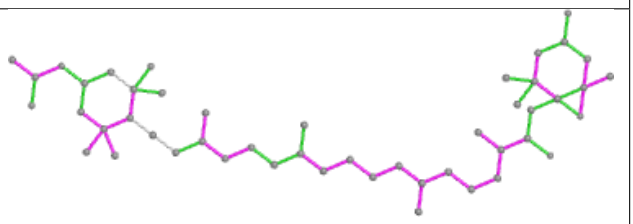

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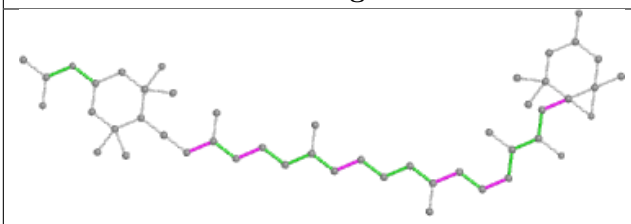

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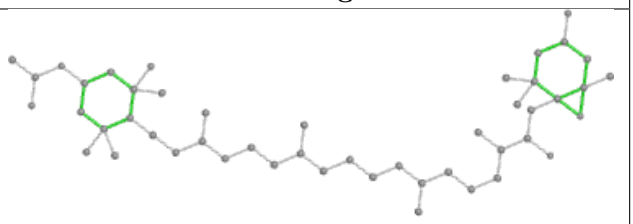
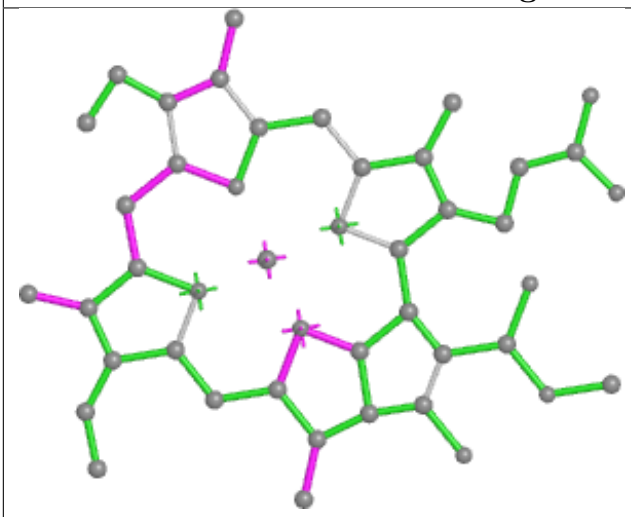


Rings

Ligand CLA 40 205



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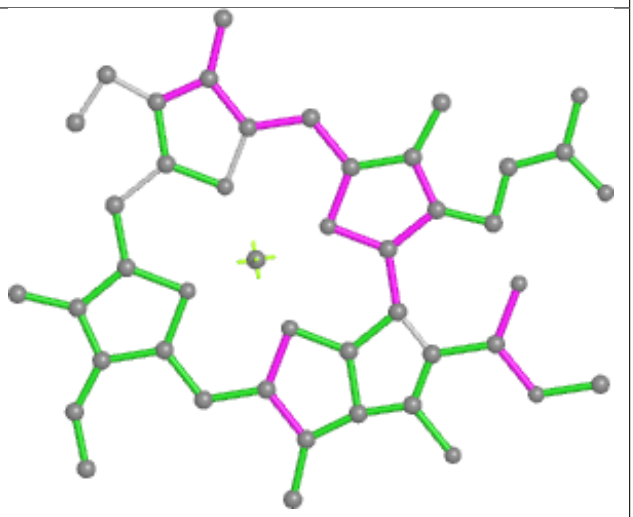

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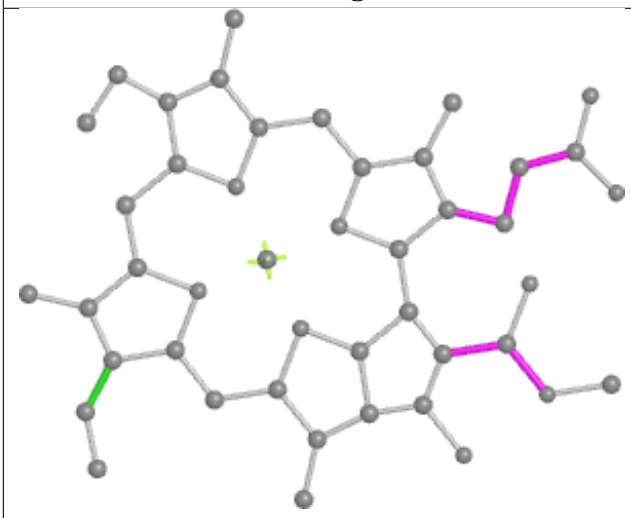

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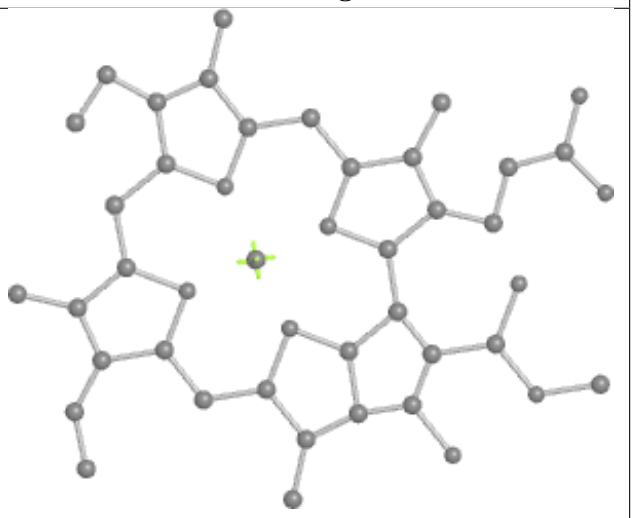
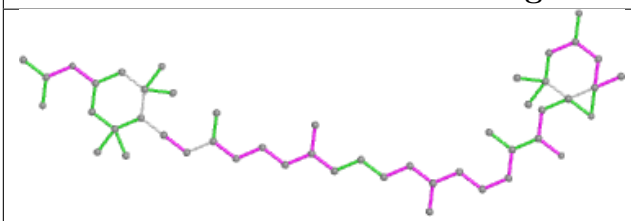


Rings

Ligand A86 41 310



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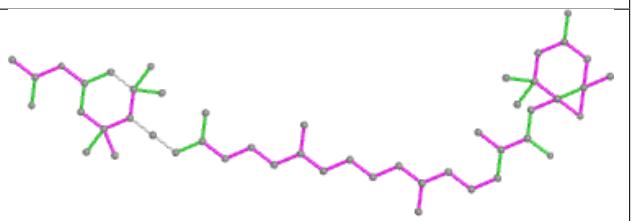

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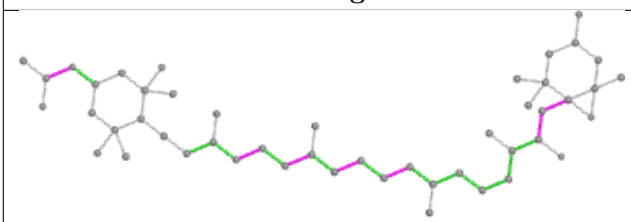

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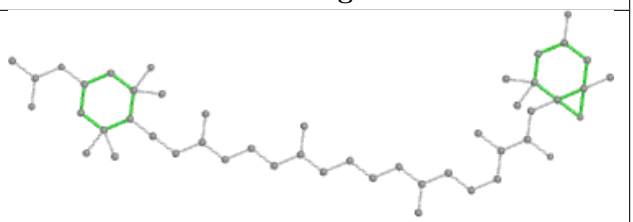
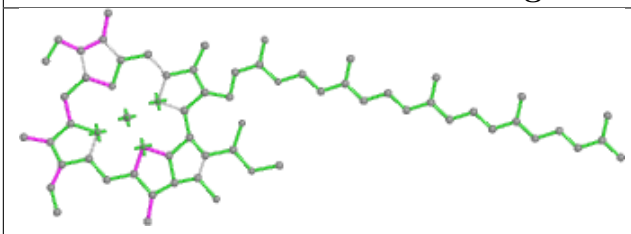


Rings

Ligand CLA B 605



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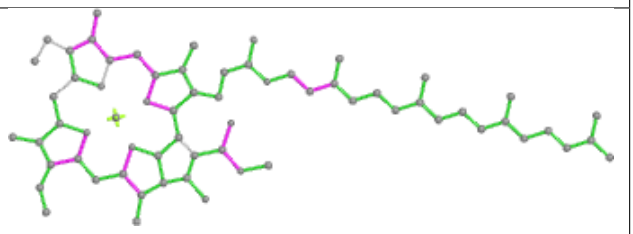
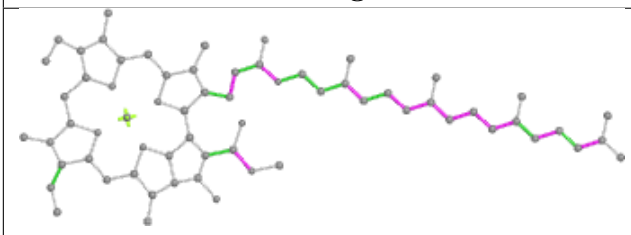


Bond angles



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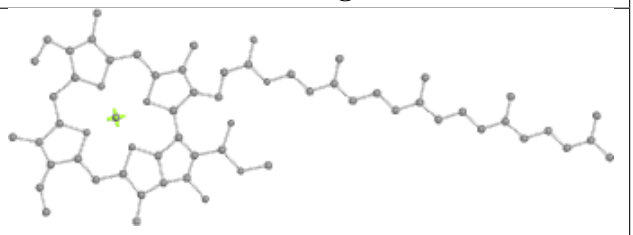
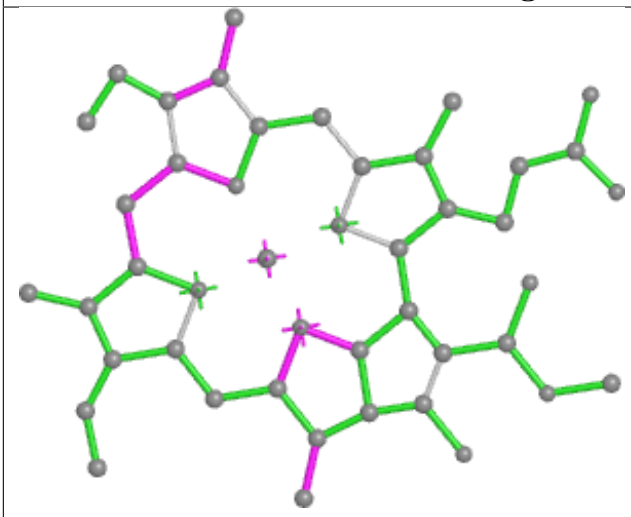


Rings

Ligand CLA 20 203



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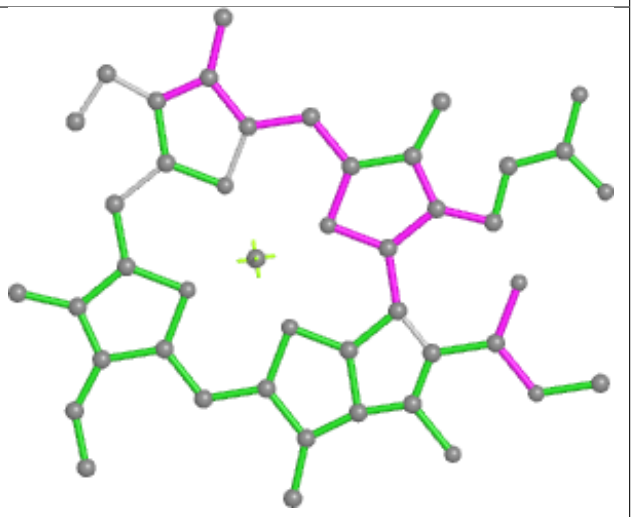
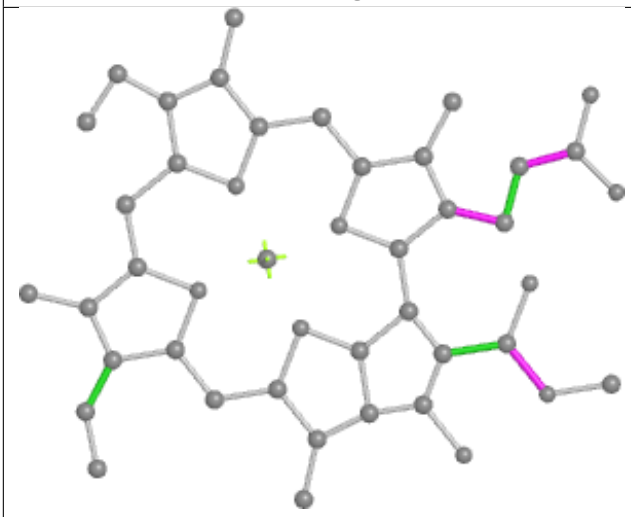


Bond angles



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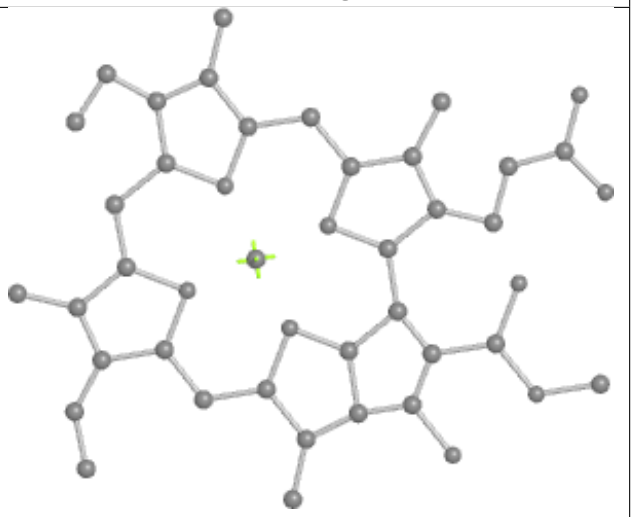
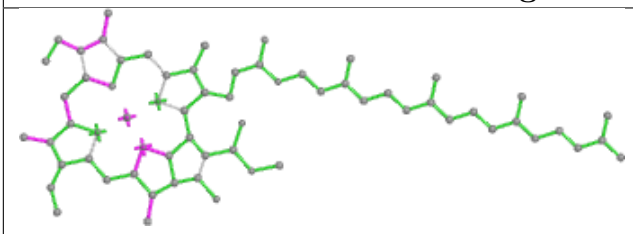
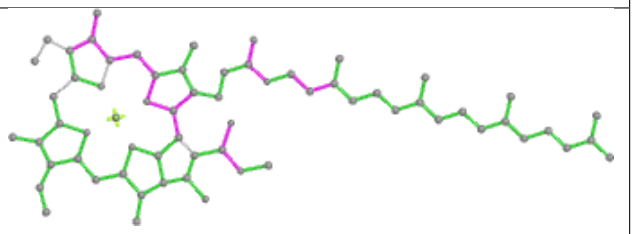


Rings

Ligand CLA 14 308



Bond lengths



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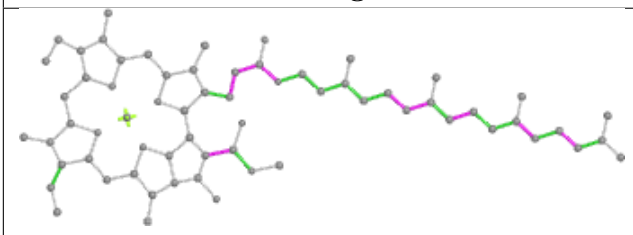
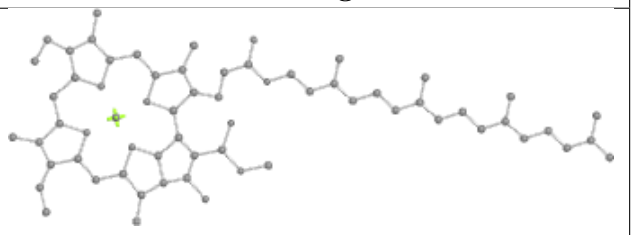
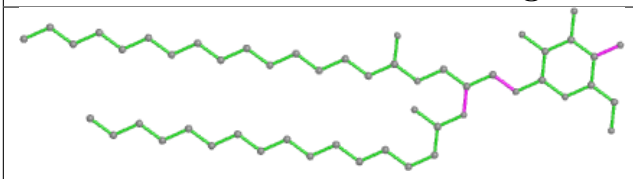


Torsions



Rings

Ligand LMG d 410



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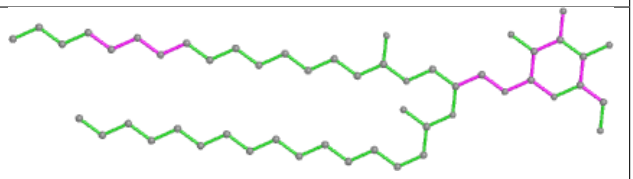

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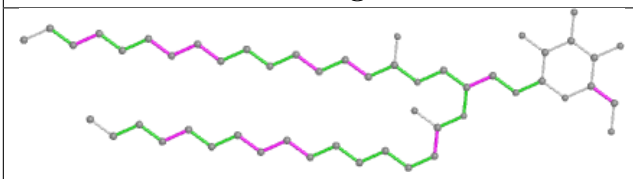

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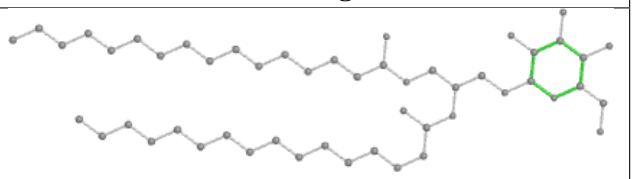
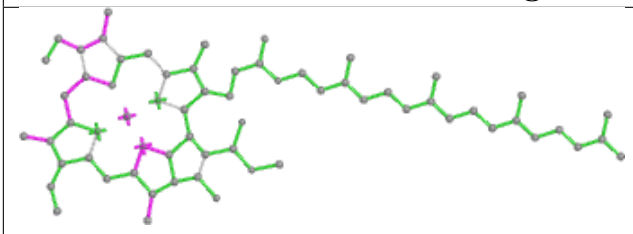


Rings

Ligand CLA D 406



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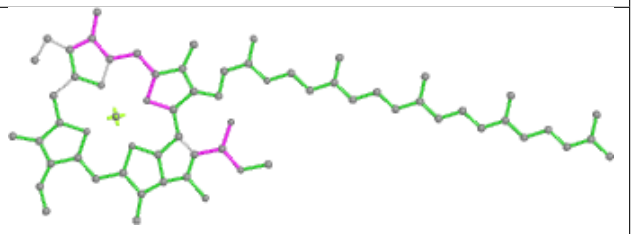

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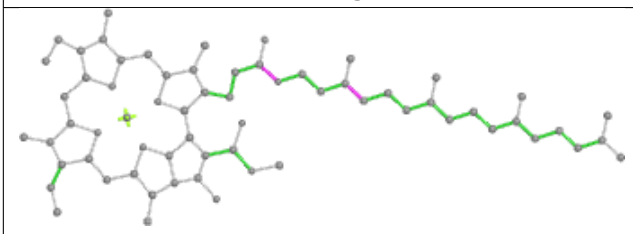

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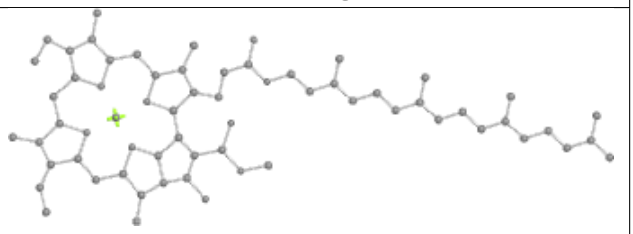
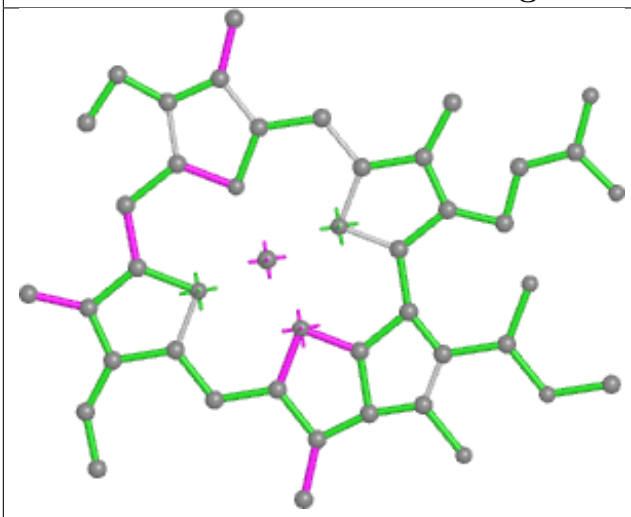


Rings

Ligand CLA 11 304



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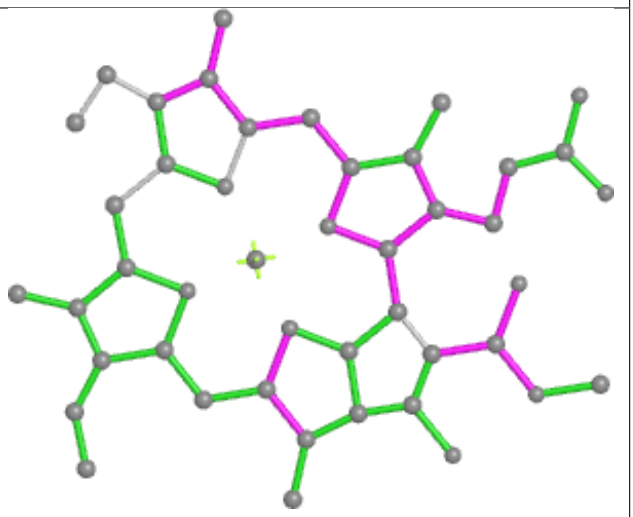

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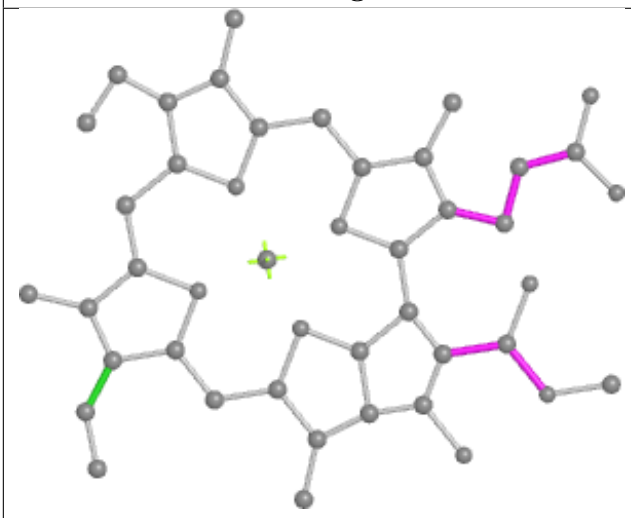

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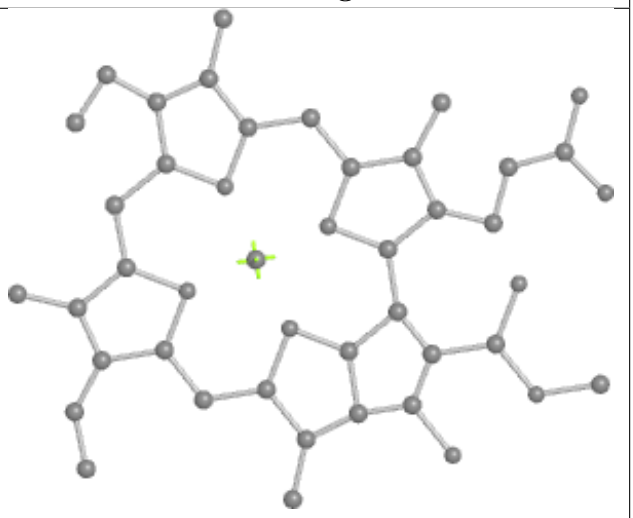
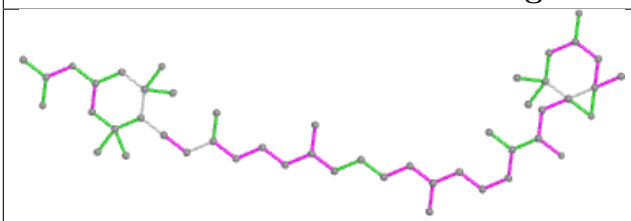


Rings

Ligand A86 17 313



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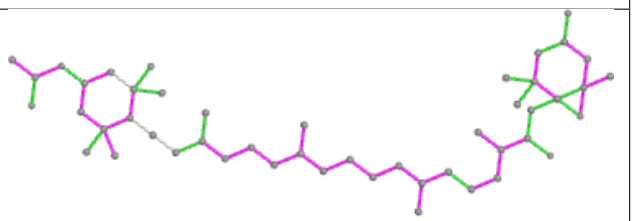

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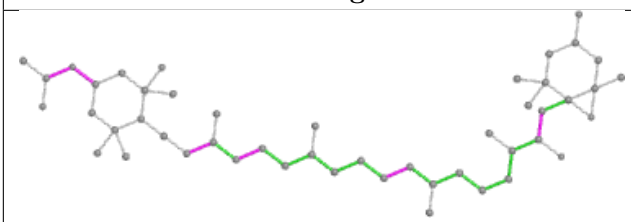

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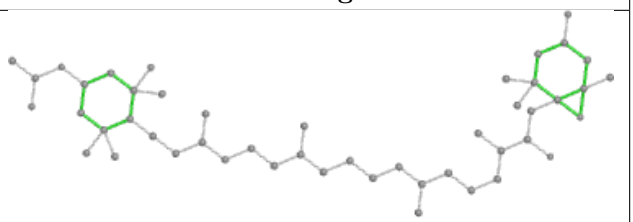
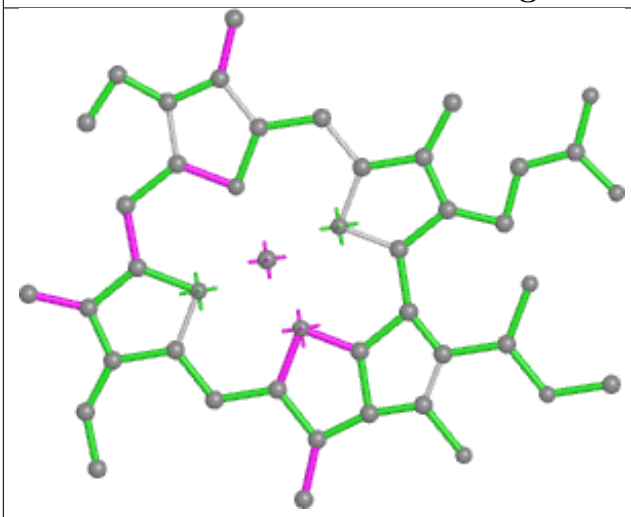


Rings

Ligand CLA 11 305



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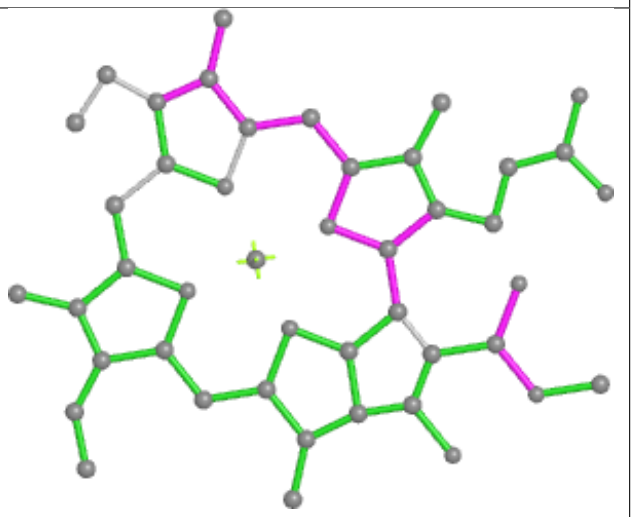

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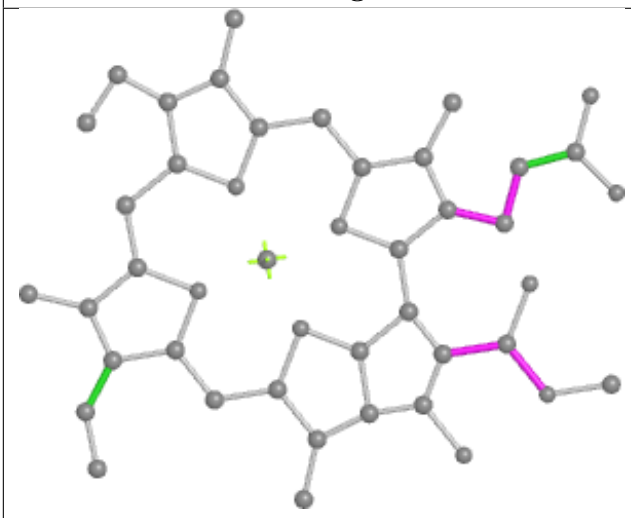

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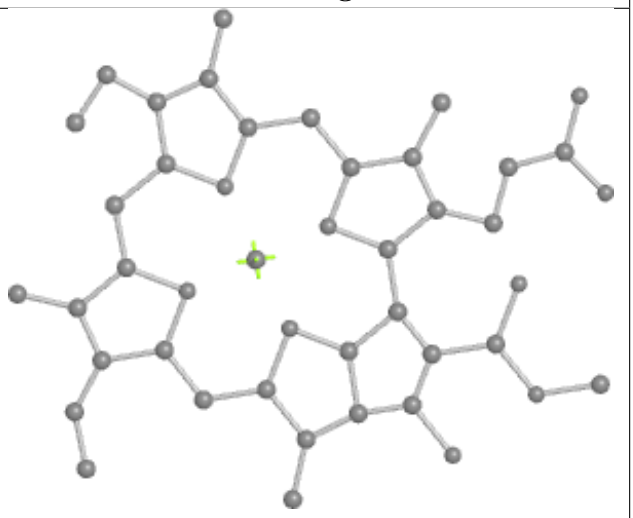
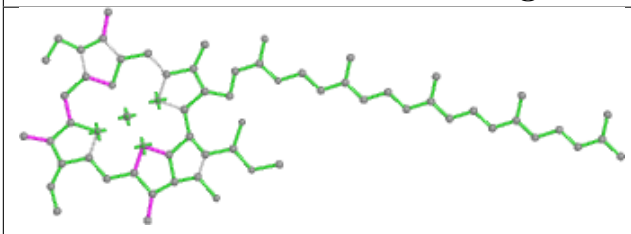


Rings

Ligand CLA 20 202



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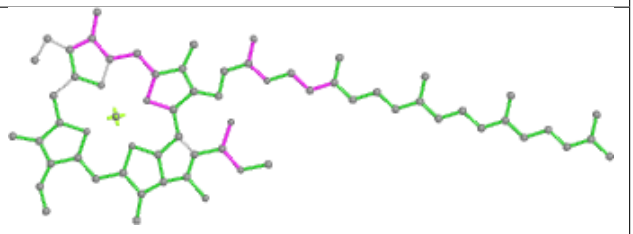

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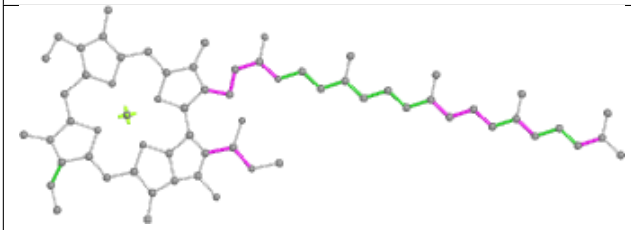

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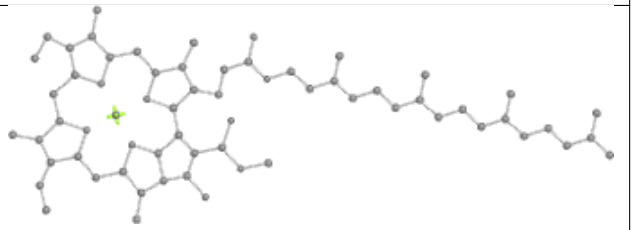
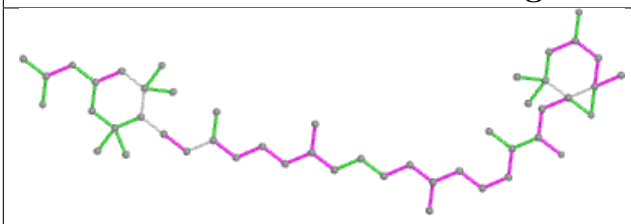


Rings

Ligand A86 37 313



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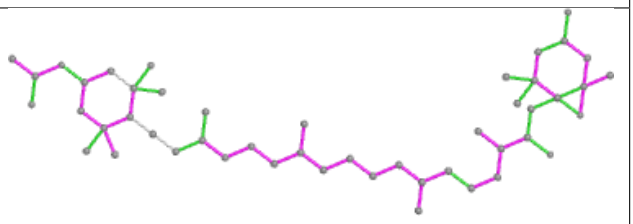

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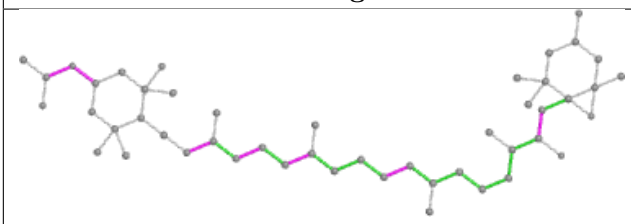

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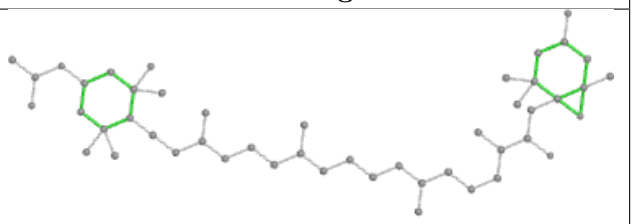
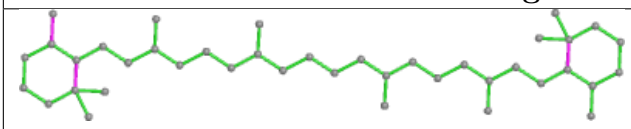


Rings

Ligand BCR B 624



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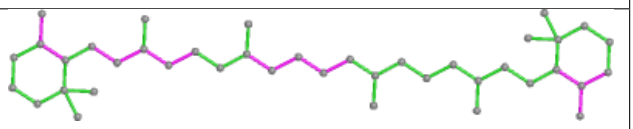

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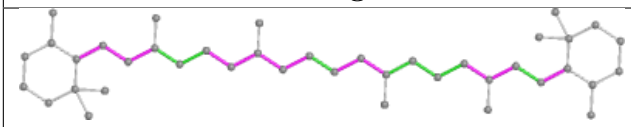

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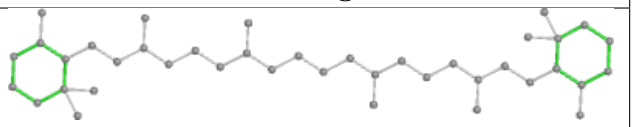
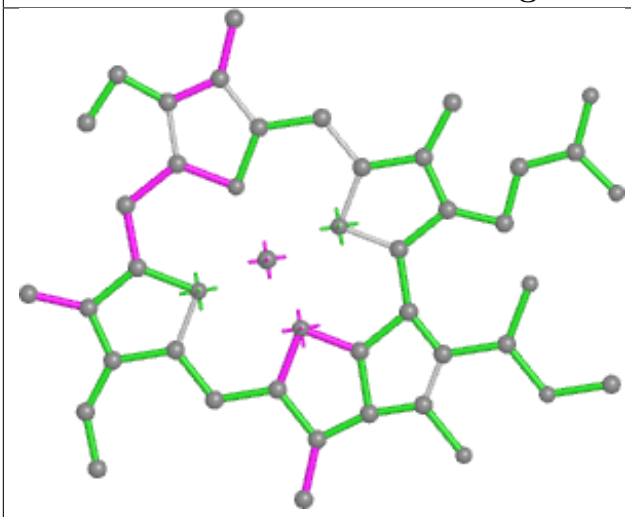


Rings

Ligand CLA 13 303



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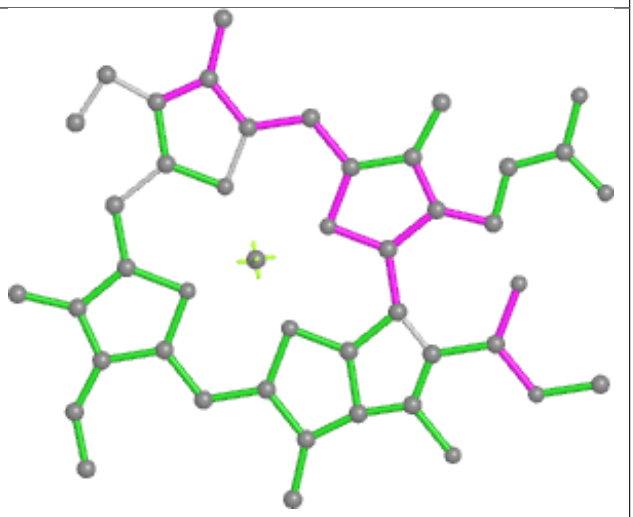

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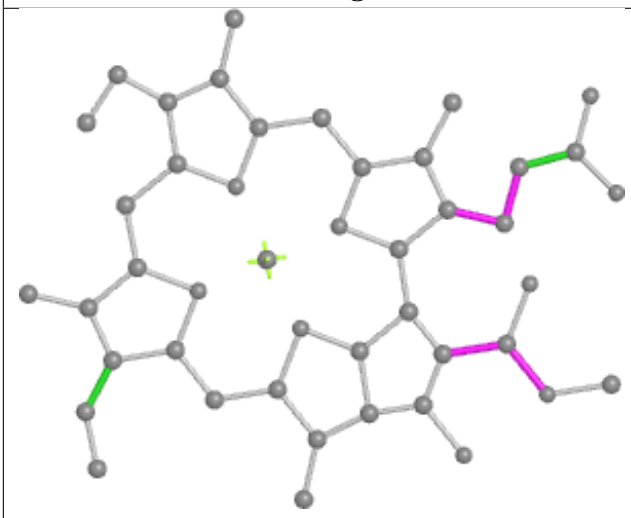

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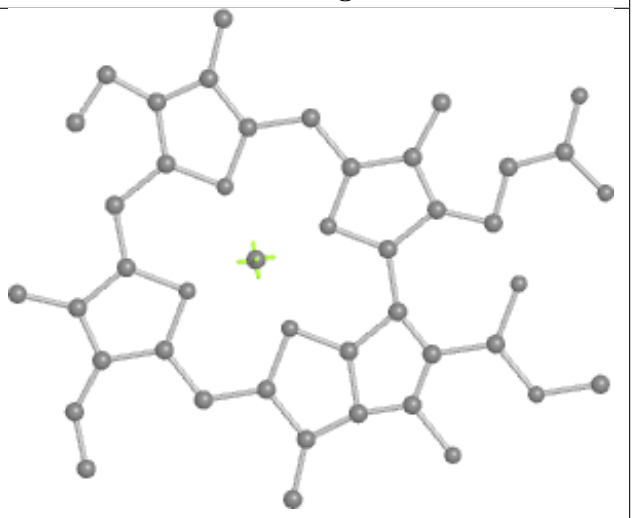
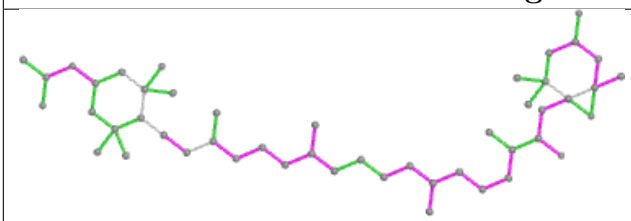


Rings

Ligand A86 41 313



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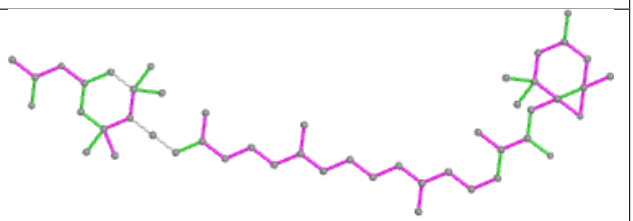

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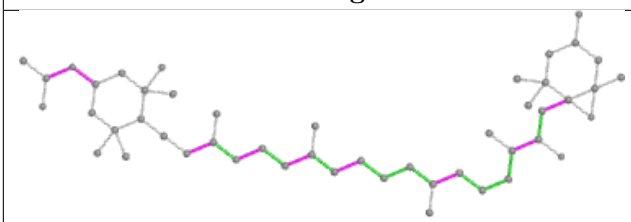

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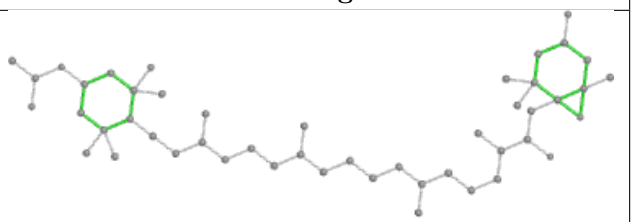
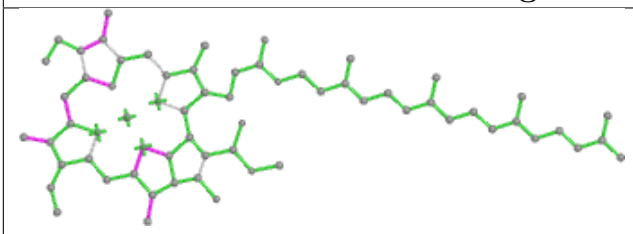


Rings

Ligand CLA 21 301



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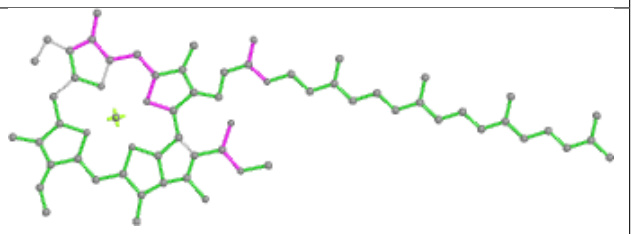
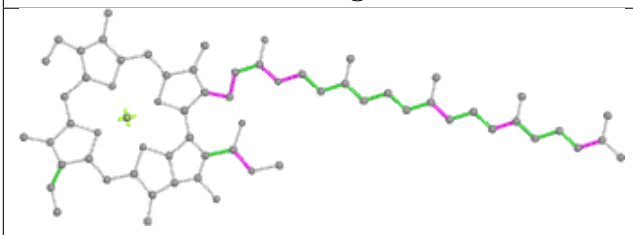


Bond angles



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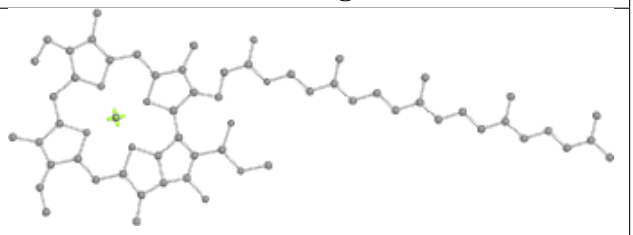
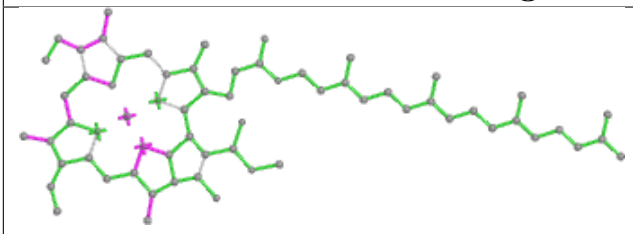


Rings

Ligand CLA 13 304



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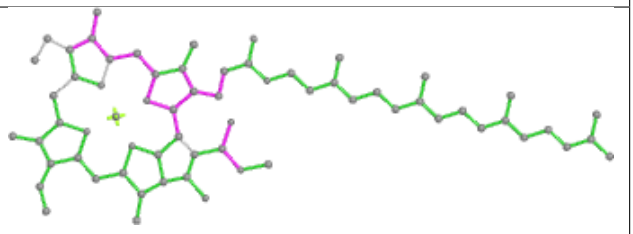
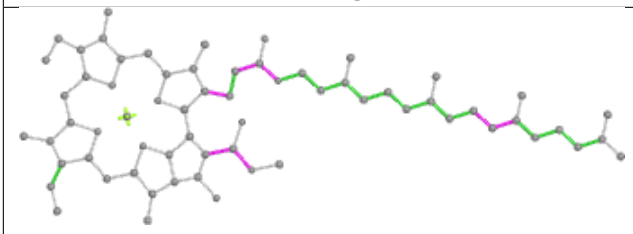
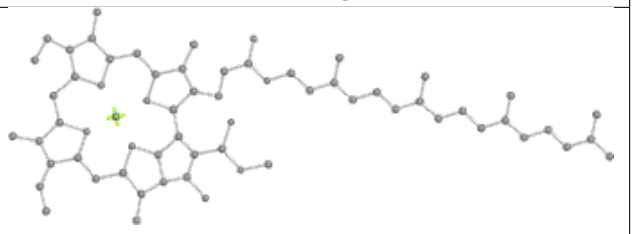


Bond angles

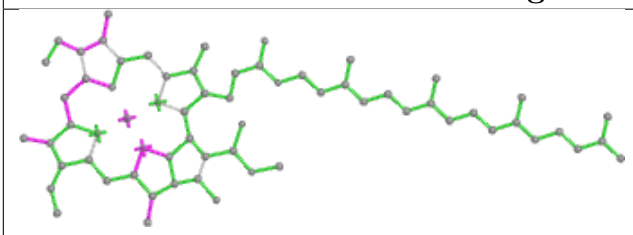


Torsions



Rings

Ligand CLA d 407



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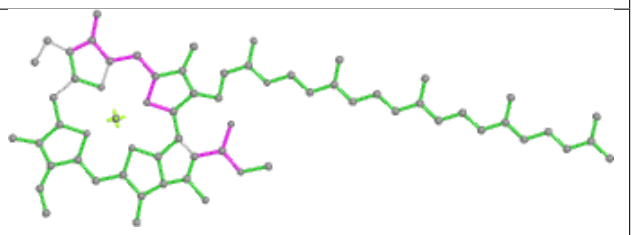
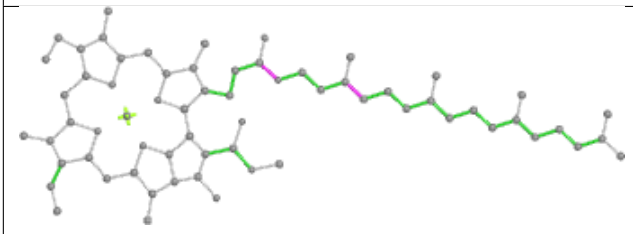


Bond angles



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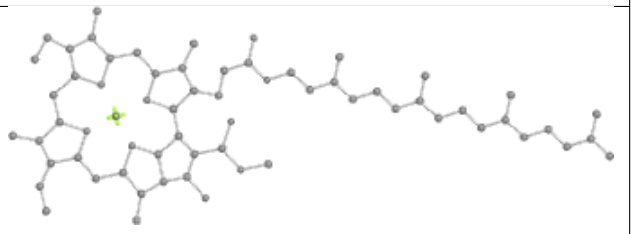
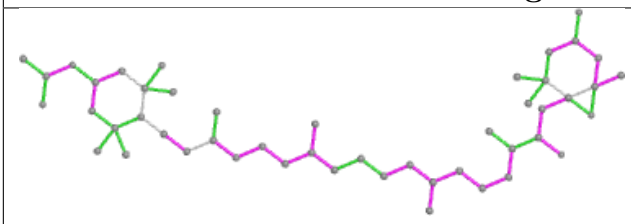
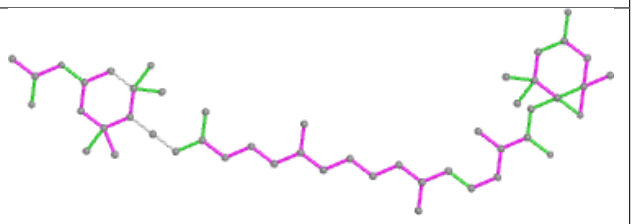


Rings

Ligand A86 35 312



Bond lengths



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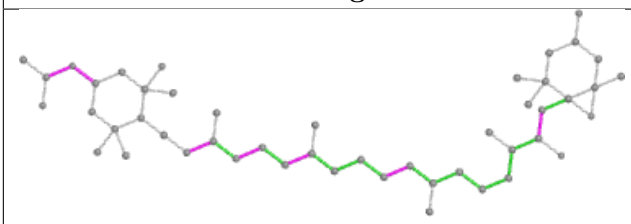
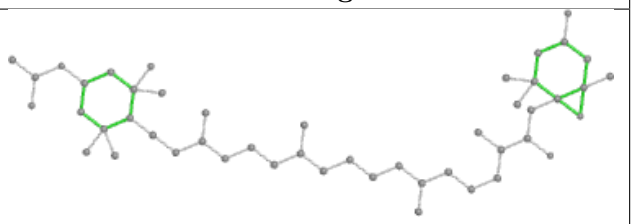
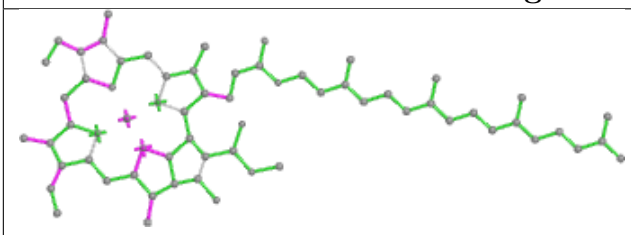


Torsions



Rings

Ligand CLA C 511



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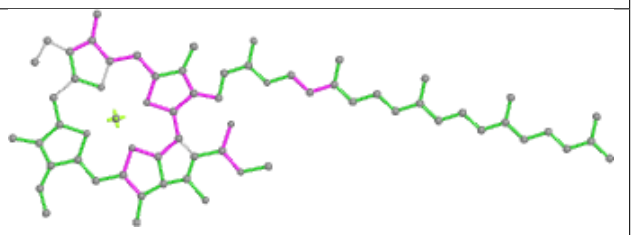

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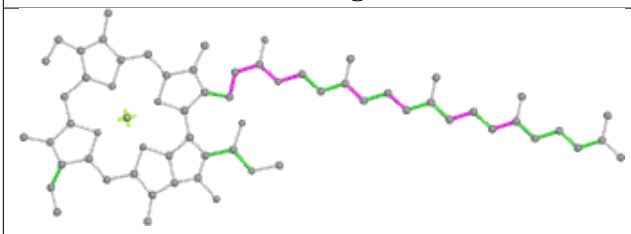

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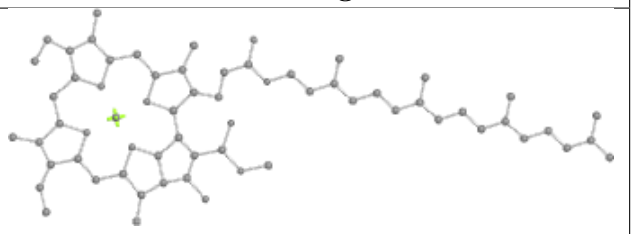
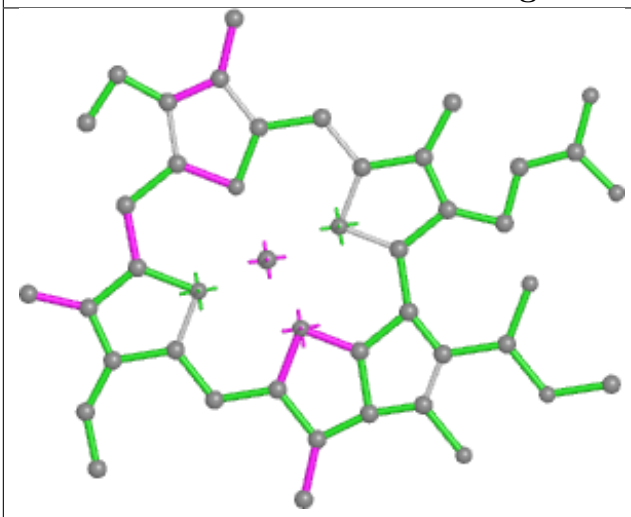


Rings

Ligand CLA 38 311



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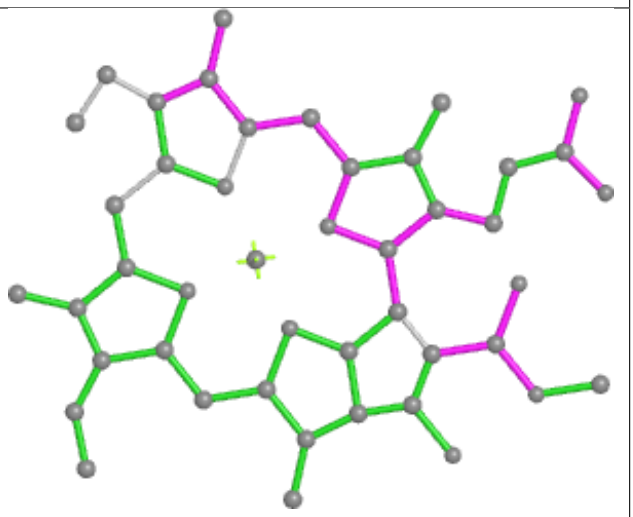

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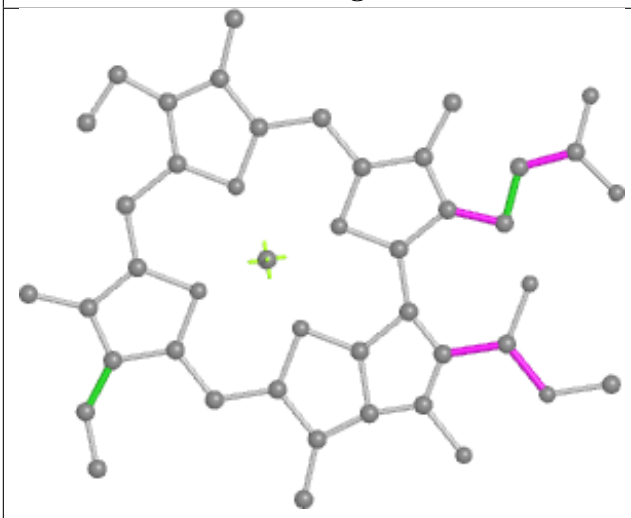

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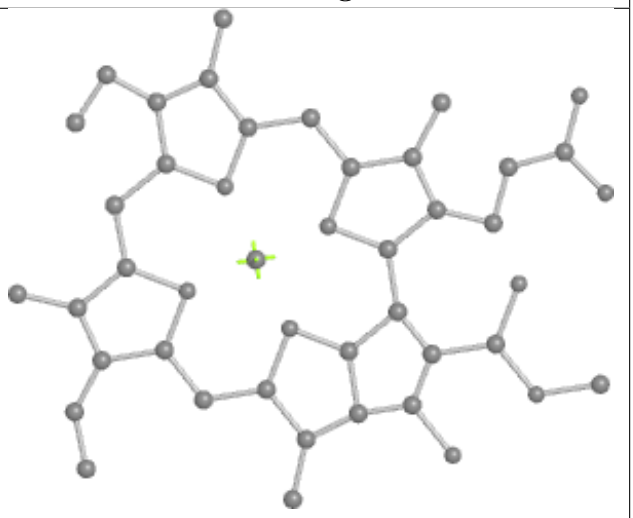
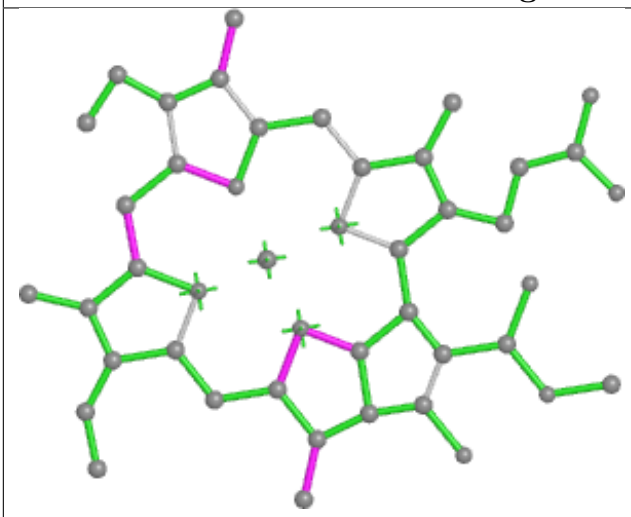


Rings

Ligand CLA 15 305



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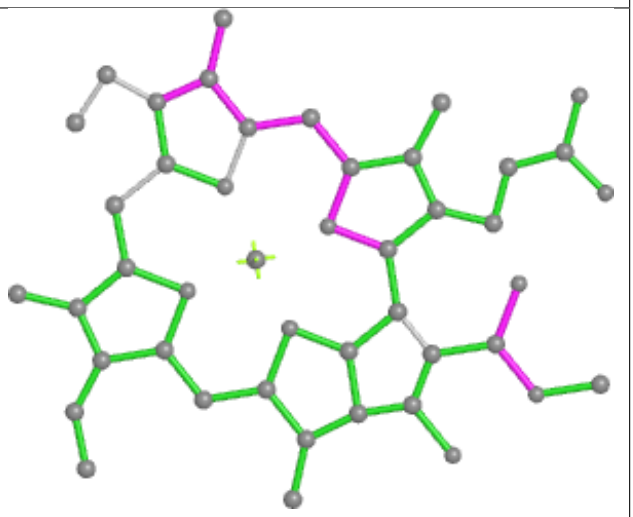

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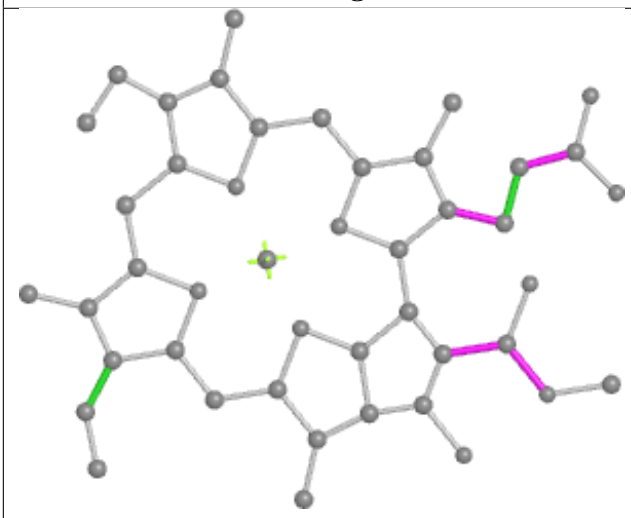

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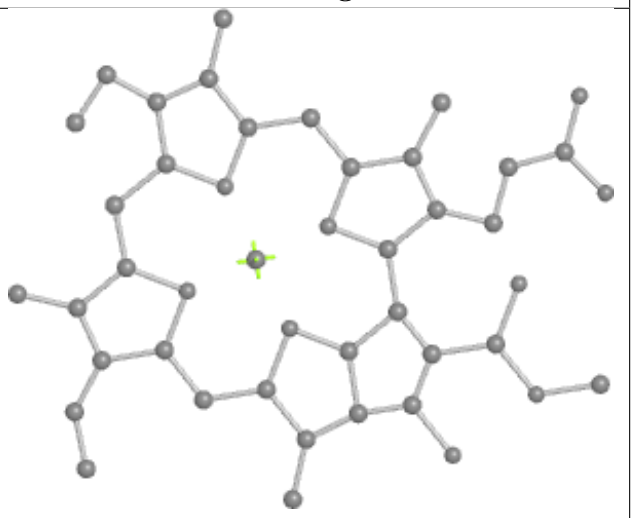
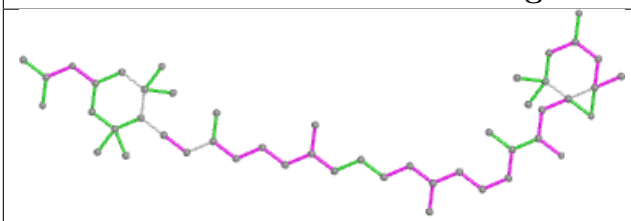


Rings

Ligand A86 11 313



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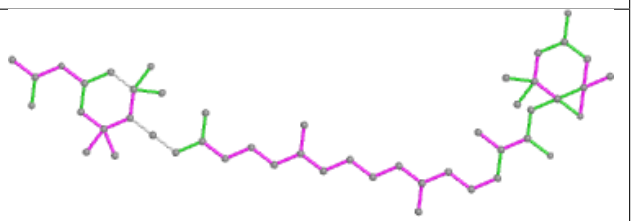

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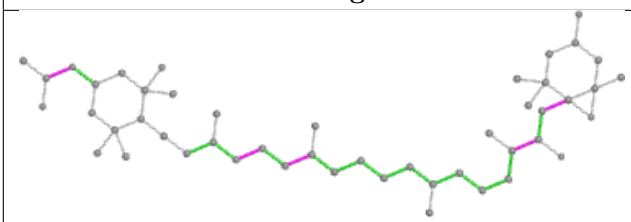

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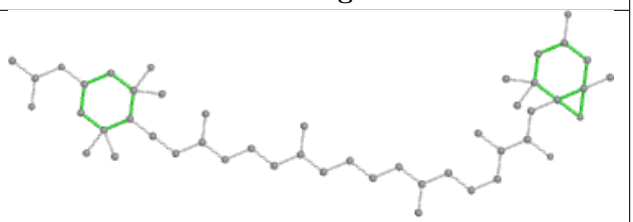
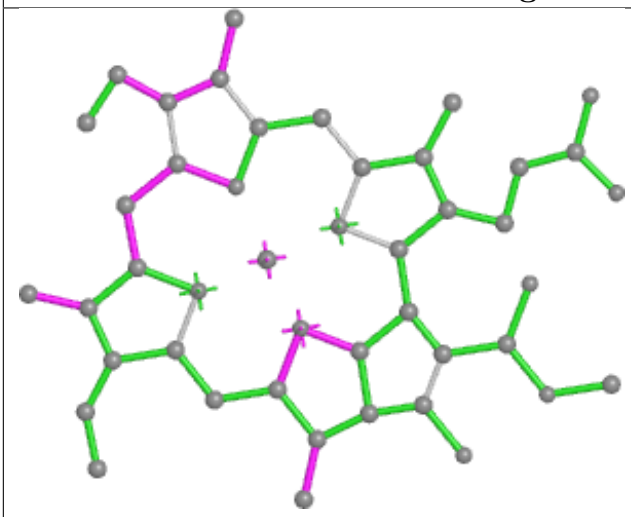


Rings

Ligand CLA 32 312



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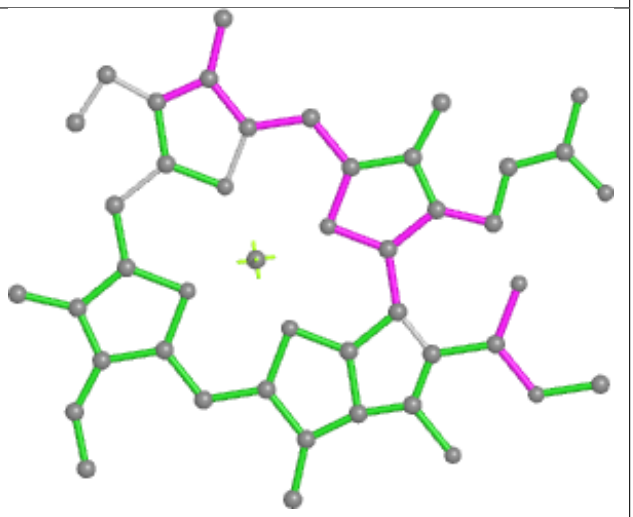

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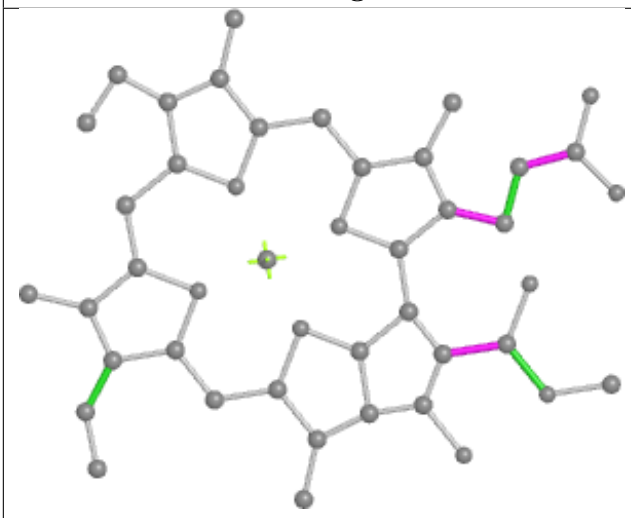

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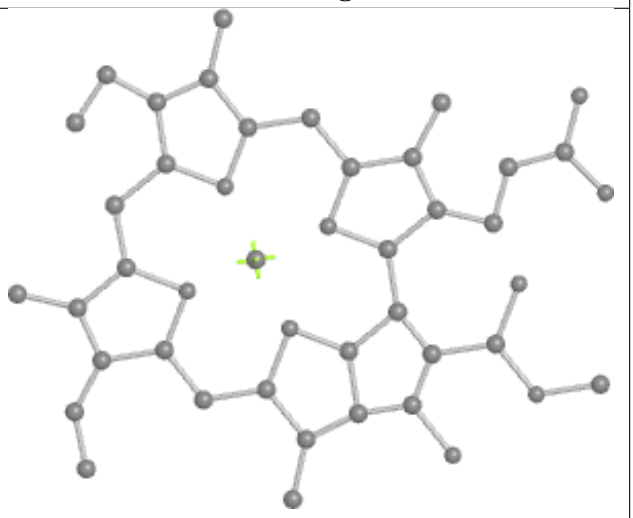
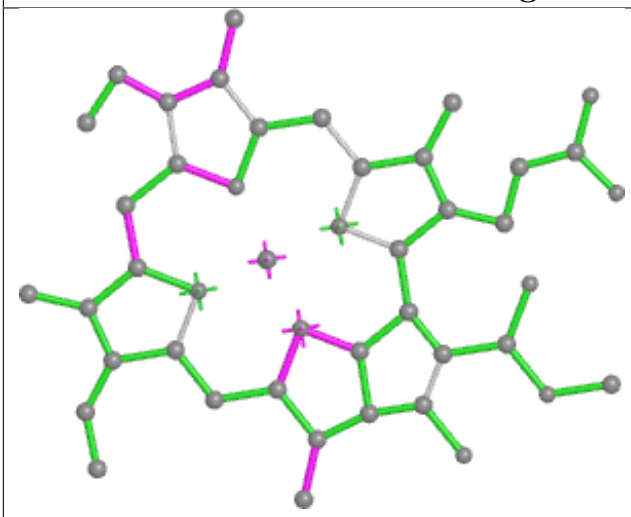


Rings

Ligand CLA 37 307



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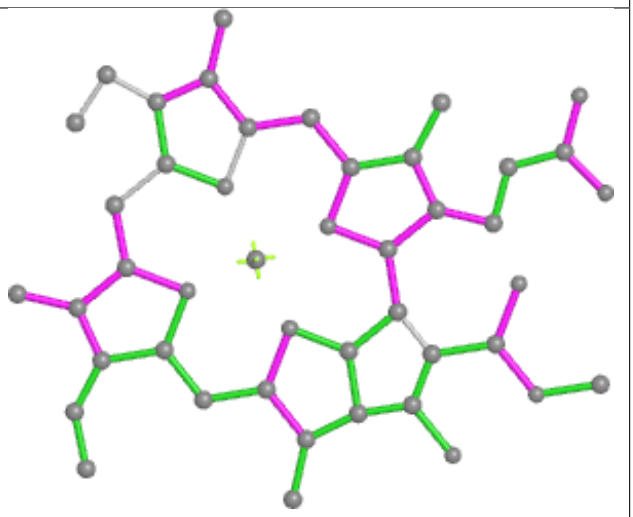

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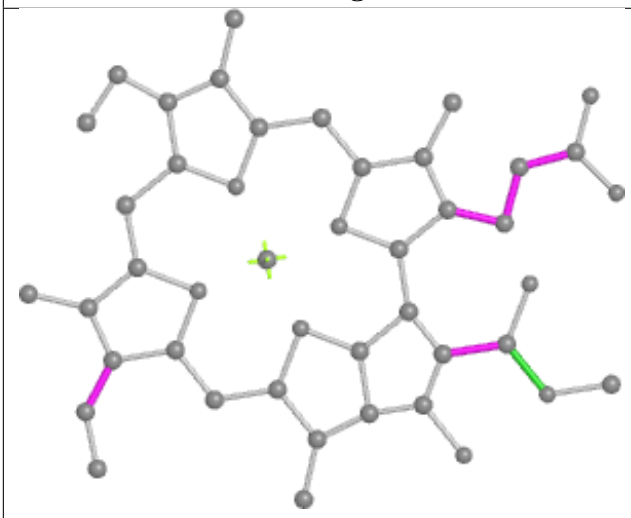

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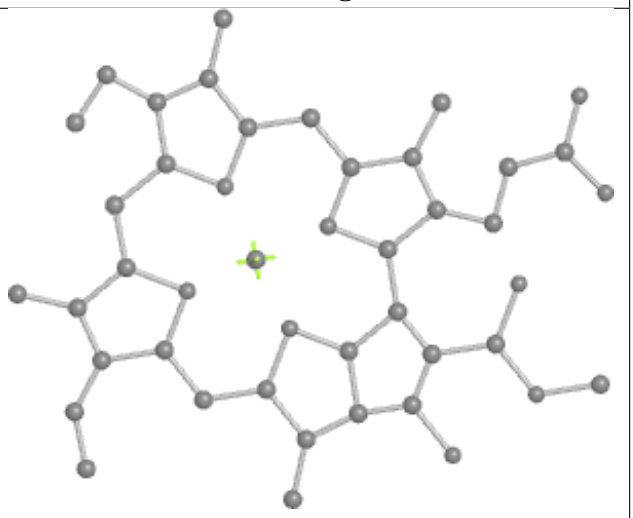
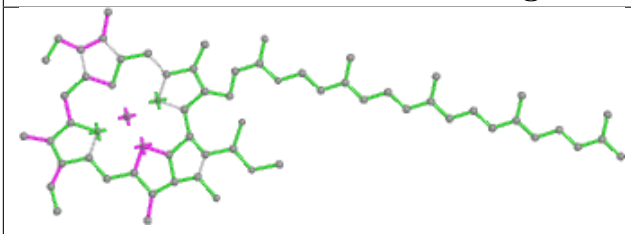


Rings

Ligand CLA m 101



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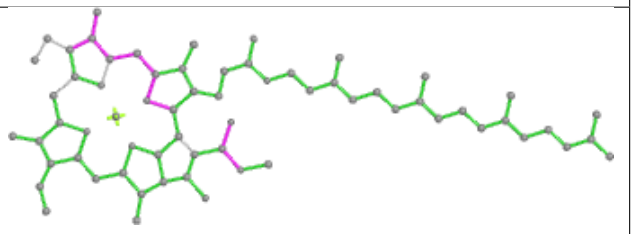

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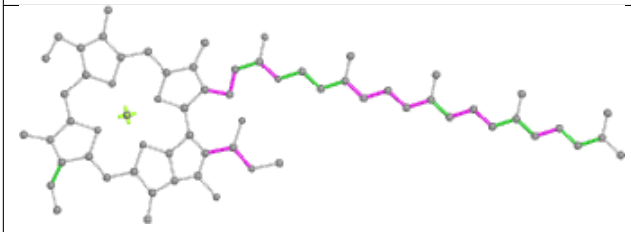

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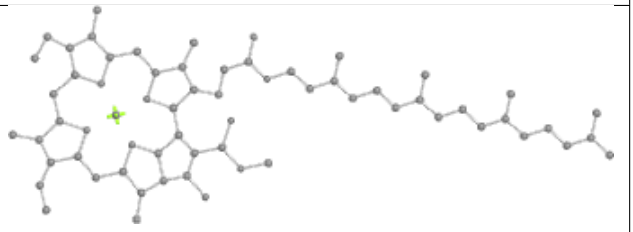
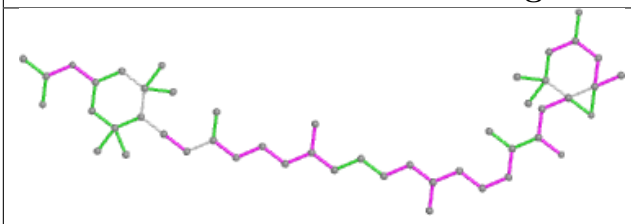


Rings

Ligand A86 17 316



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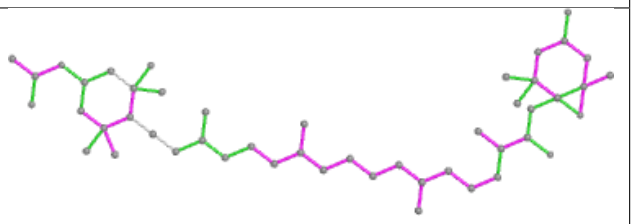

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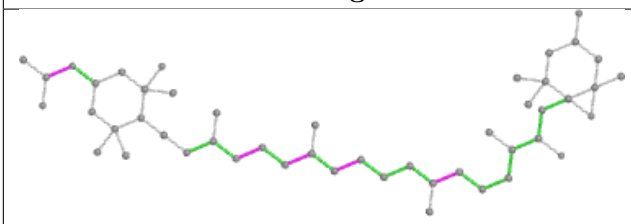

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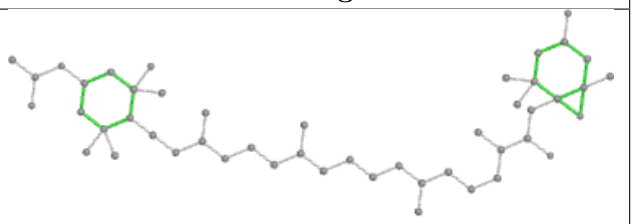
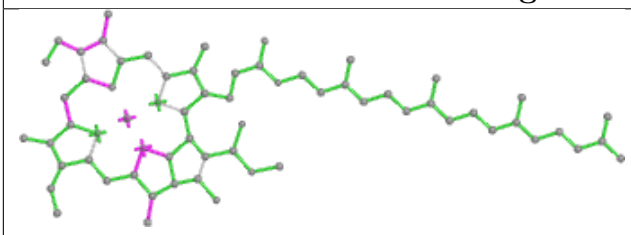


Rings

Ligand CLA 16 301



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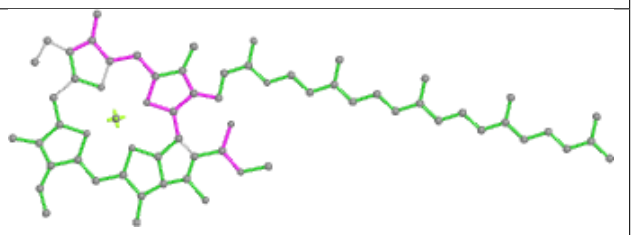

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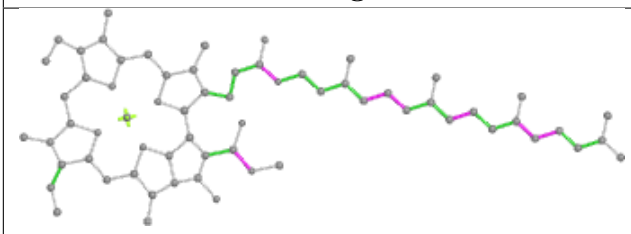

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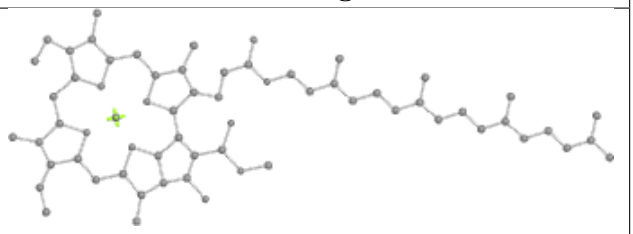
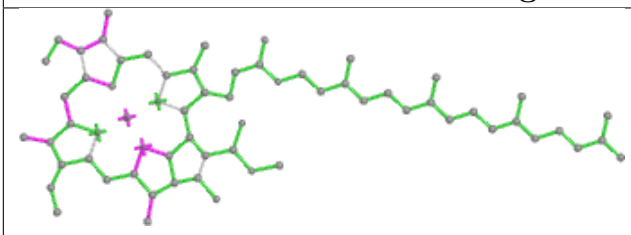


Rings

Ligand CLA 34 302



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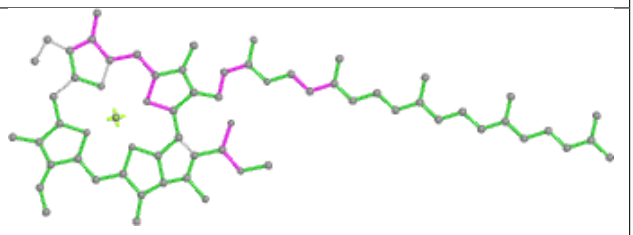

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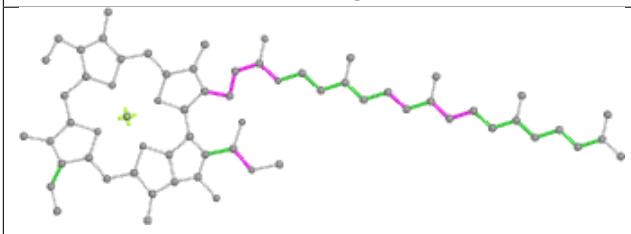

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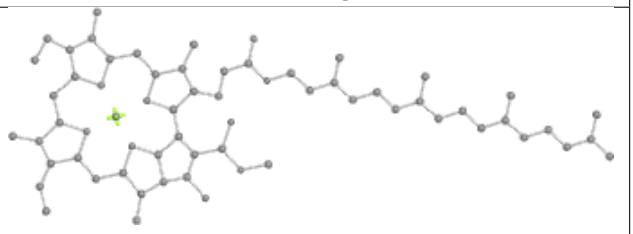
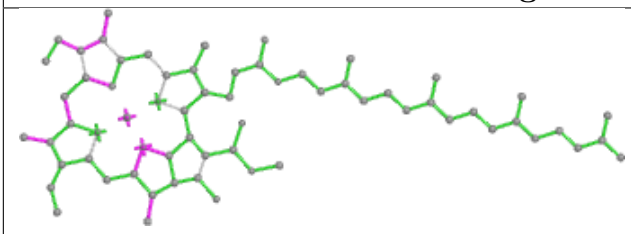


Rings

Ligand CLA 20 204



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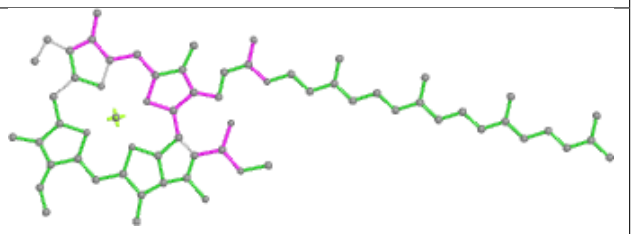

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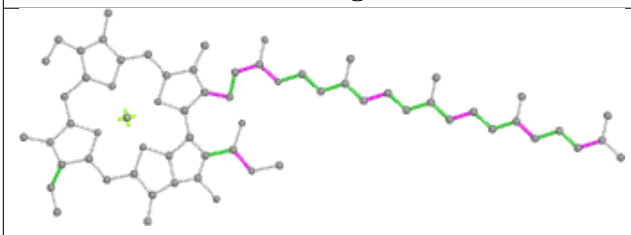

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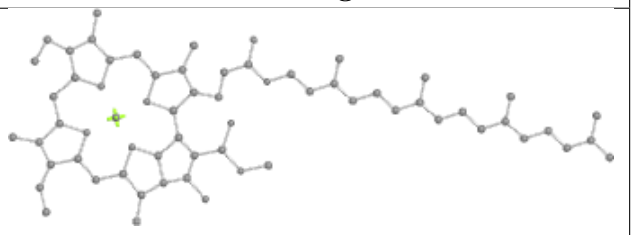
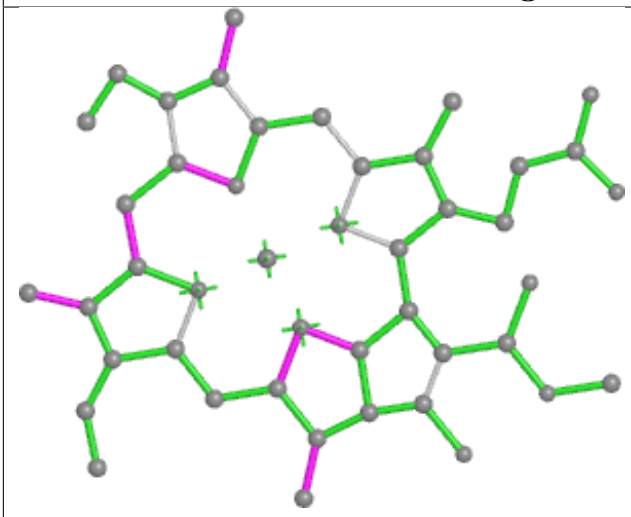


Rings

Ligand CLA 35 304



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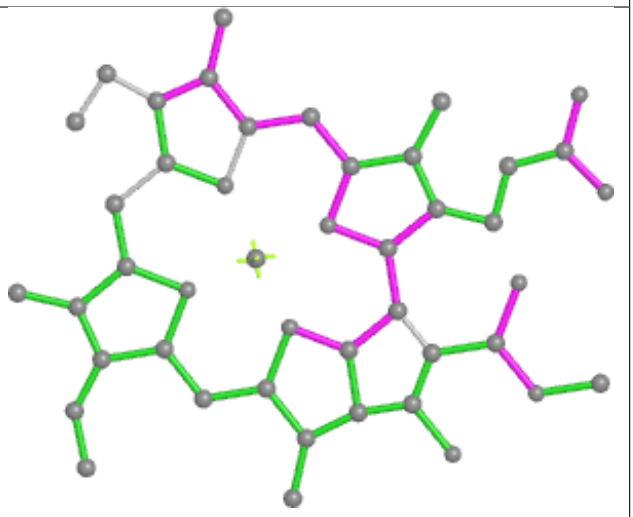

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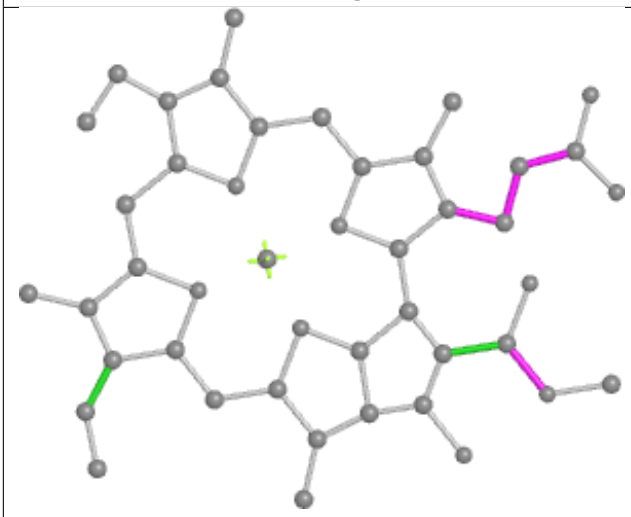

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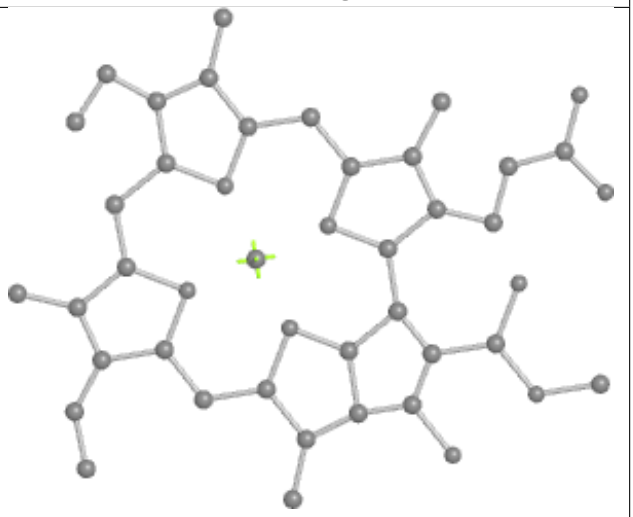
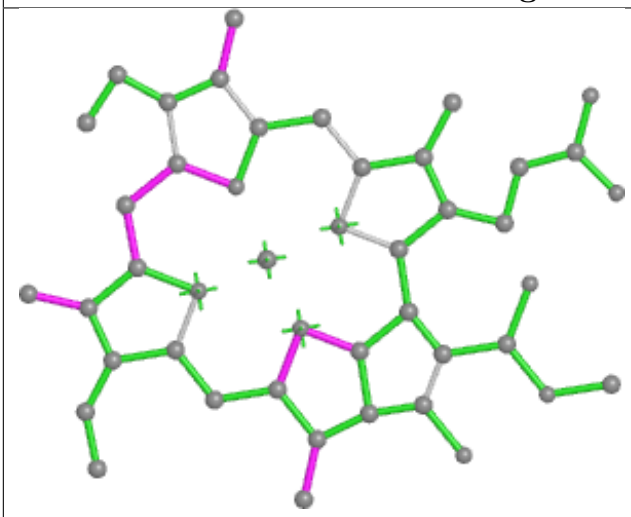


Rings

Ligand CLA 18 304



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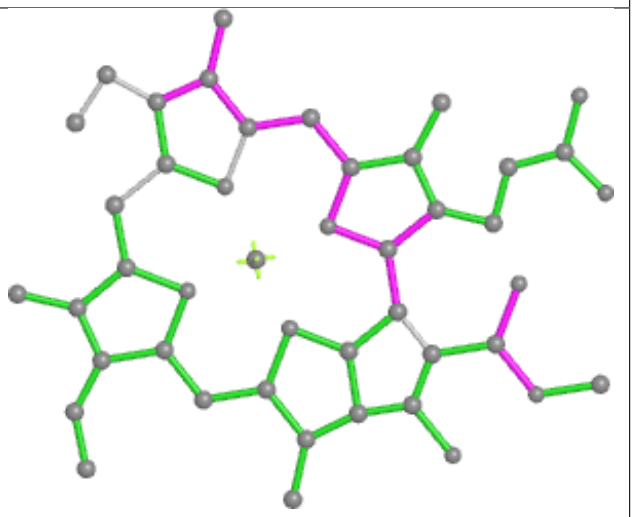
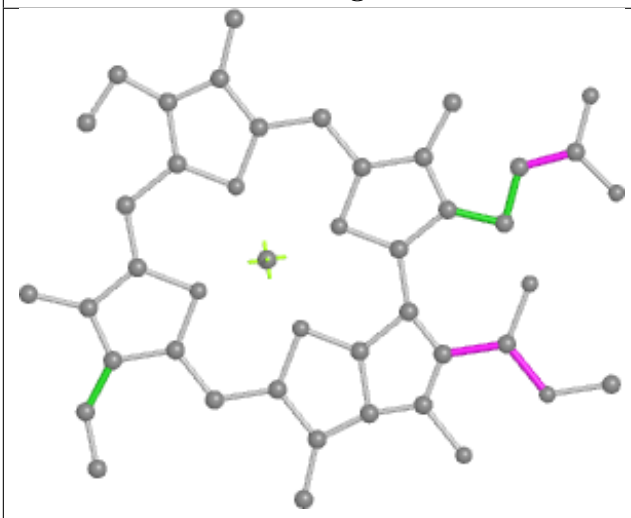


Bond angles



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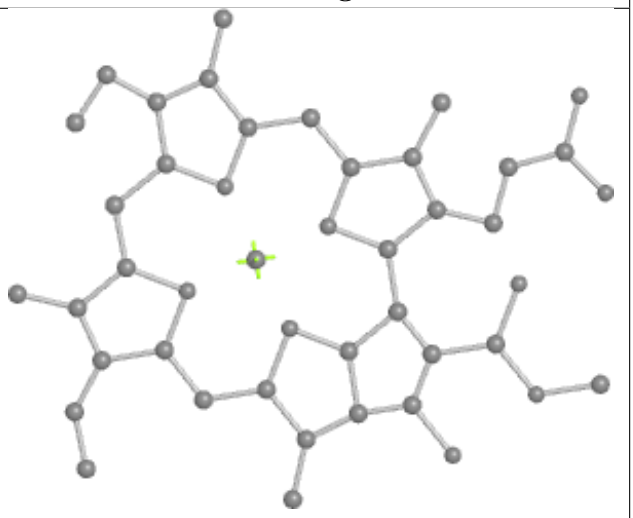
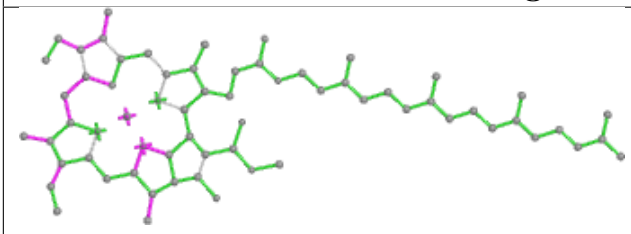
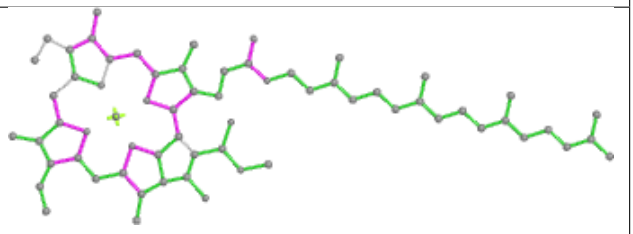


Rings

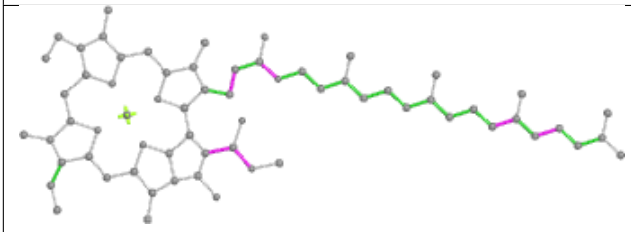
Ligand CLA C 503



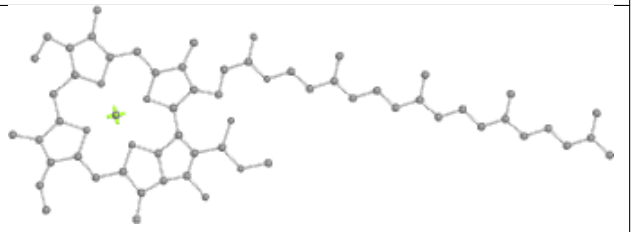
Bond lengths



Bond angles

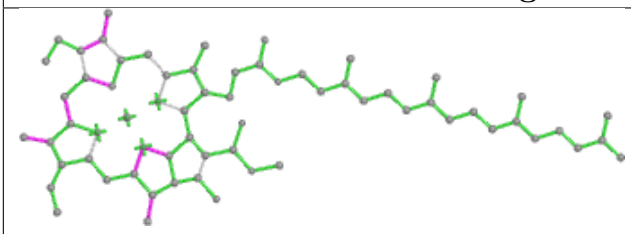


Torsions



Rings

Ligand CLA 18 305



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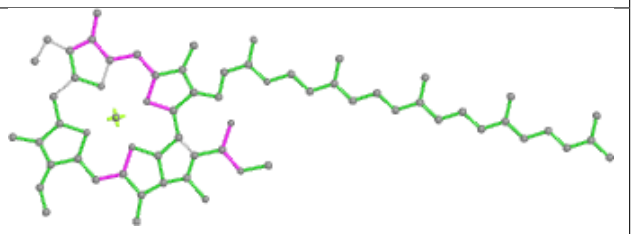

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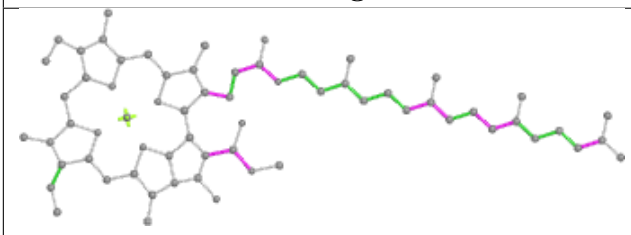

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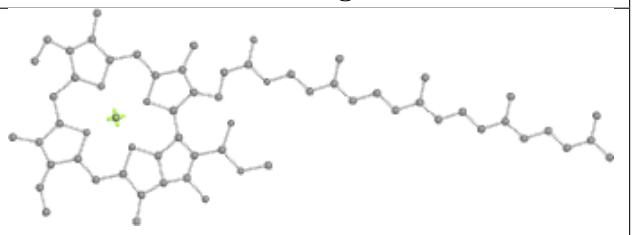
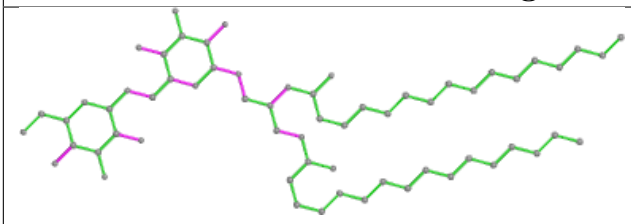


Rings

Ligand DGD C 517



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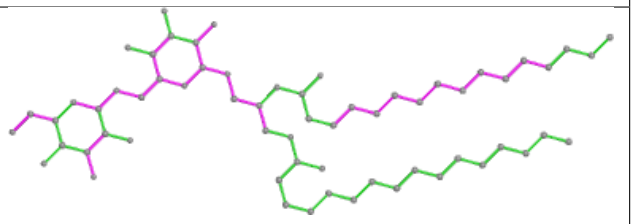

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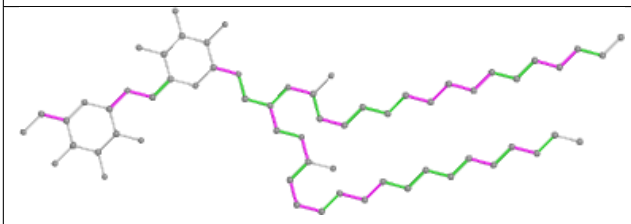

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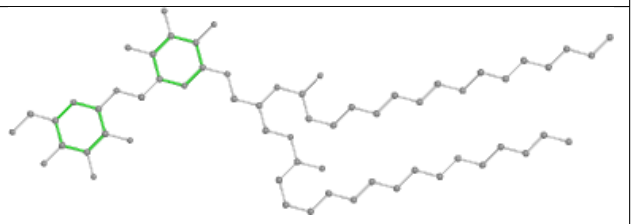
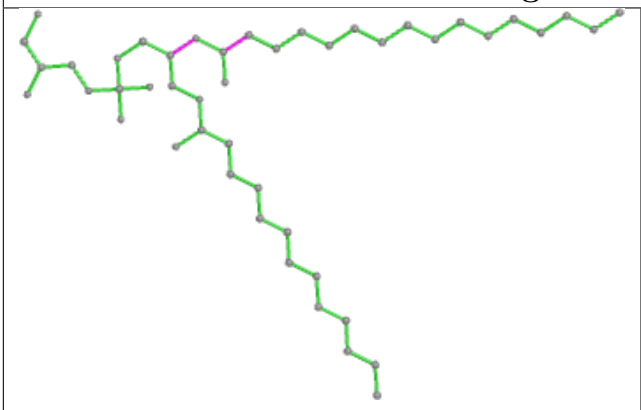


Rings

Ligand LHG A 408



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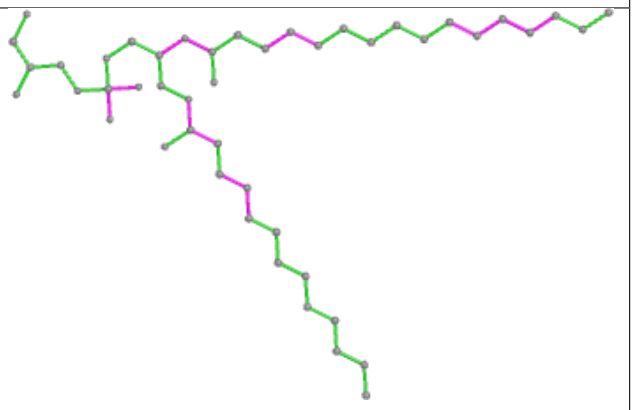

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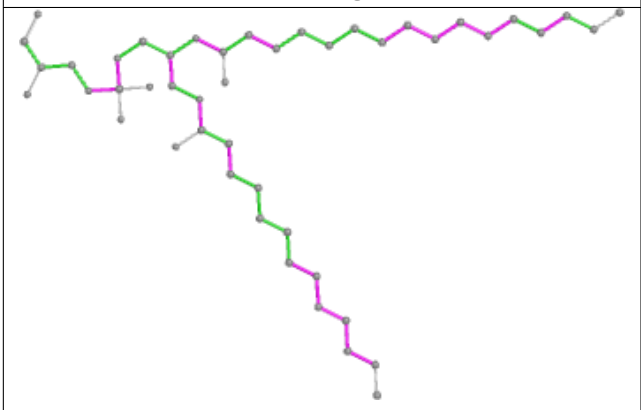

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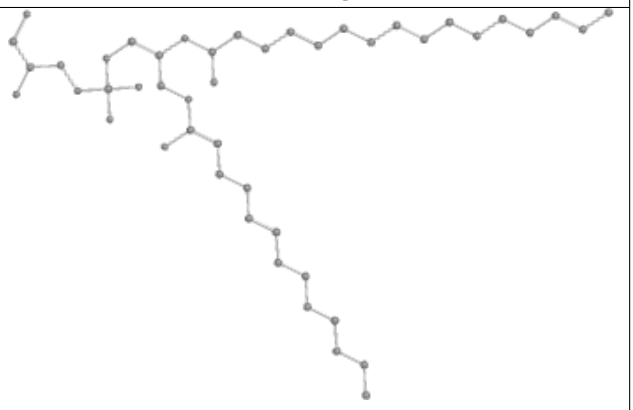
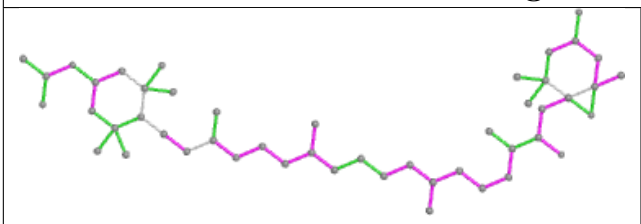


Rings

Ligand A86 15 312



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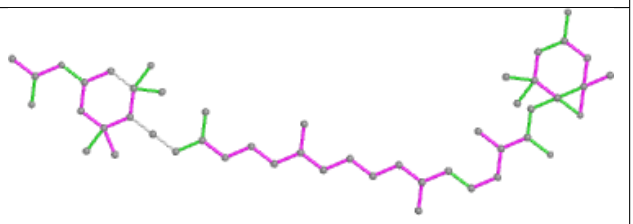

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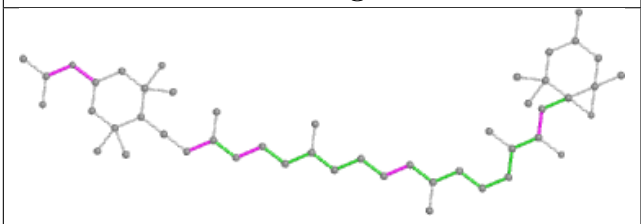

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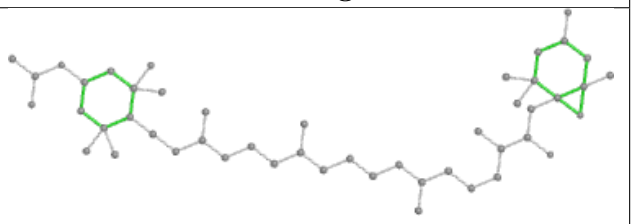
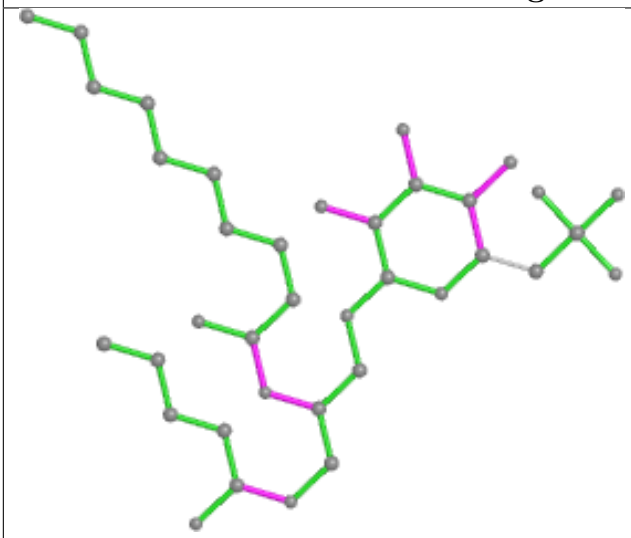


Rings

Ligand SQD b 620



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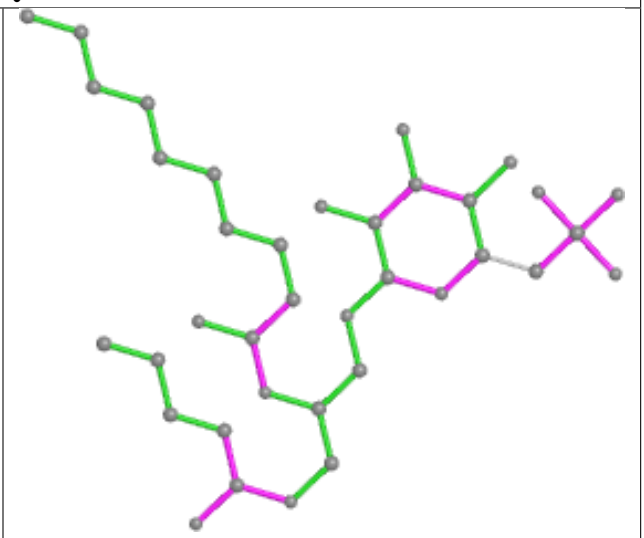
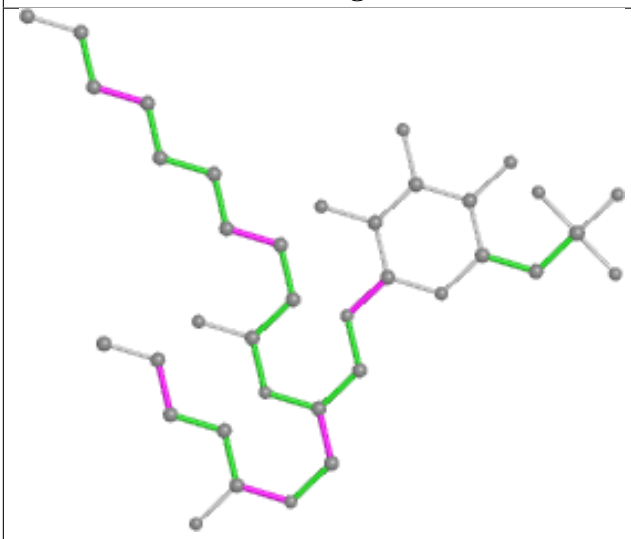


Bond angles



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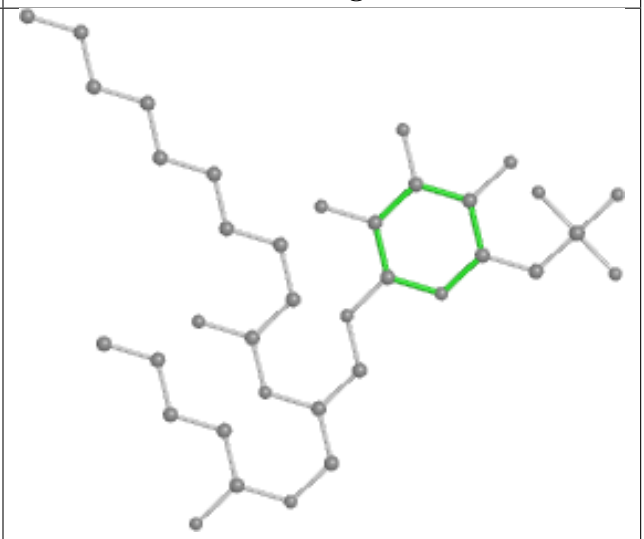
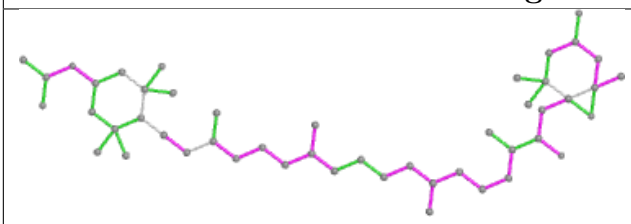


Rings

Ligand A86 17 312



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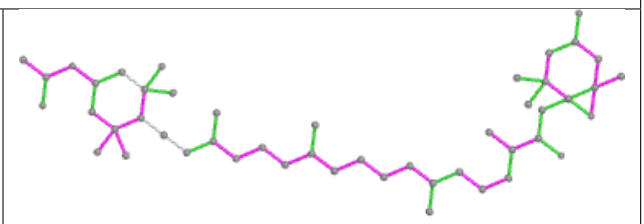
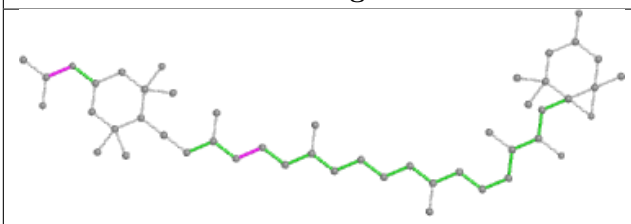


Bond angles



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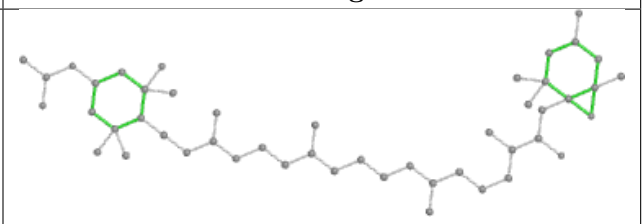
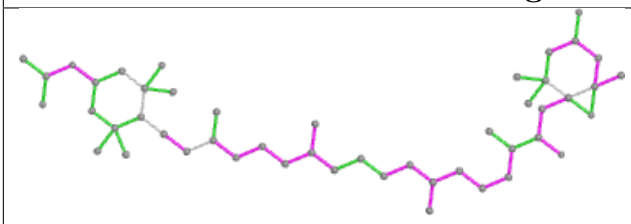


Rings

Ligand A86 37 312



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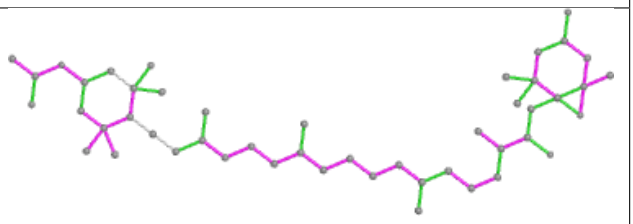

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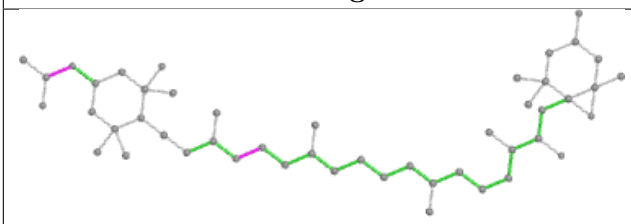

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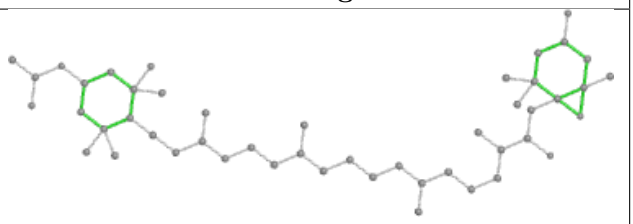
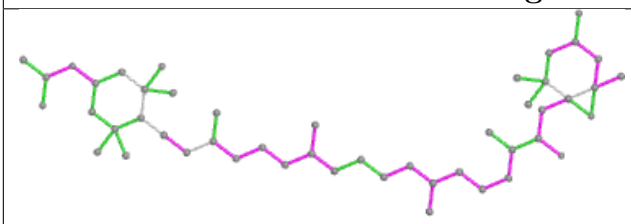


Rings

Ligand A86 11 314



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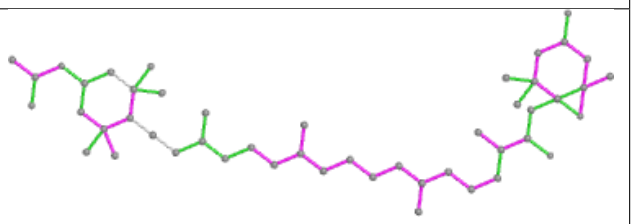

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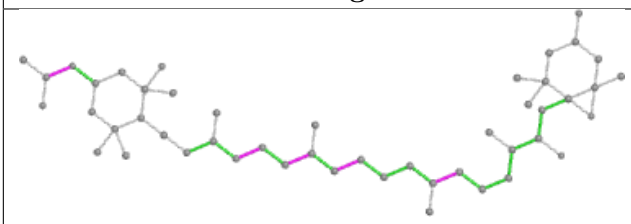

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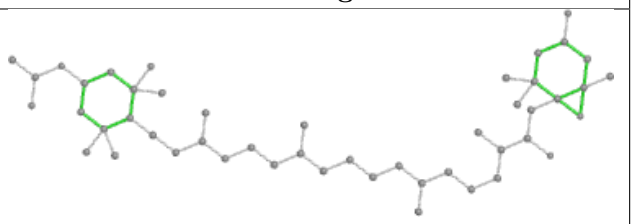
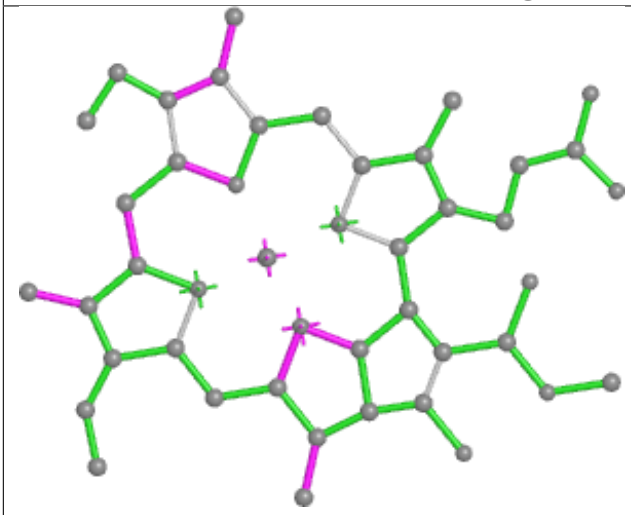


Rings

Ligand CLA 14 310



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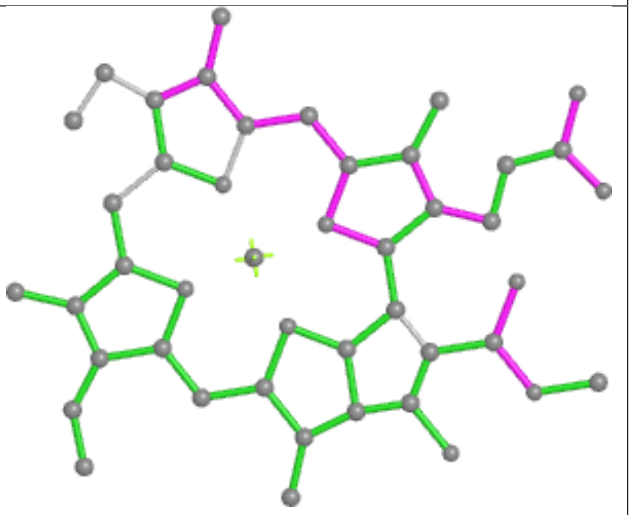

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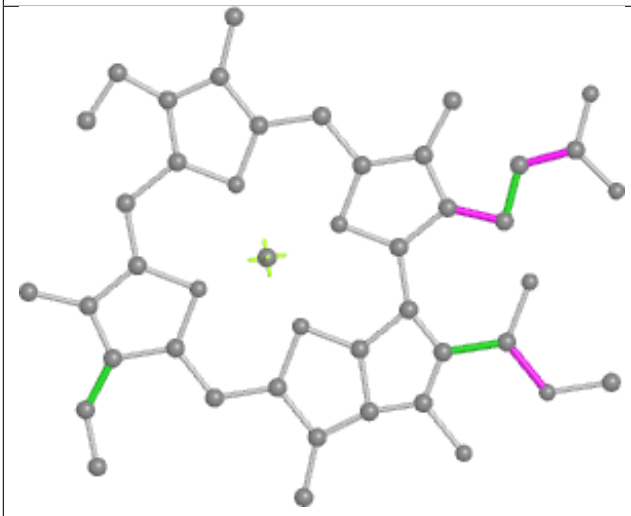

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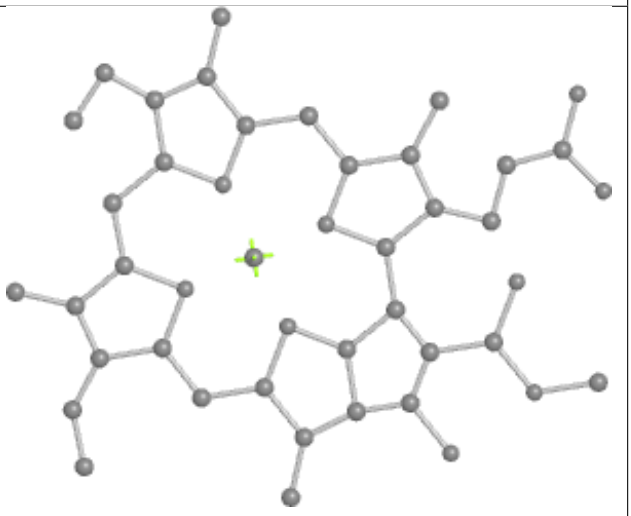
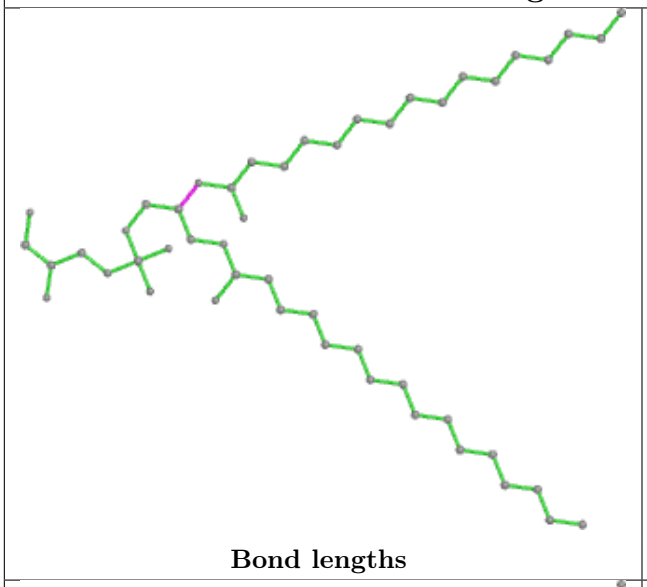


Rings

Ligand LHG d 409



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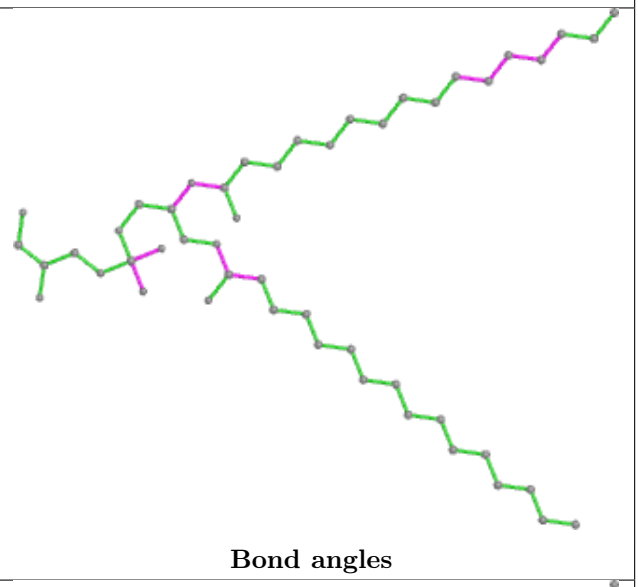

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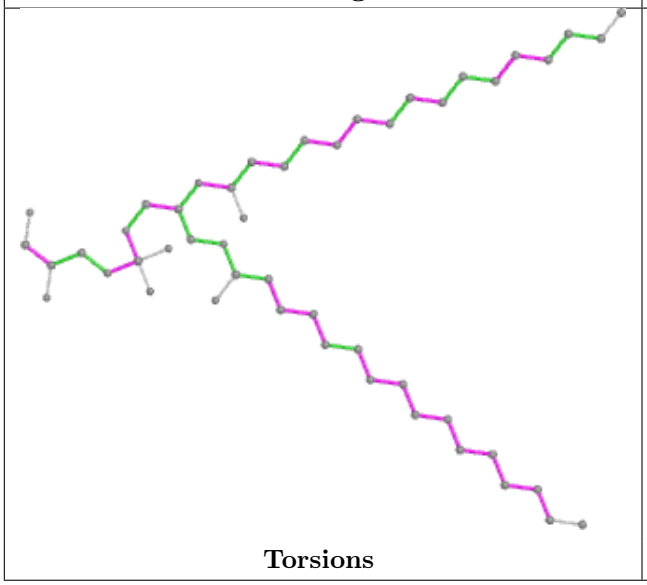

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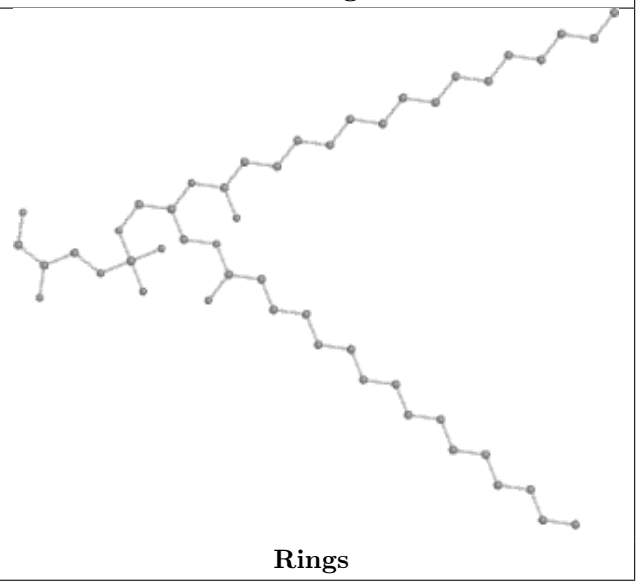
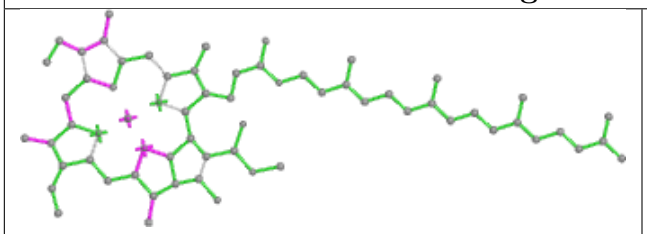


Rings

Ligand CLA 12 307



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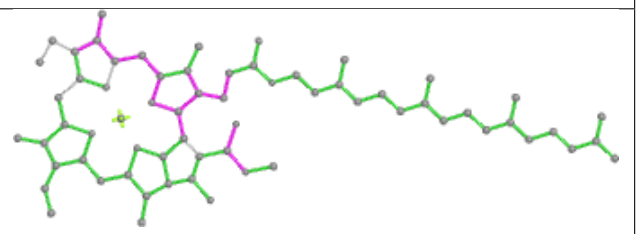

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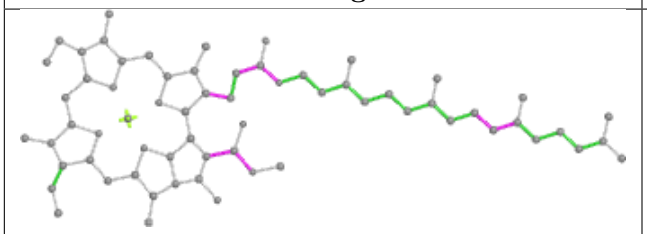

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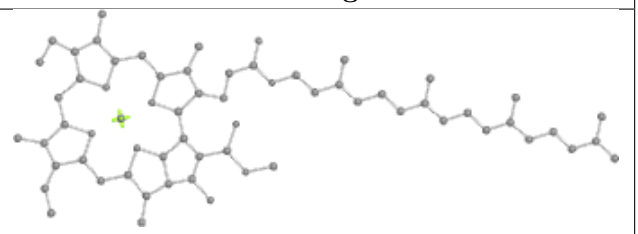
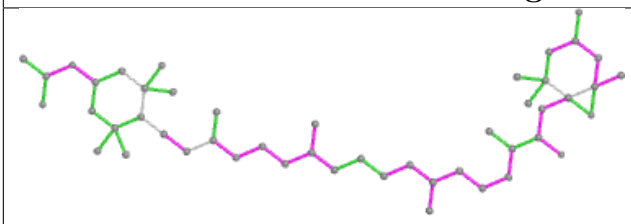


Rings

Ligand A86 18 313



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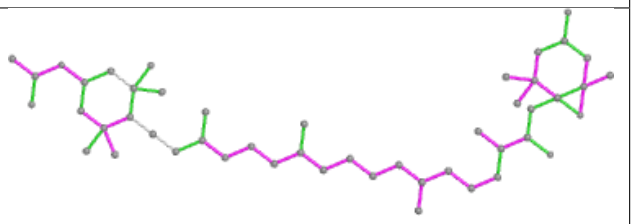
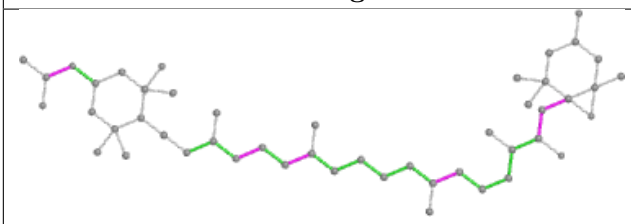


Bond angles



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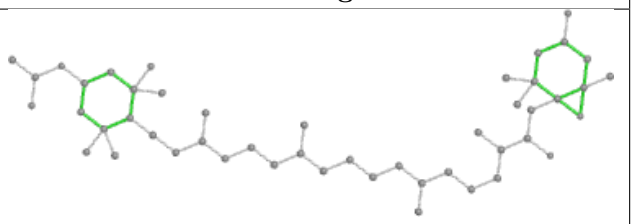
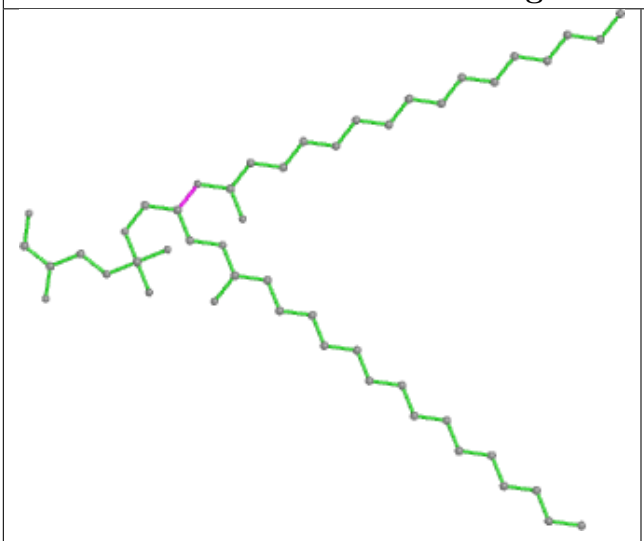


Rings

Ligand LHG b 621



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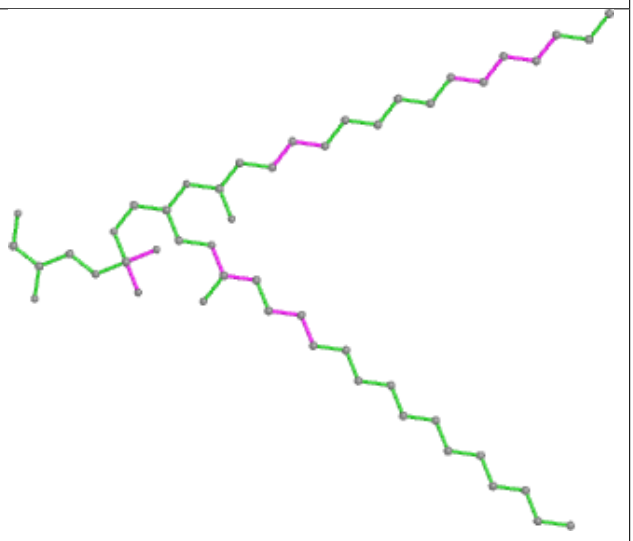
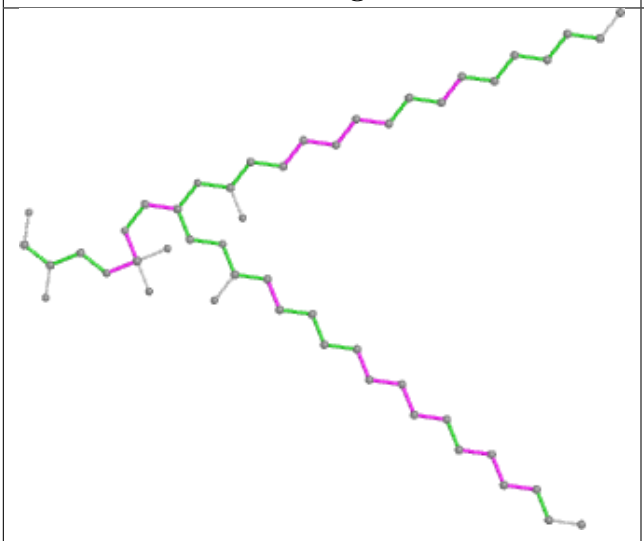
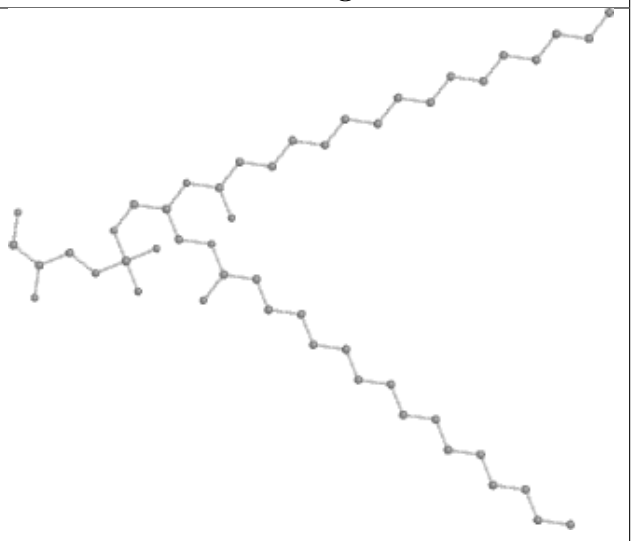


Bond angles

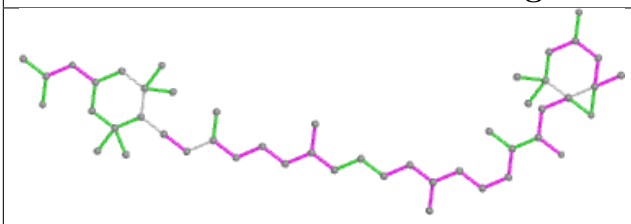


Torsions

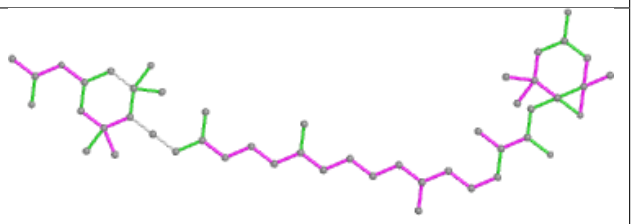


Rings

Ligand A86 15 310



Bond lengths



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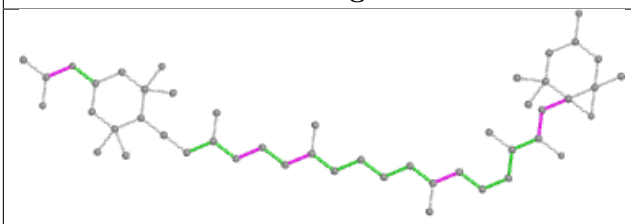
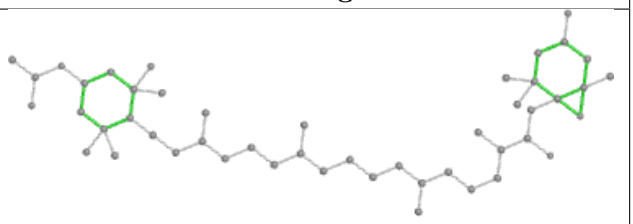
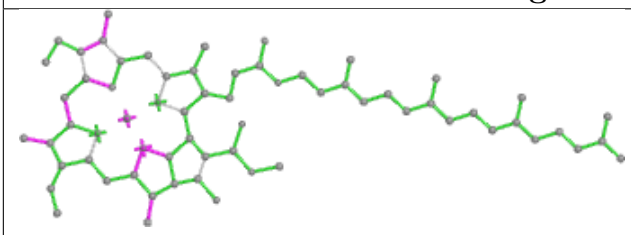


Torsions



Rings

Ligand CLA c 513



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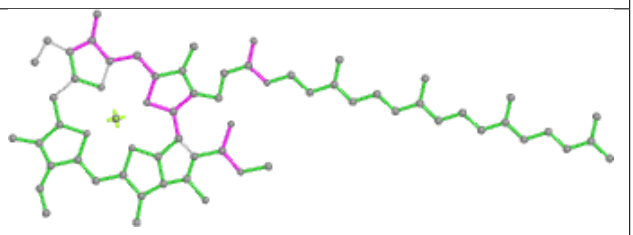

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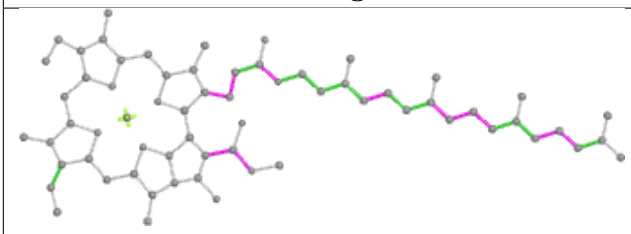

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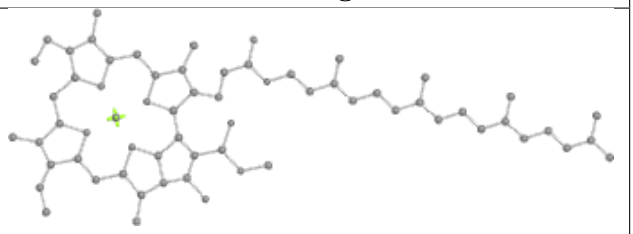
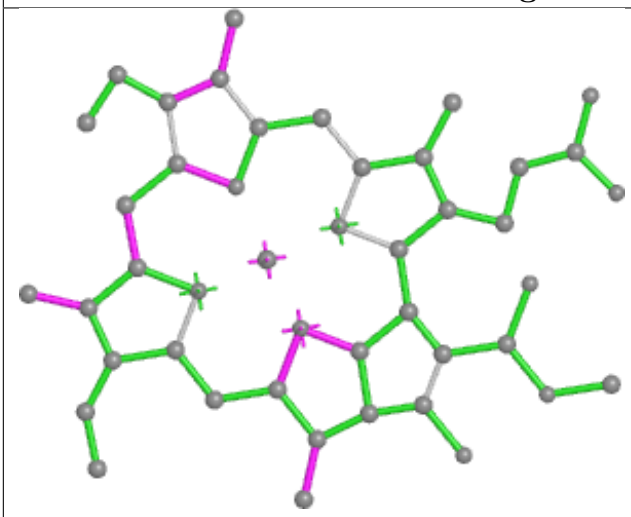


Rings

Ligand CLA 16 308



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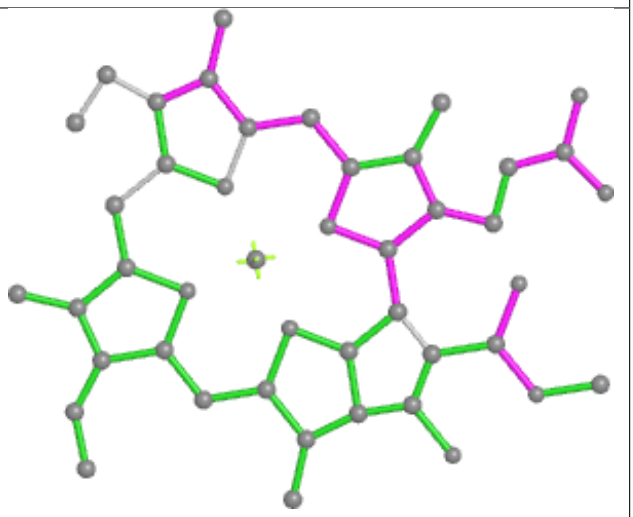

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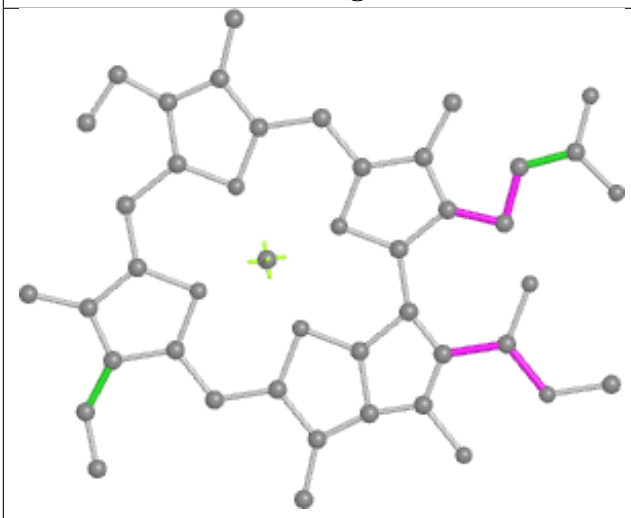

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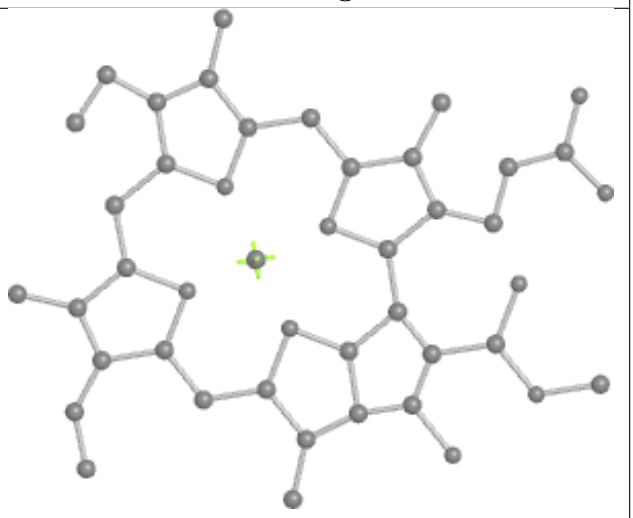
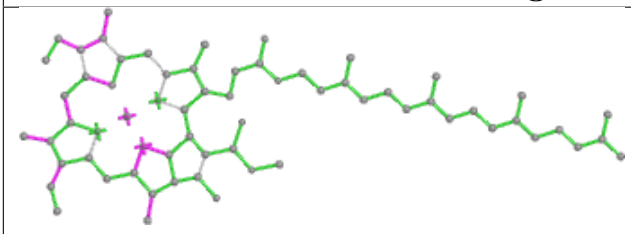


Rings

Ligand CLA b 610



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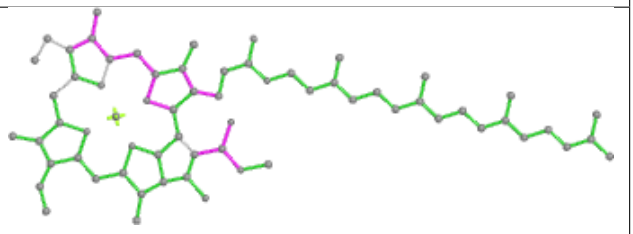

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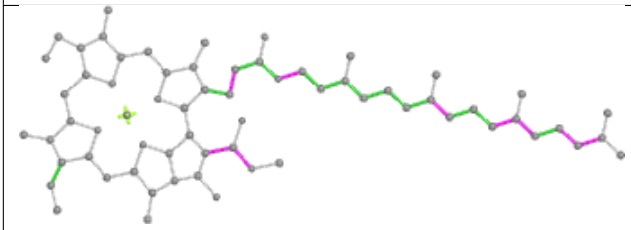

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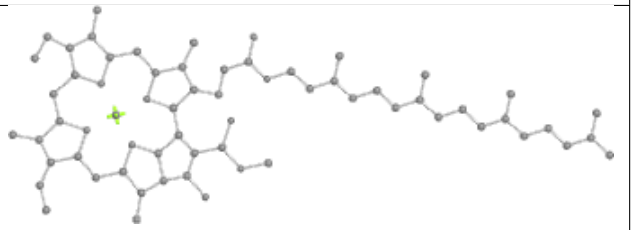
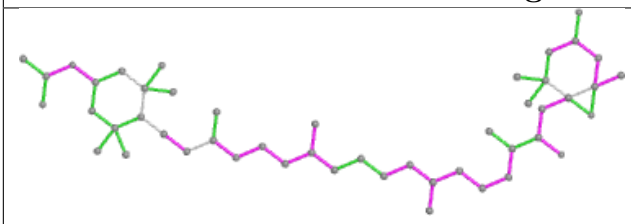


Rings

Ligand A86 34 311



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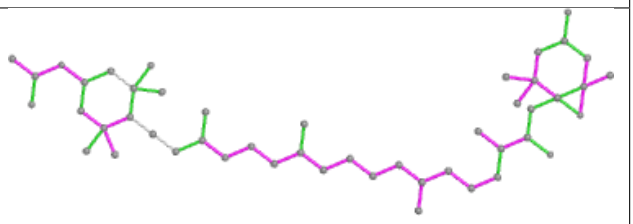

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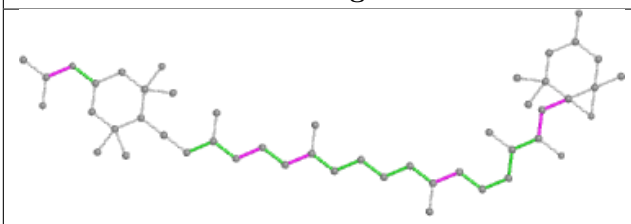

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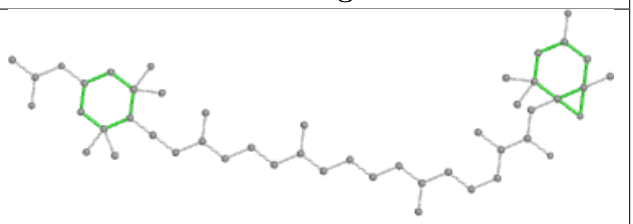
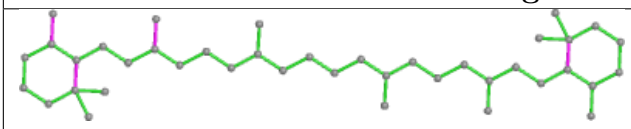


Rings

Ligand BCR Y 101



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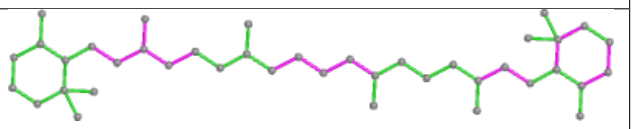

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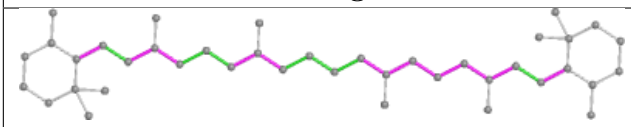

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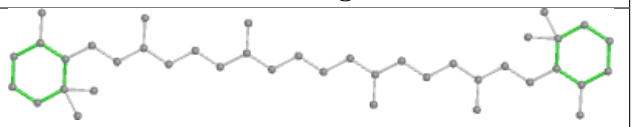
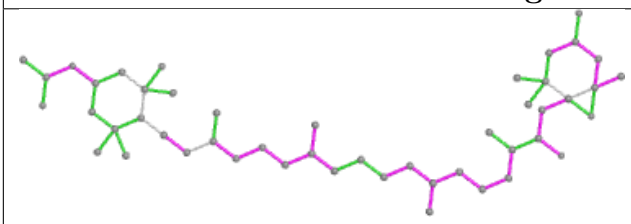


Rings

Ligand A86 38 302



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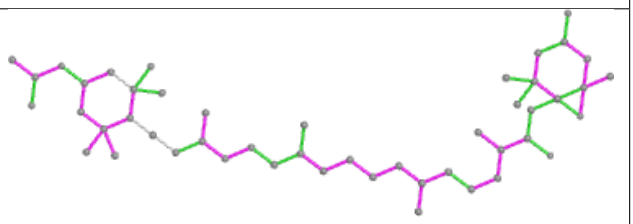

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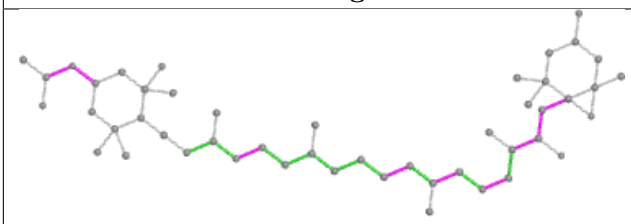

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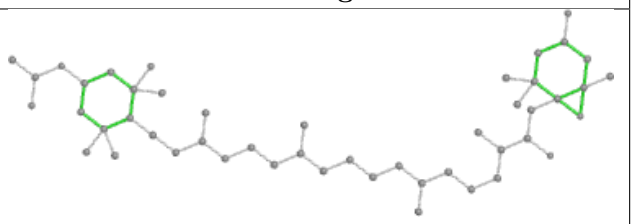
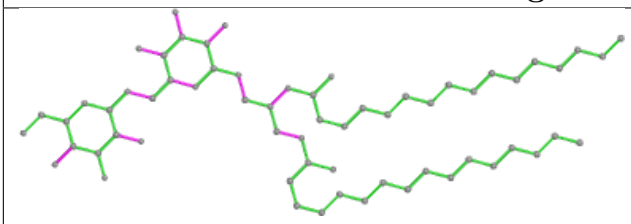


Rings

Ligand DGD j 101



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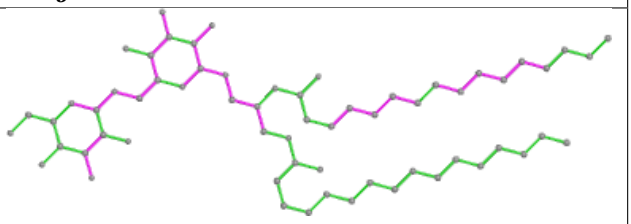

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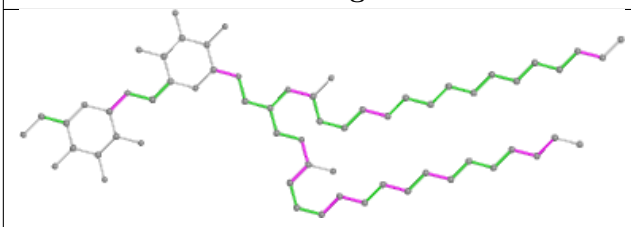

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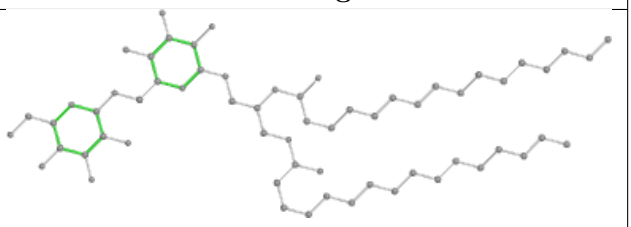
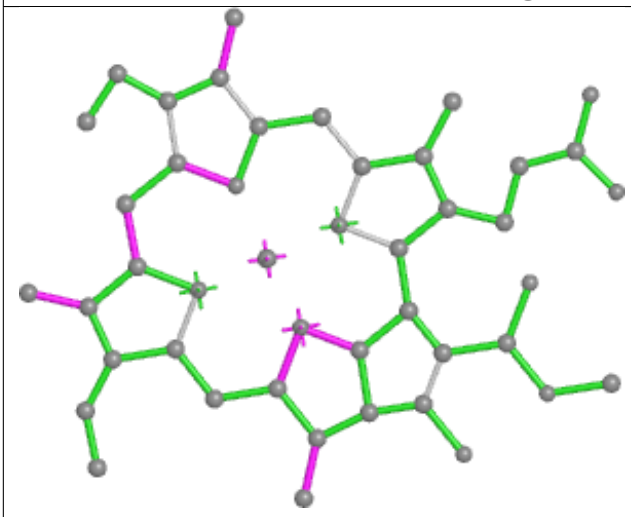


Rings

Ligand CLA 13 306



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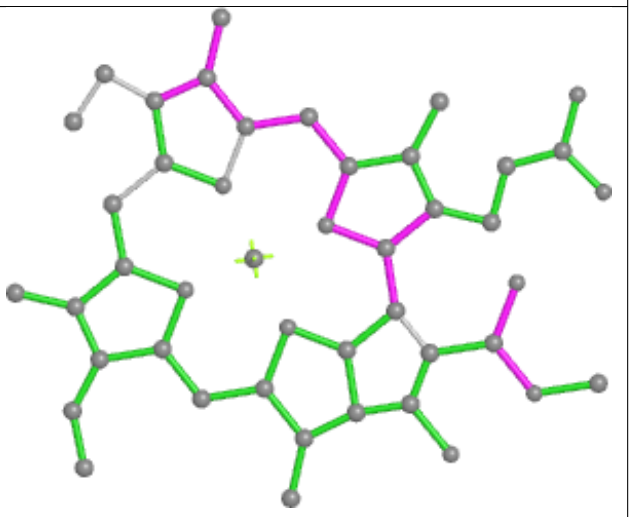

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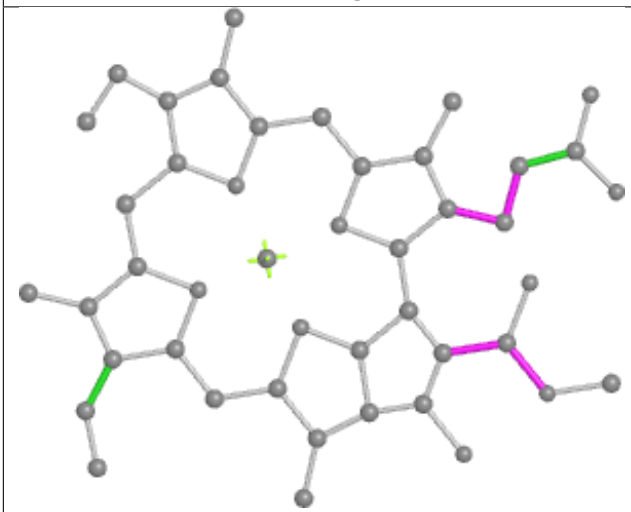

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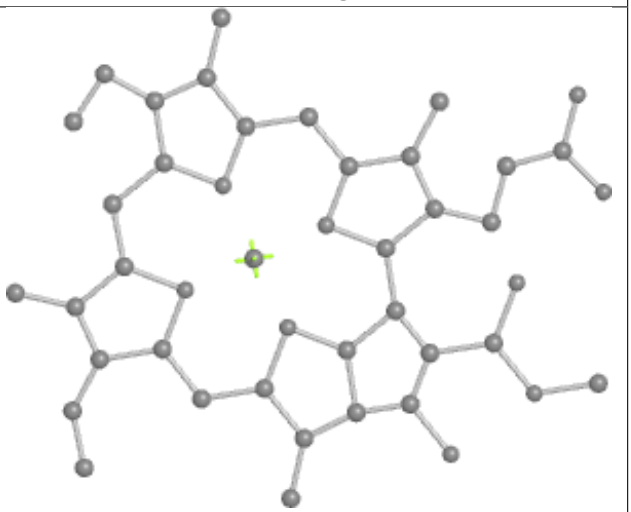
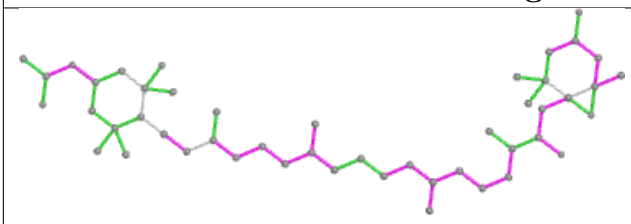


Rings

Ligand A86 14 312



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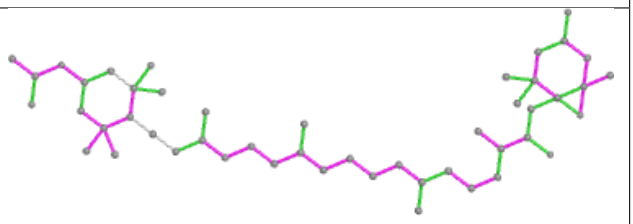

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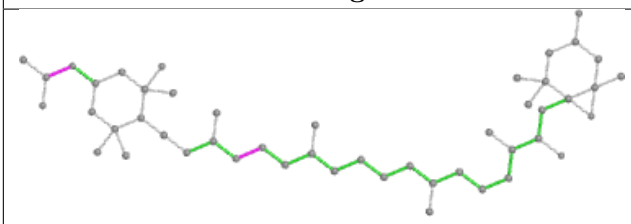

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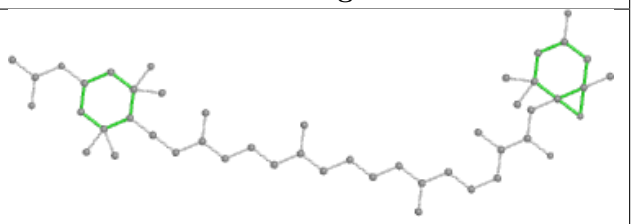
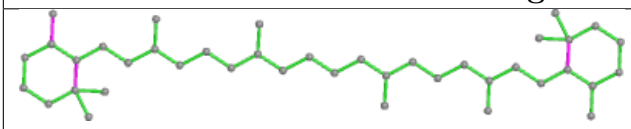


Rings

Ligand BCR c 520



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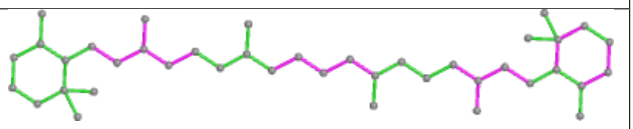

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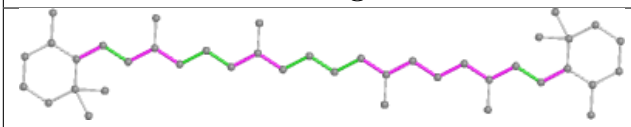

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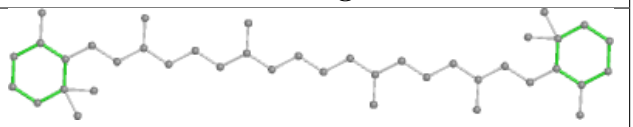
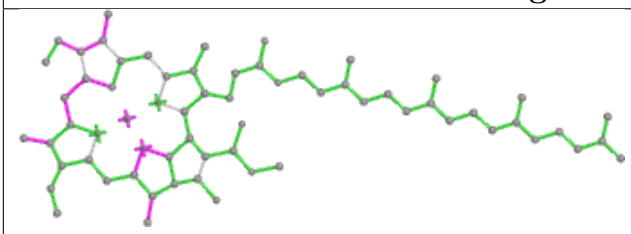


Rings

Ligand CLA c 522



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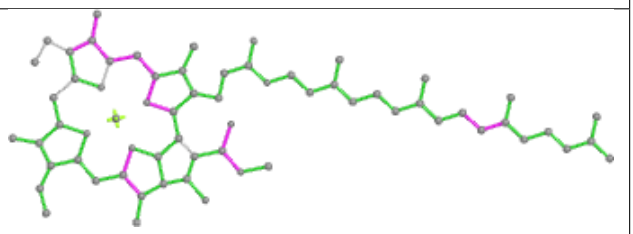
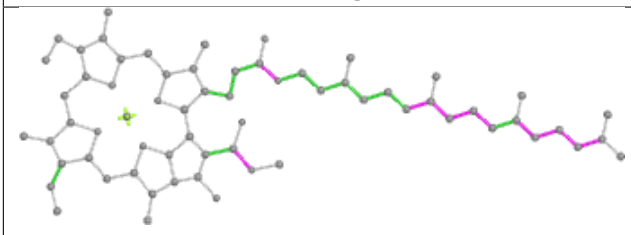


Bond angles



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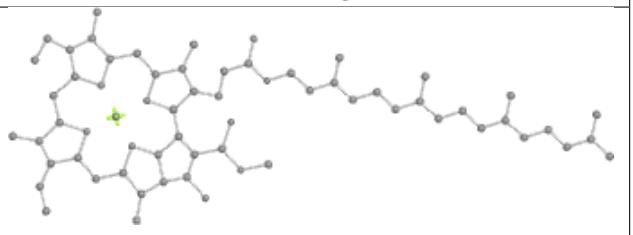
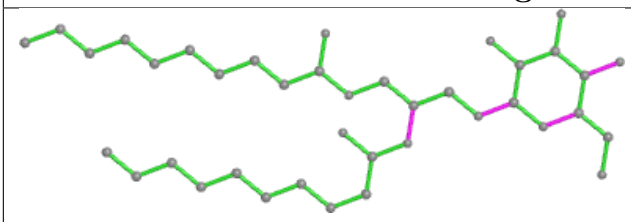


Rings

Ligand LMG 32 301



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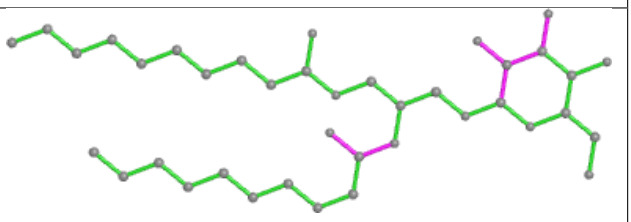

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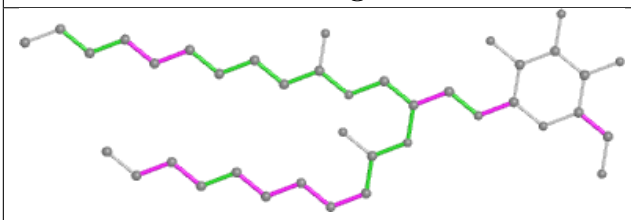

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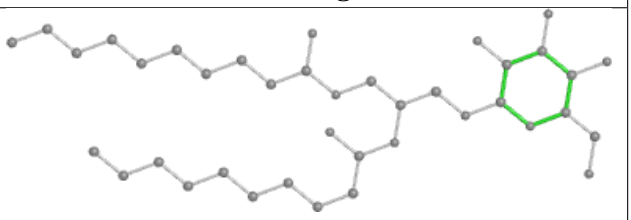
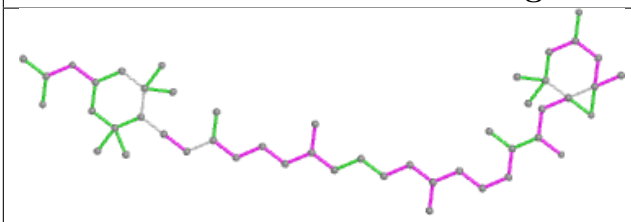


Rings

Ligand A86 12 316



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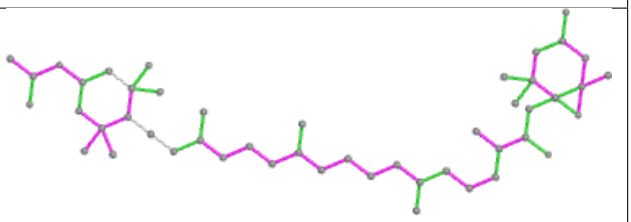

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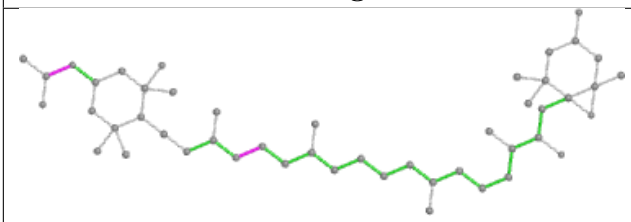

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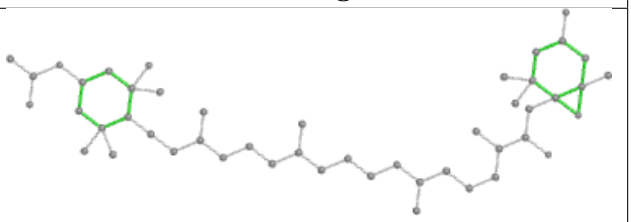
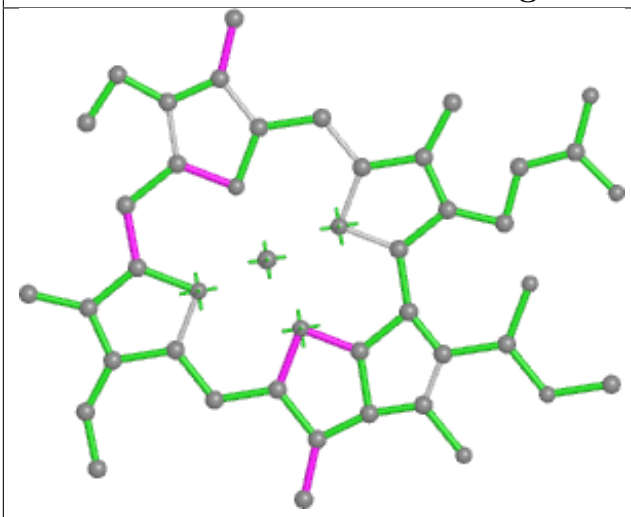
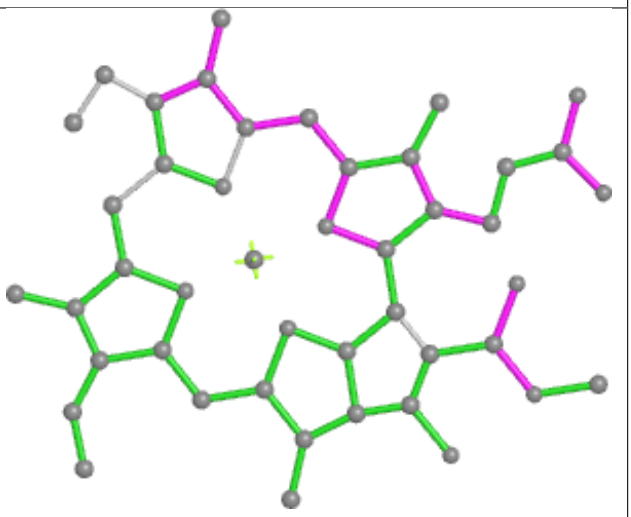


Rings

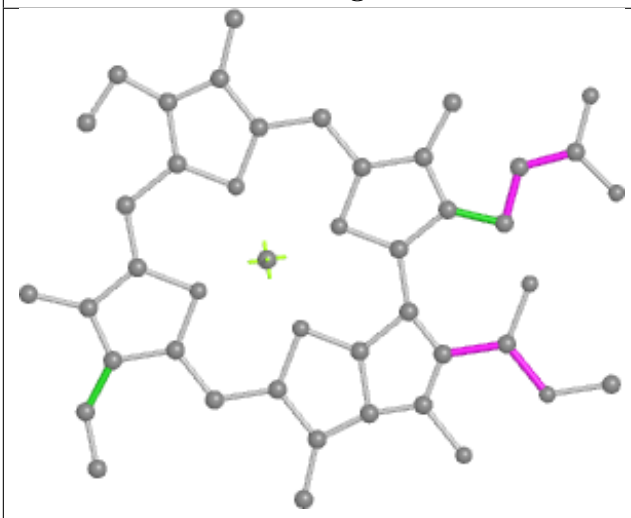
Ligand CLA 18 307



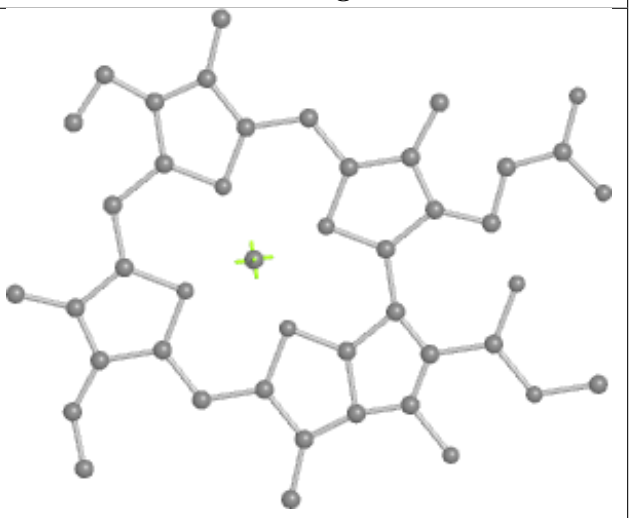
Bond lengths



Bond angles

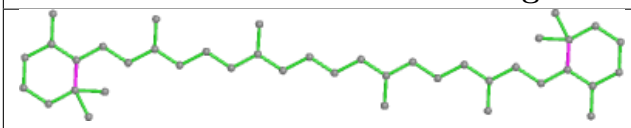


Torsions



Rings

Ligand BCR A 409



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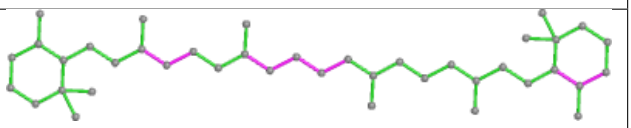

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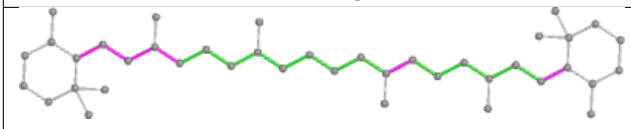
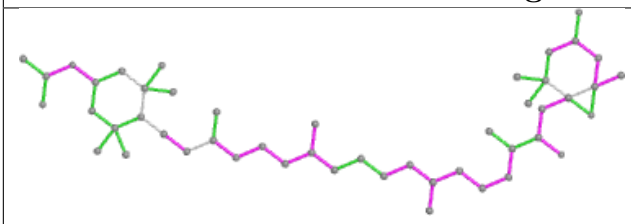


Torsions

Rings

Ligand A86 14 311



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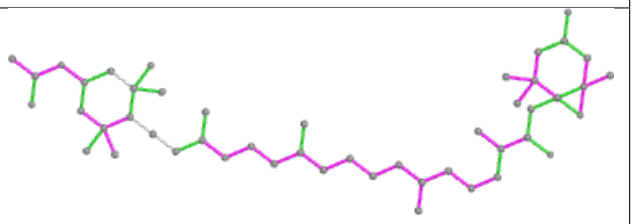

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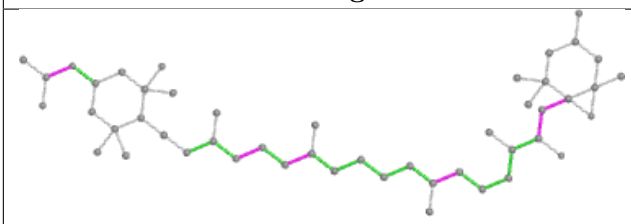

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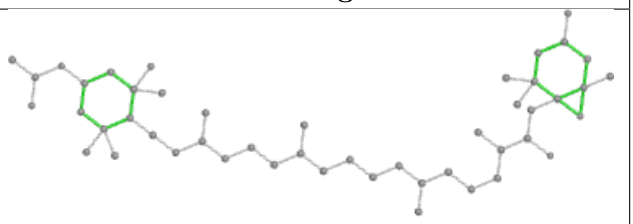
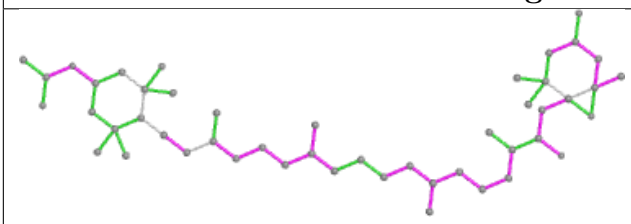


Rings

Ligand A86 15 313



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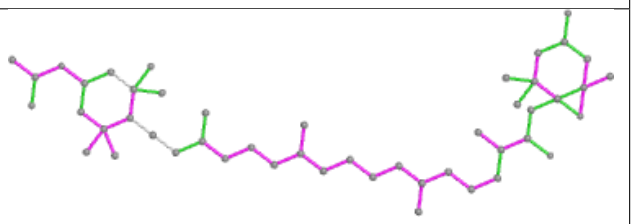

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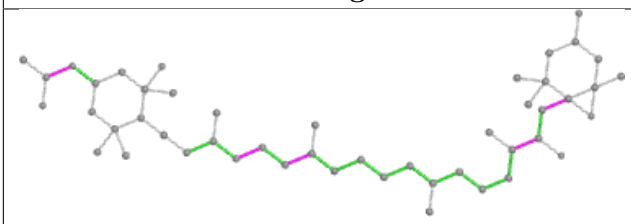

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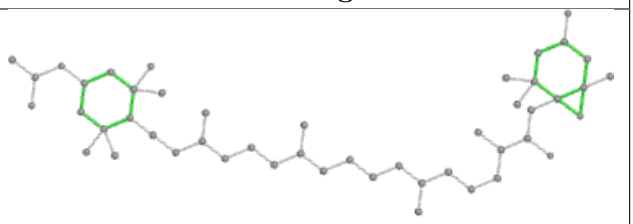
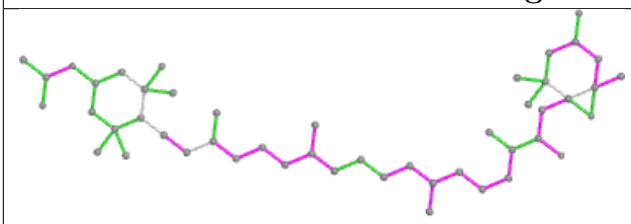


Rings

Ligand A86 39 310



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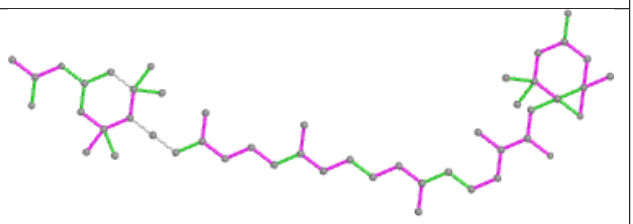
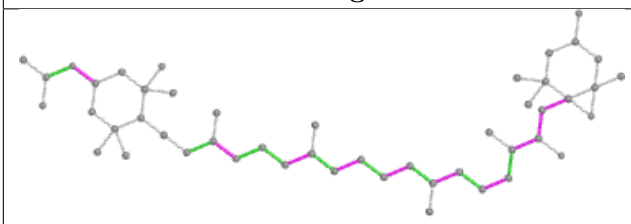


Bond angles



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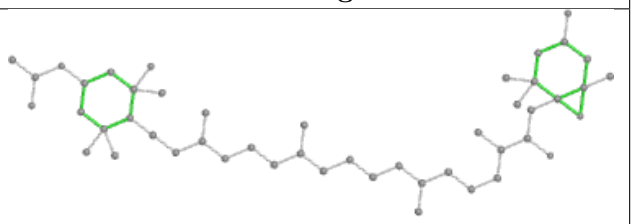
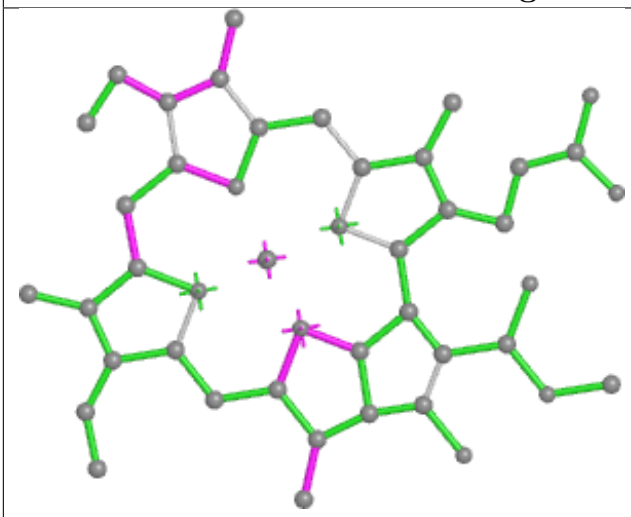


Rings

Ligand CLA 17 307



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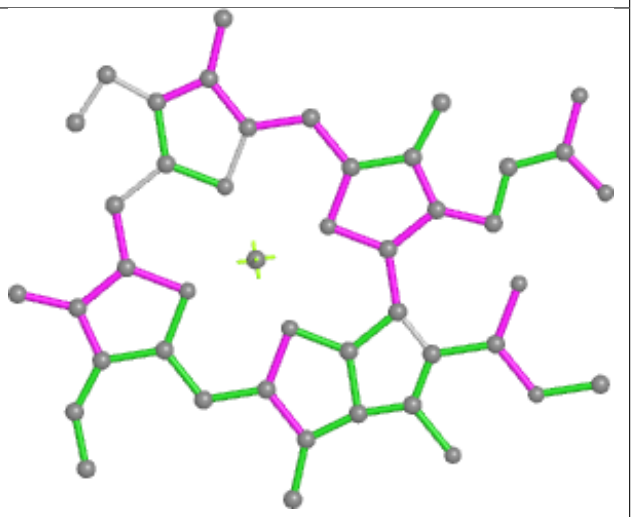

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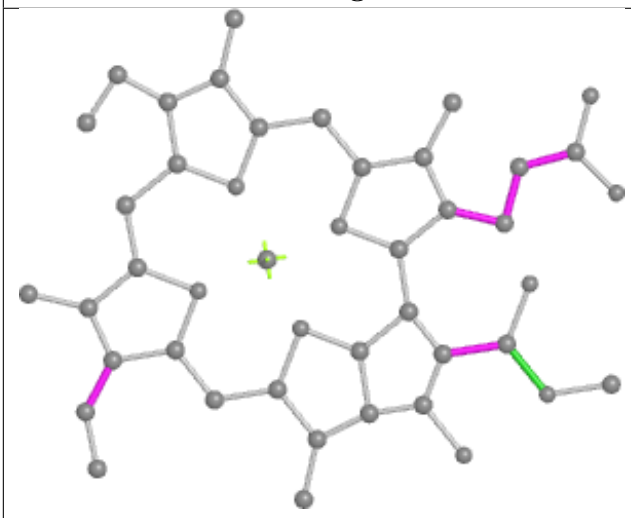

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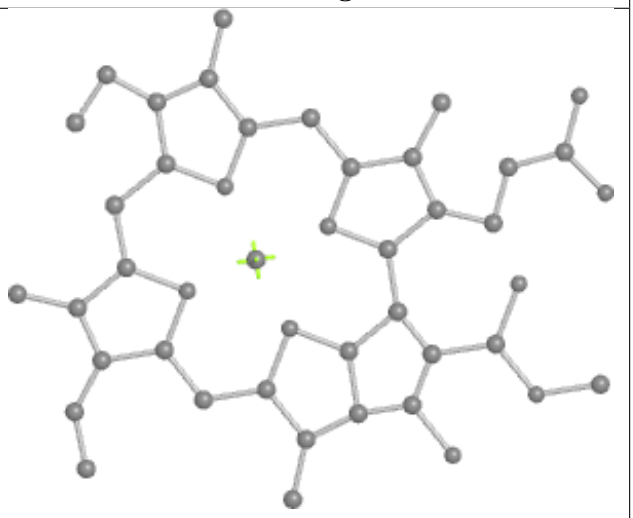
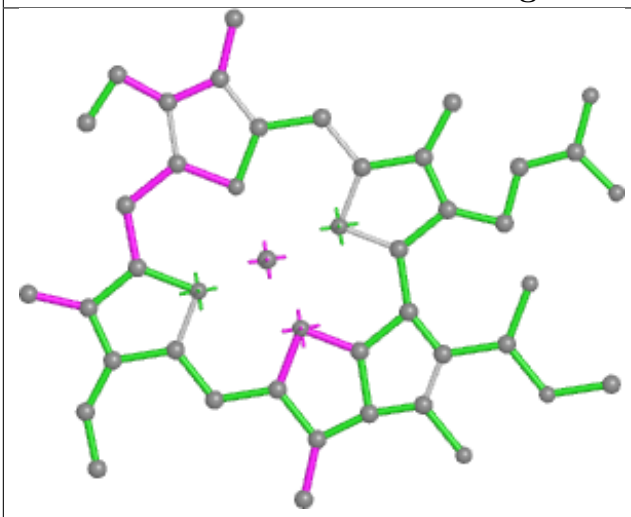


Rings

Ligand CLA 31 302



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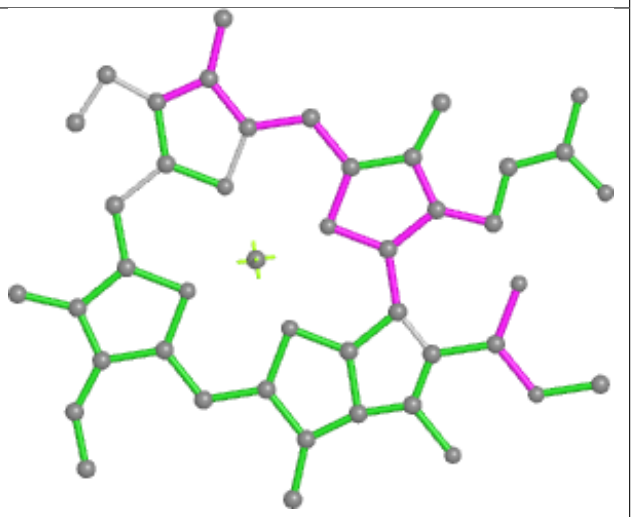
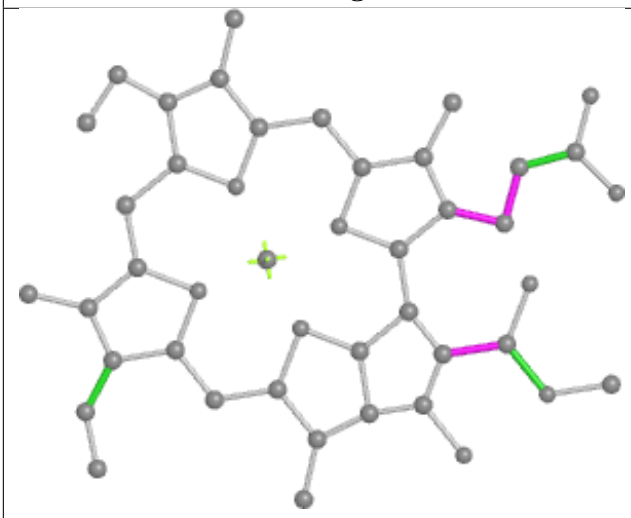


Bond angles



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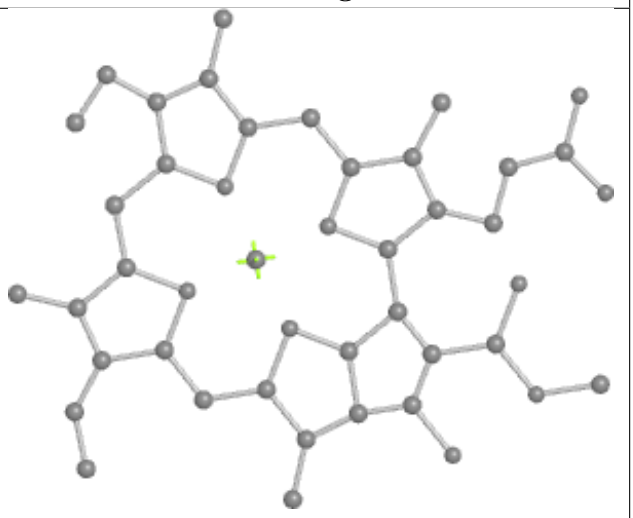
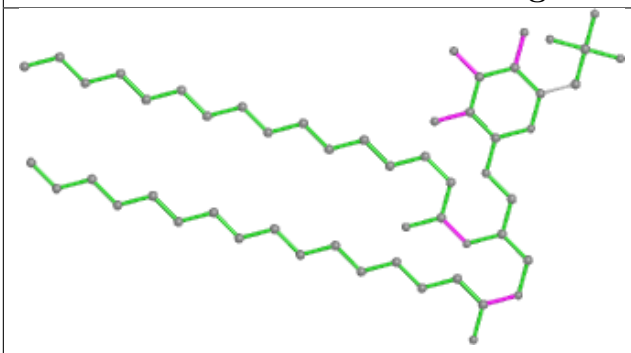


Rings

Ligand SQD a 405



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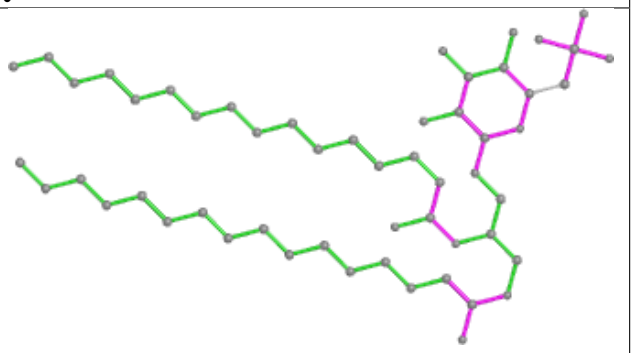
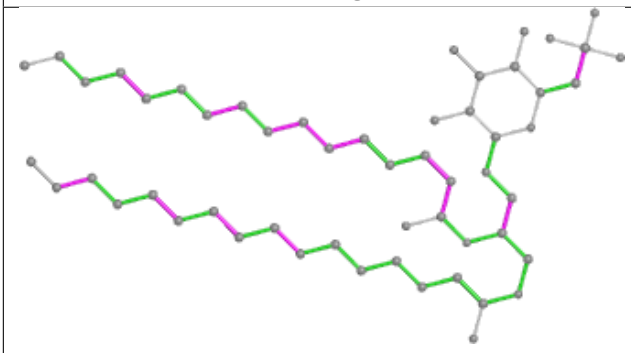


Bond angles



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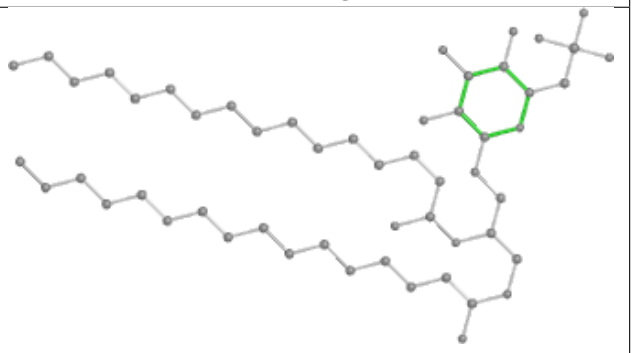
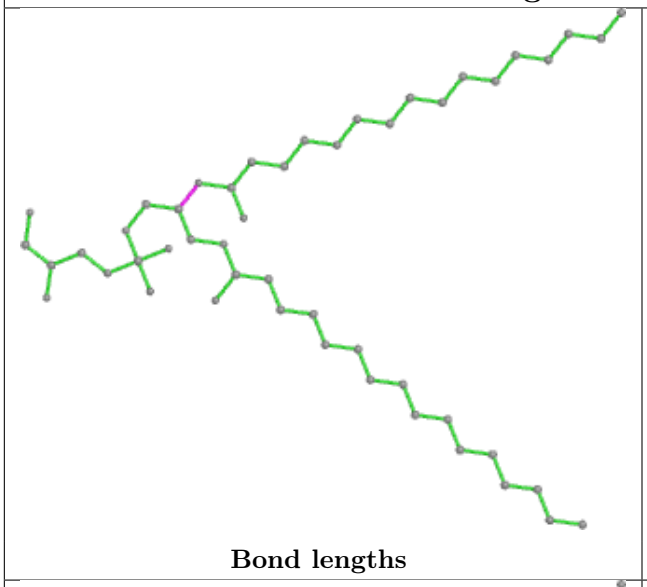


Rings

Ligand LHG B 622



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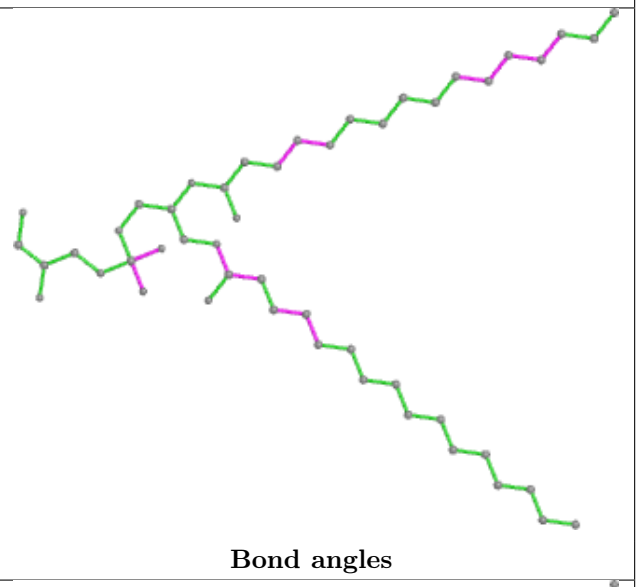
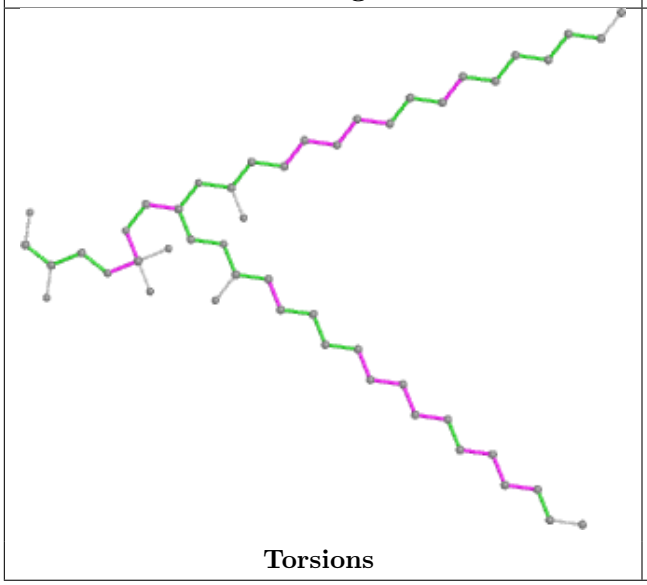


Bond angles



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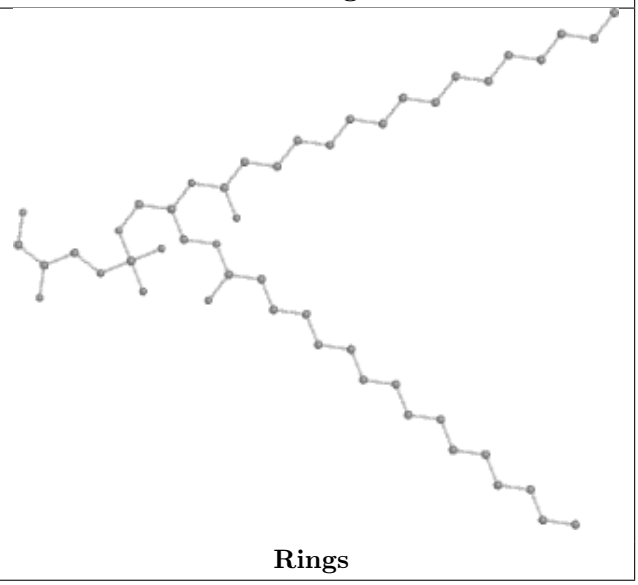
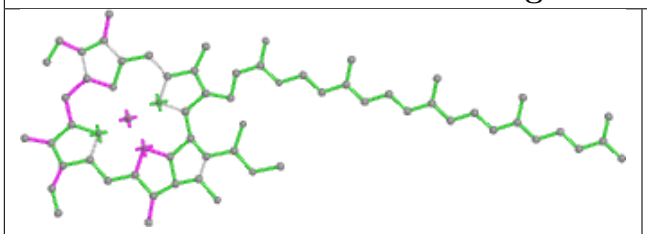


Rings

Ligand CLA C 502



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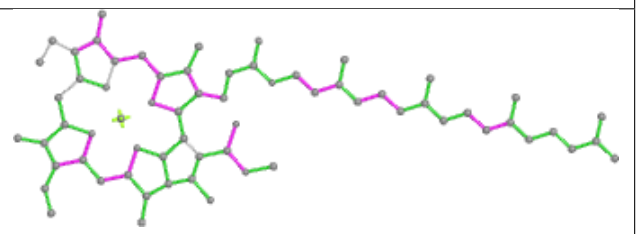
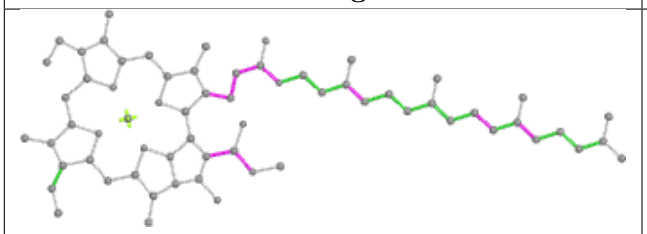
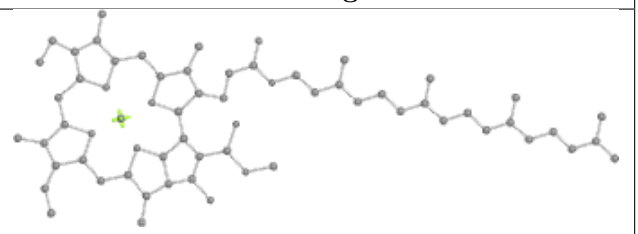


Bond angles

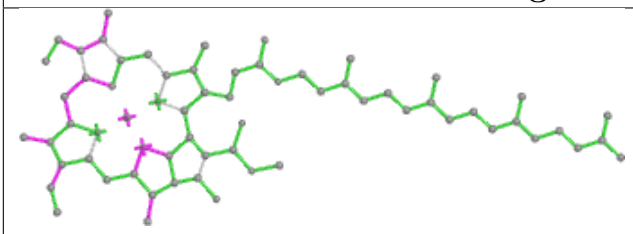


Torsions



Rings

Ligand CLA c 508



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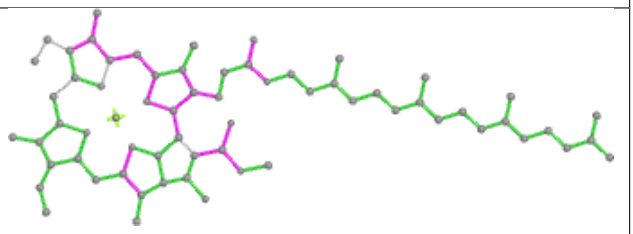
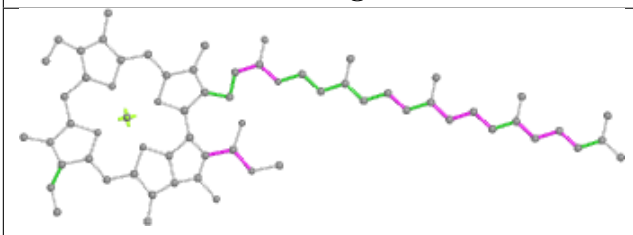


Bond angles



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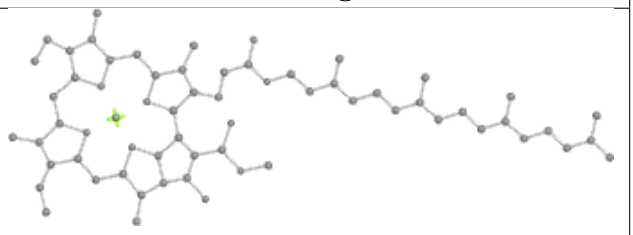
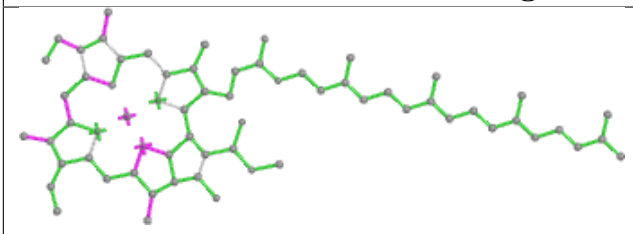


Rings

Ligand CLA 12 305



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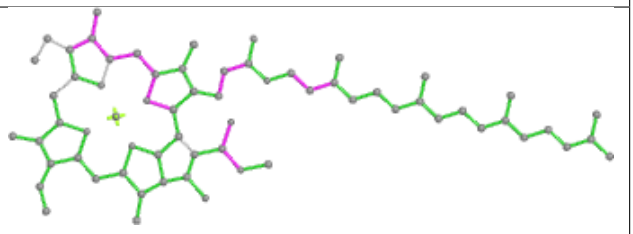
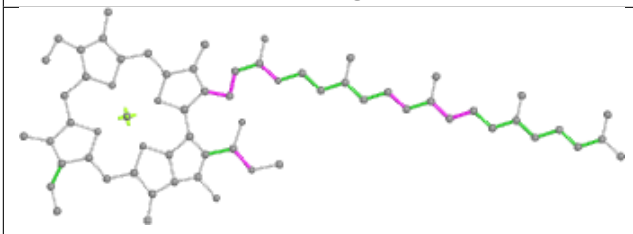


Bond angles



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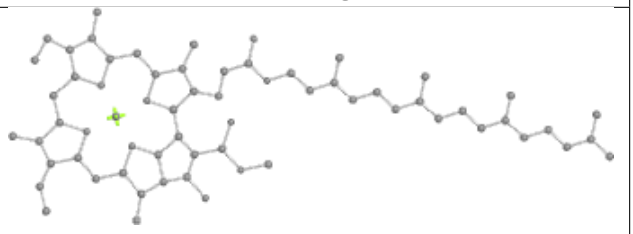
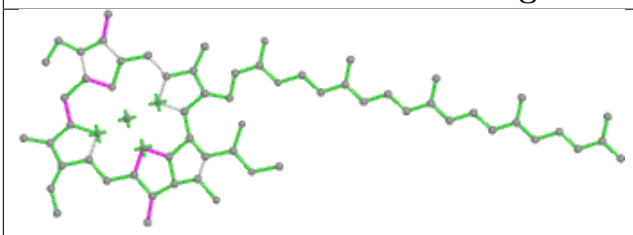


Rings

Ligand CLA 41 307



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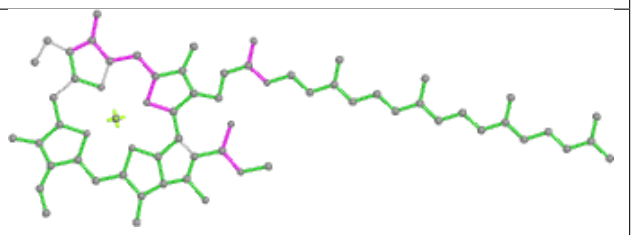
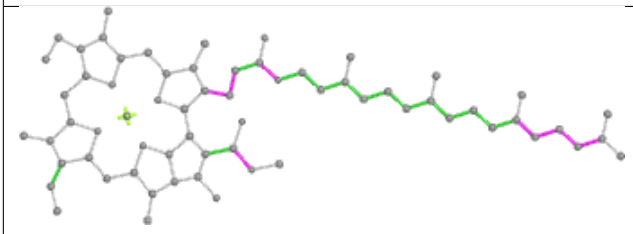


Bond angles



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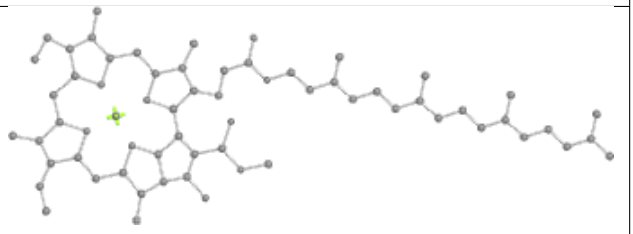
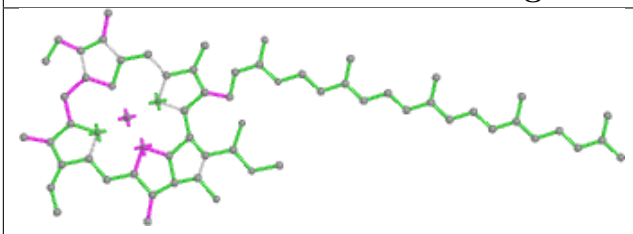


Rings

Ligand CLA B 613



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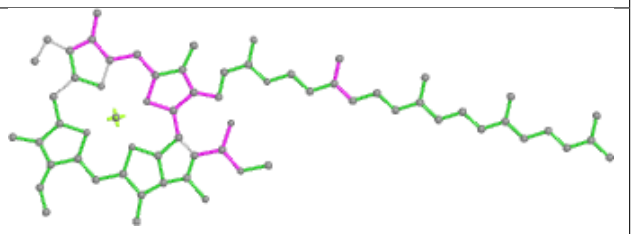
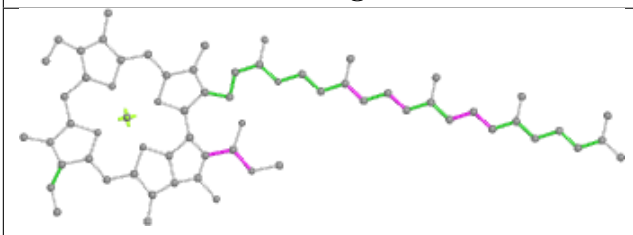


Bond angles



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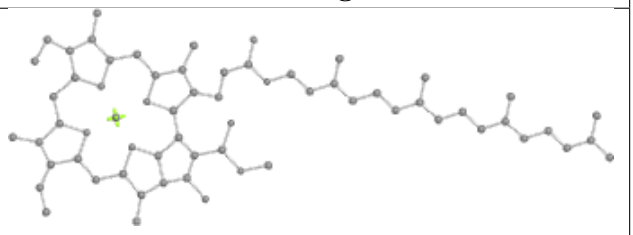
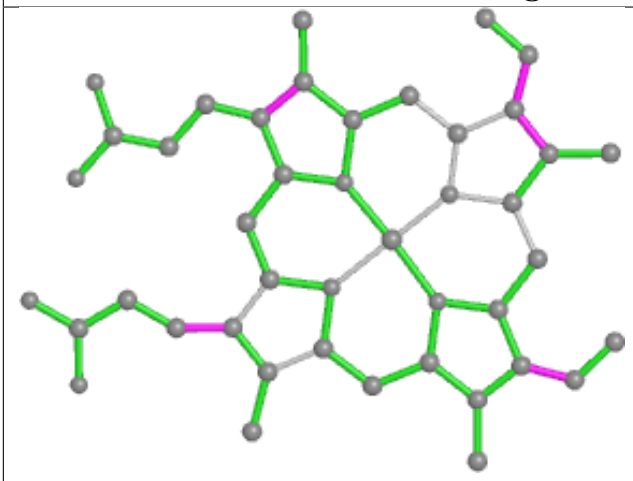


Rings

Ligand HEM e 101



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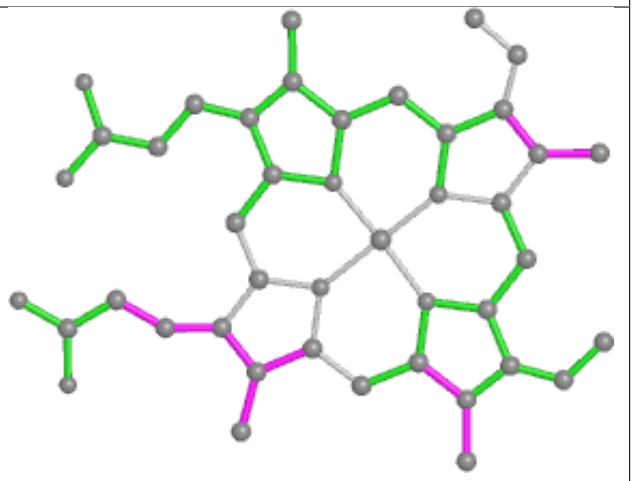
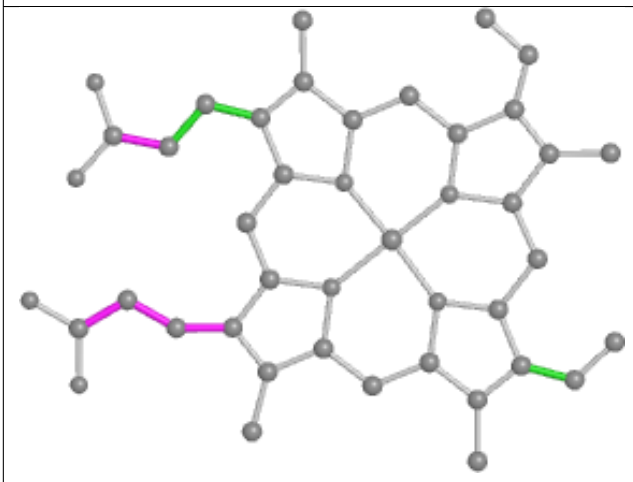
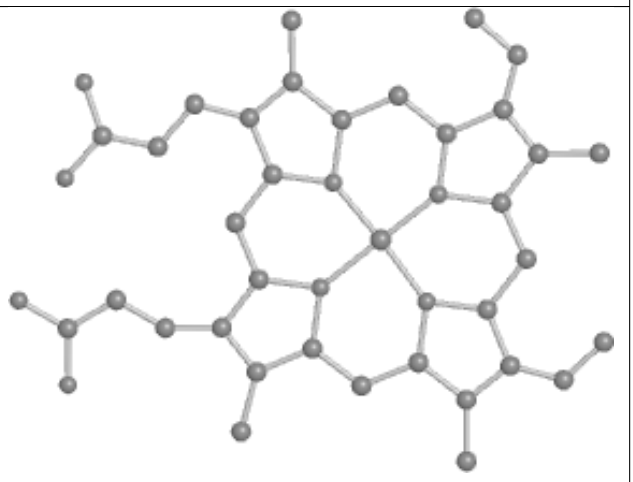


Bond angles

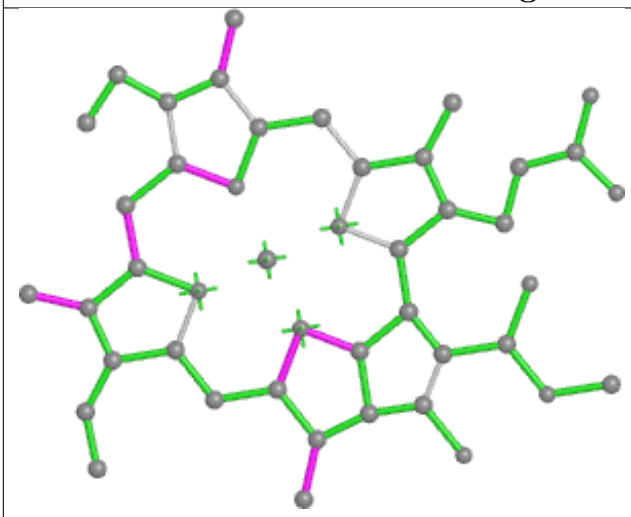


Torsions



Rings

Ligand CLA 12 309



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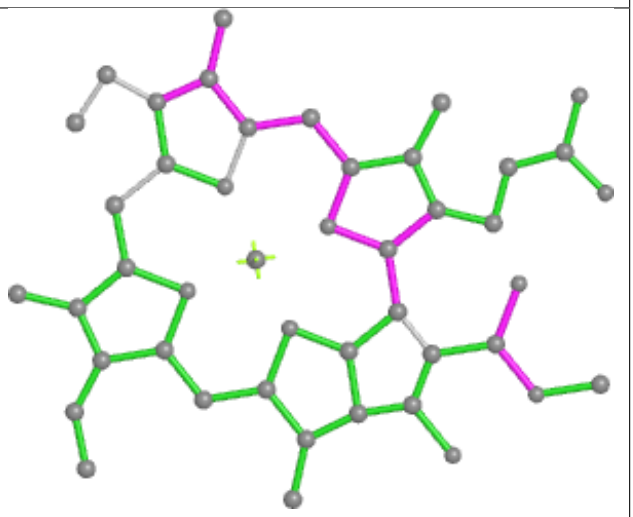

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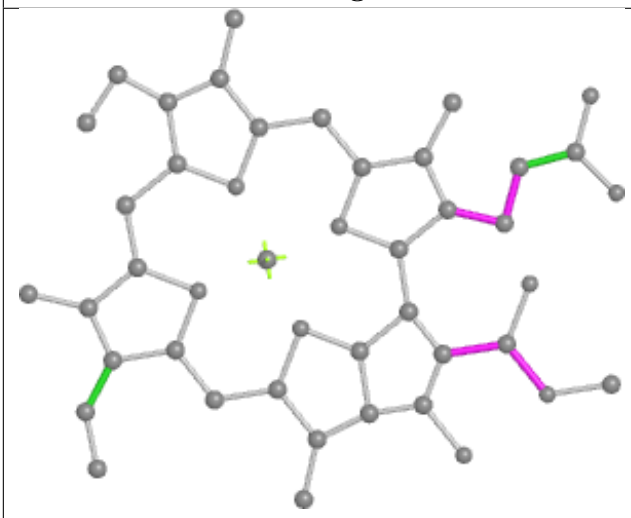

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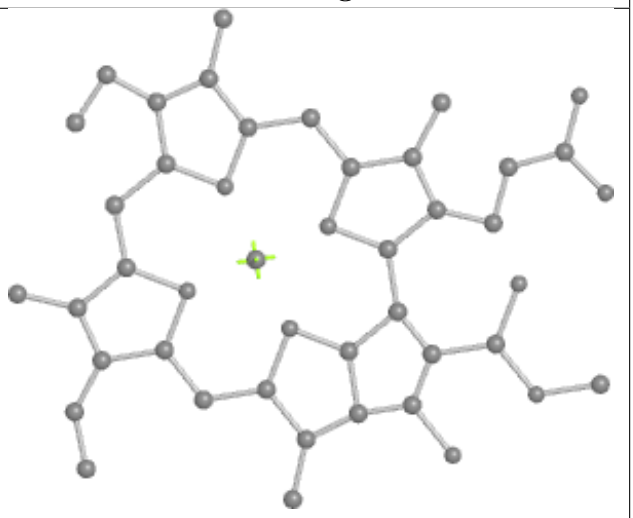
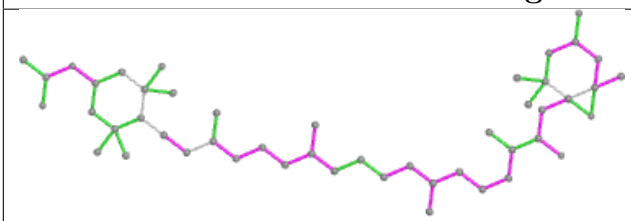


Rings

Ligand A86 21 311



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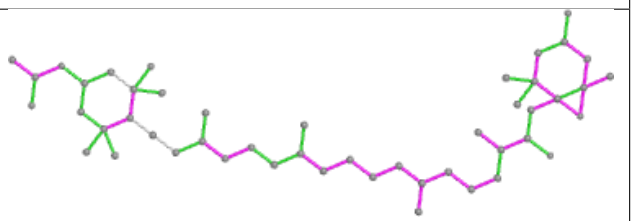

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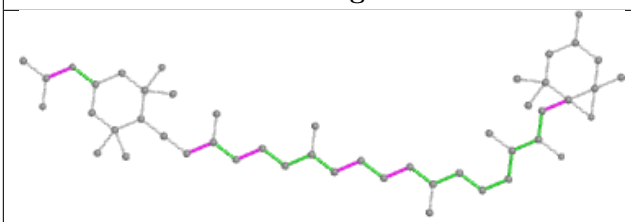

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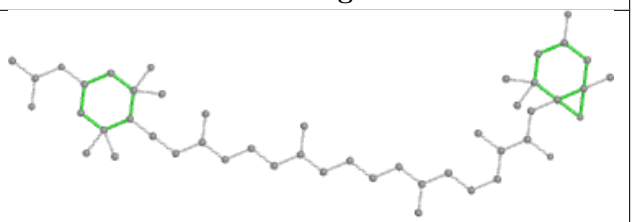
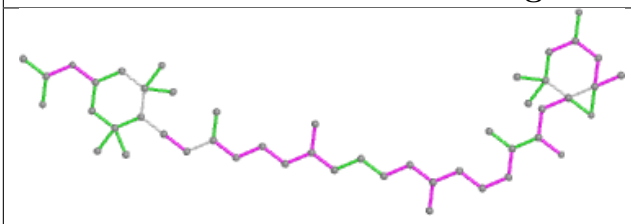


Rings

Ligand A86 32 317



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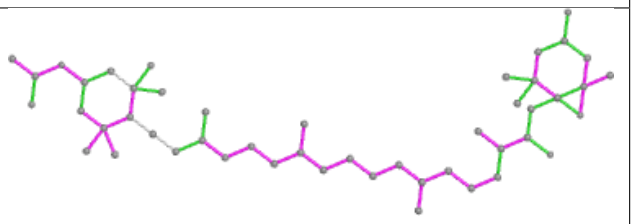

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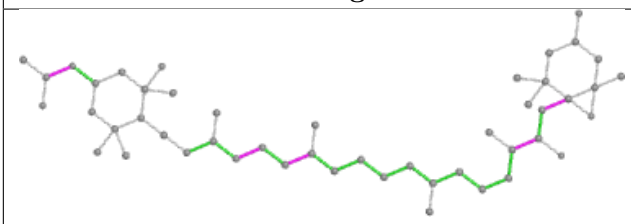

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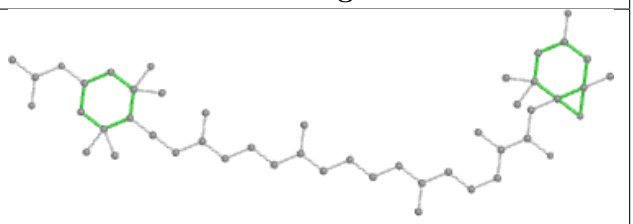
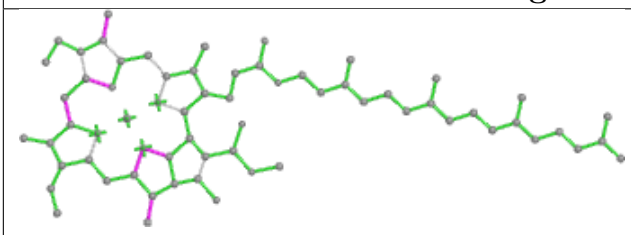


Rings

Ligand CLA c 524



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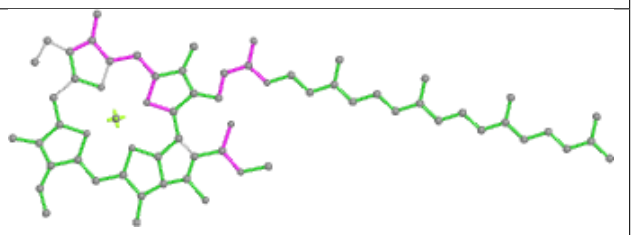

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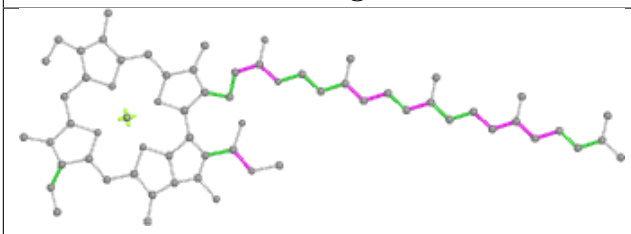

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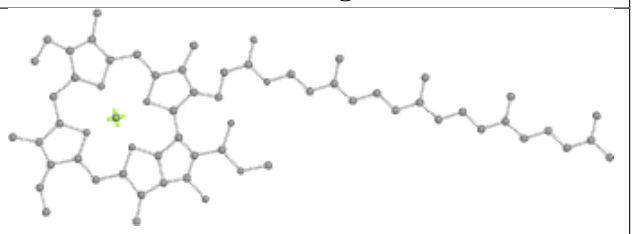
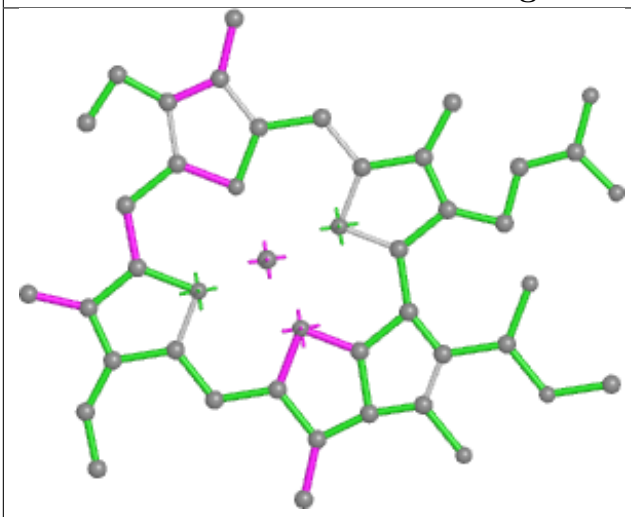


Rings

Ligand CLA 36 308



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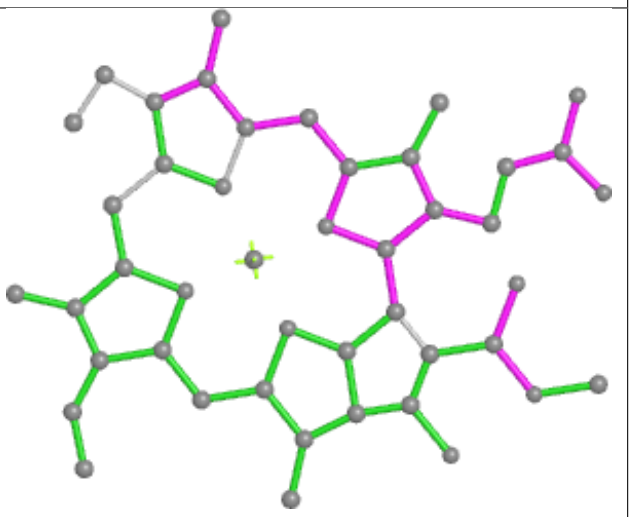
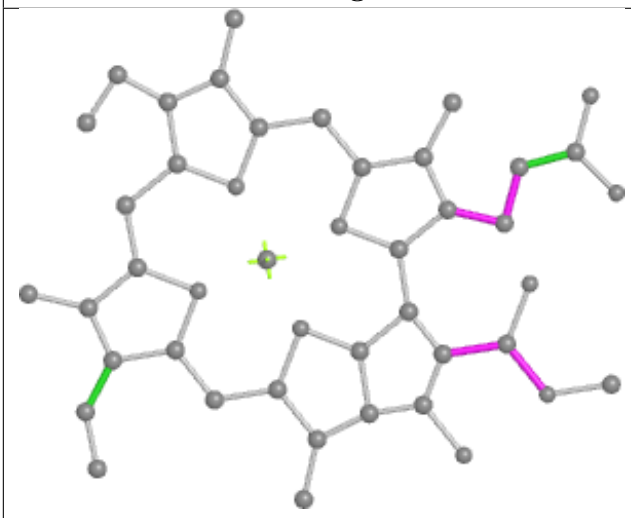


Bond angles



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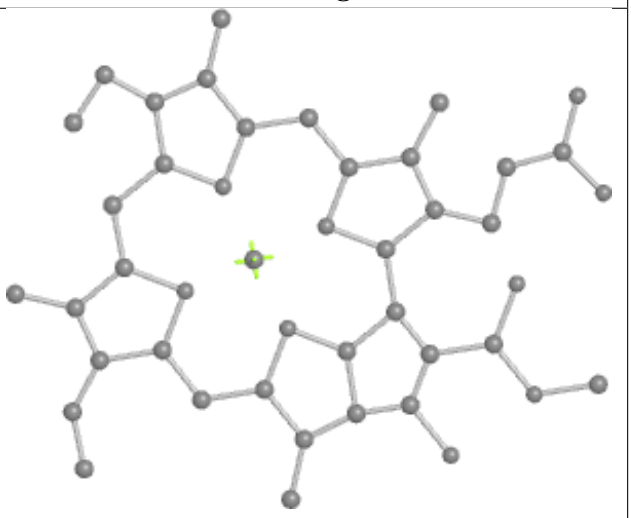
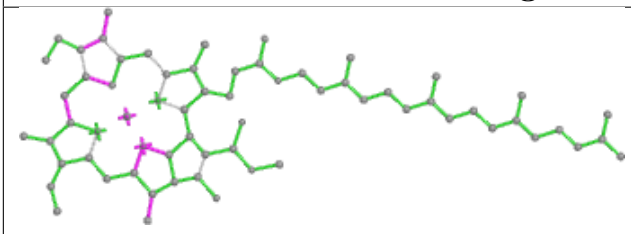


Rings

Ligand CLA 20 209



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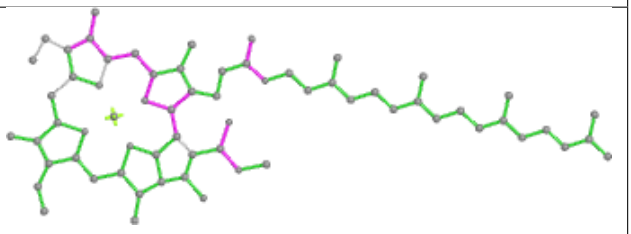
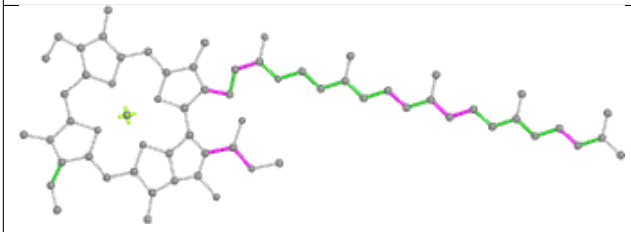


Bond angles



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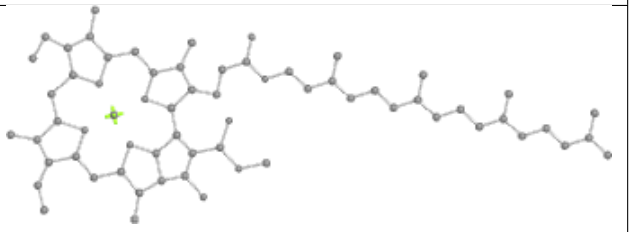
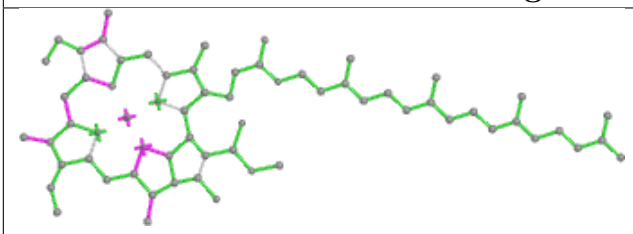


Rings

Ligand CLA w 102



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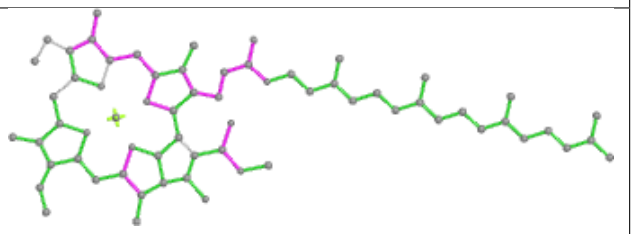

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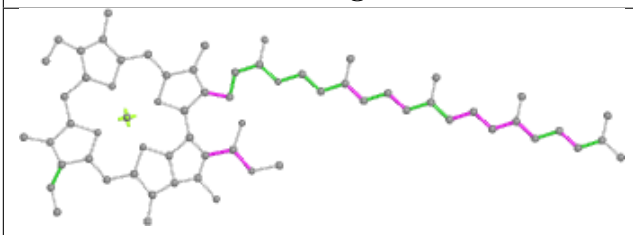

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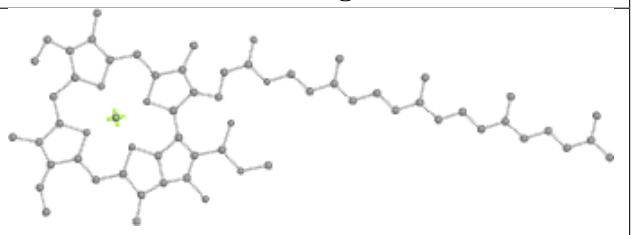
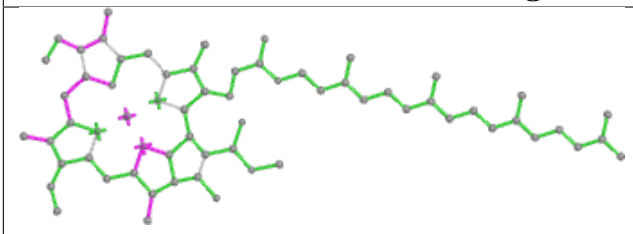


Rings

Ligand CLA C 509



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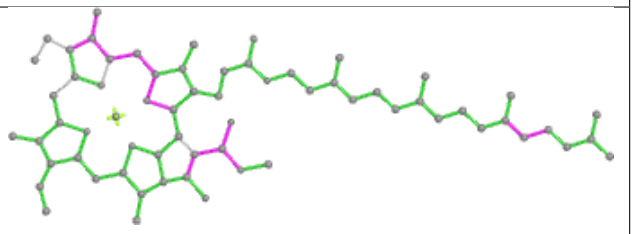

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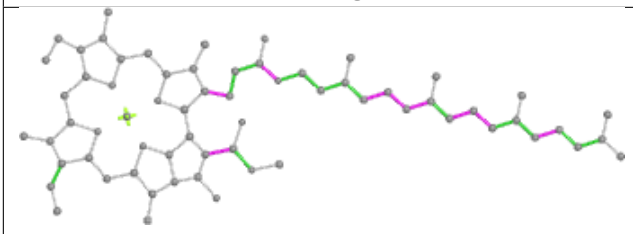

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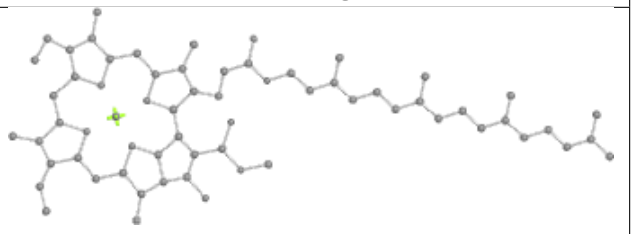
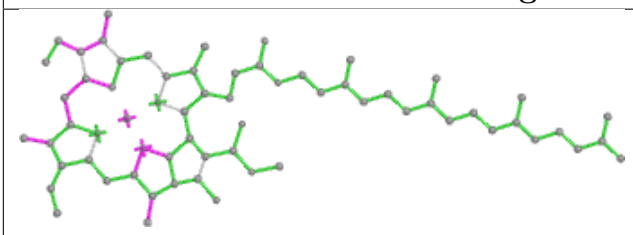


Rings

Ligand CLA 34 304



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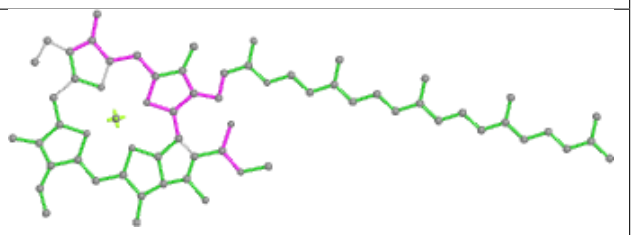
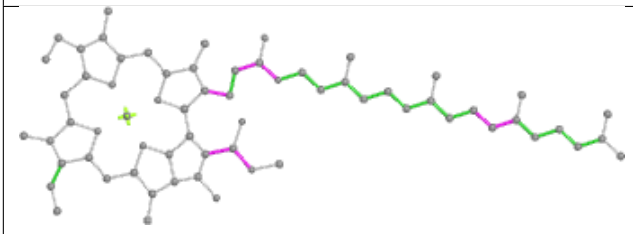


Bond angles



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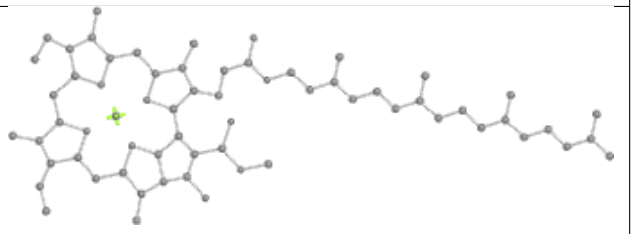
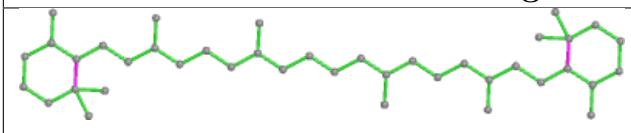


Rings

Ligand BCR A 405



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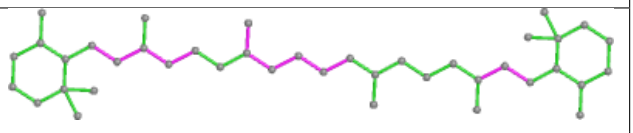
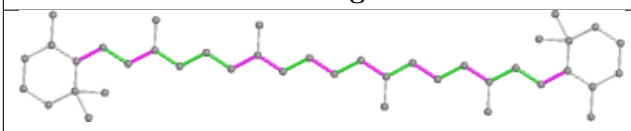


Bond angles



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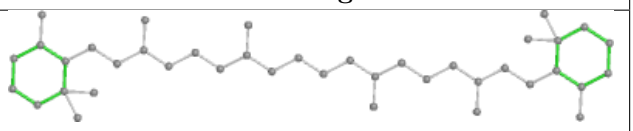
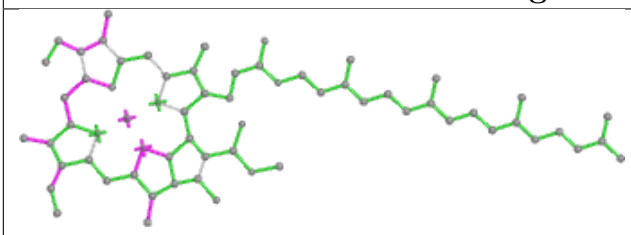


Rings

Ligand CLA c 503



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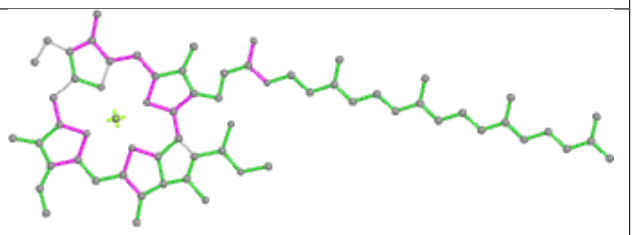
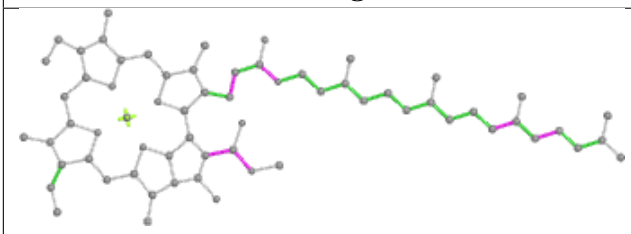


Bond angles



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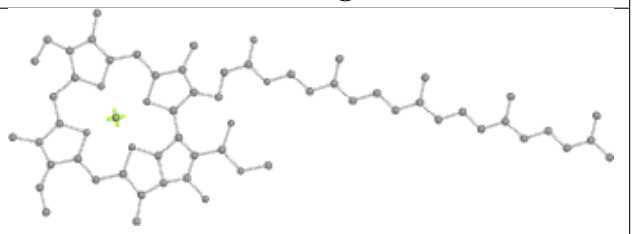
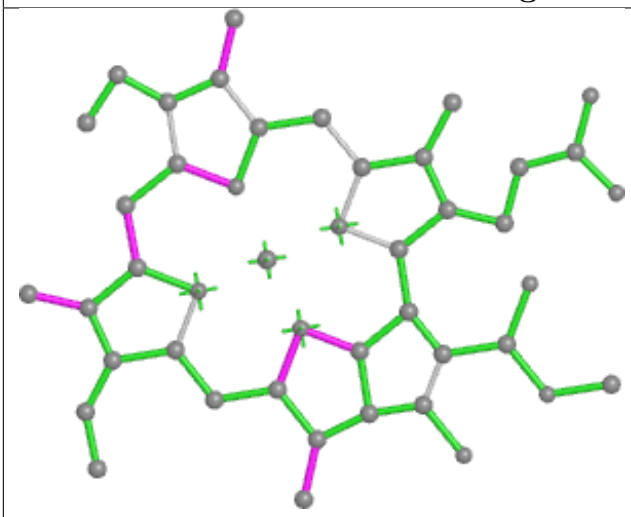


Rings

Ligand CLA 15 304



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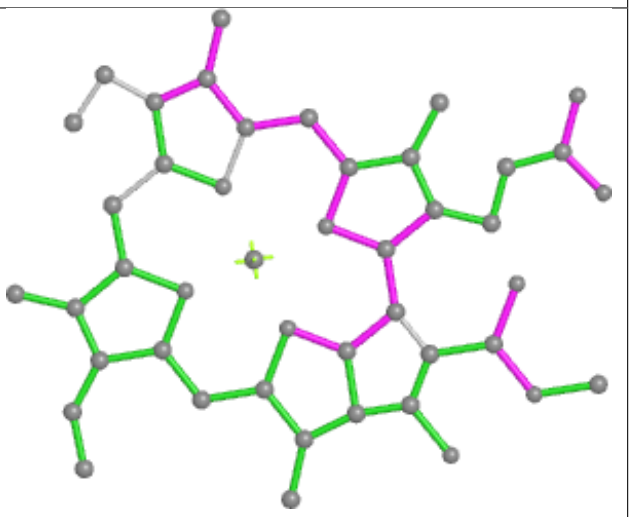
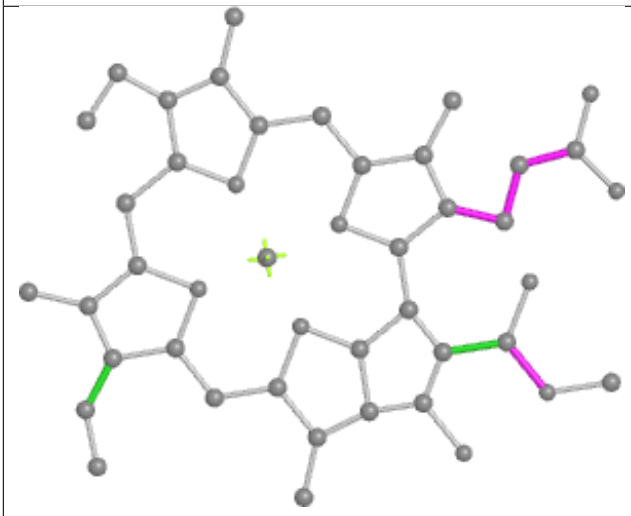


Bond angles



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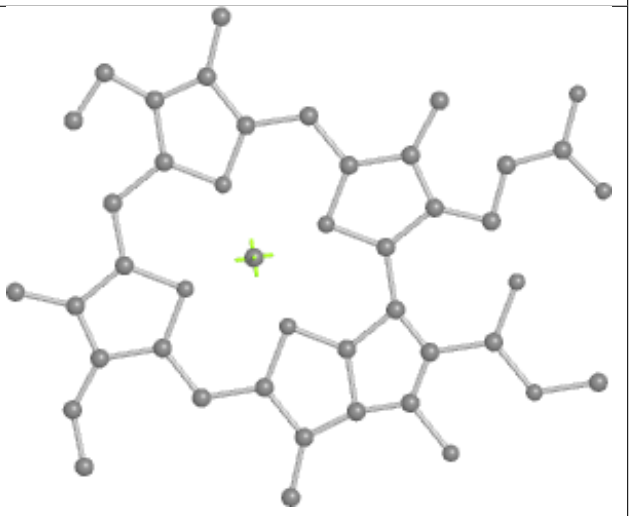
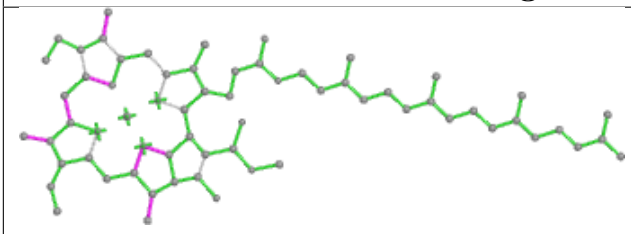


Rings

Ligand CLA 35 303



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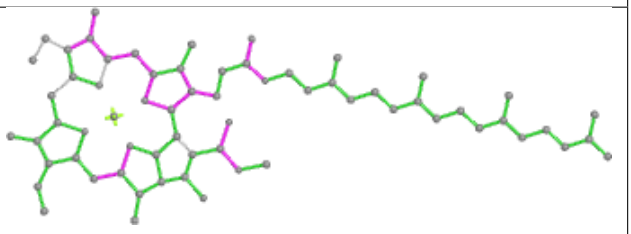
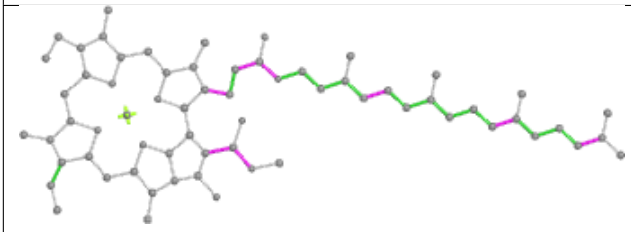


Bond angles



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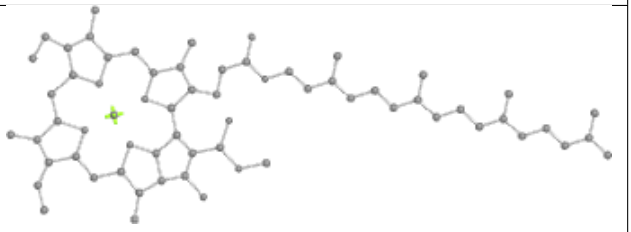
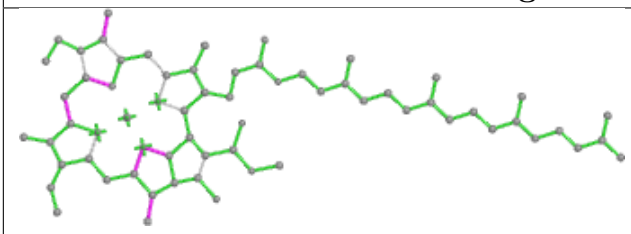


Rings

Ligand CLA W 103



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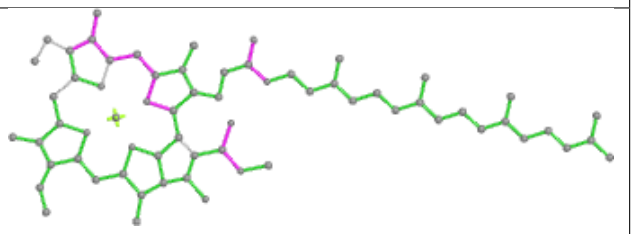
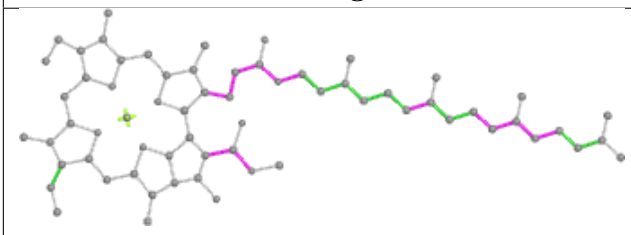
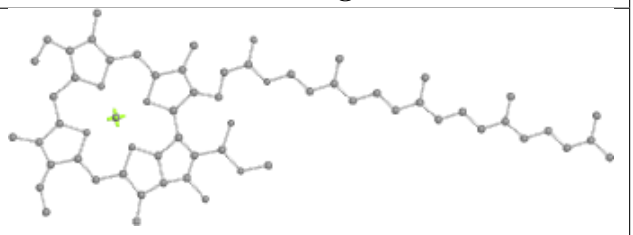


Bond angles

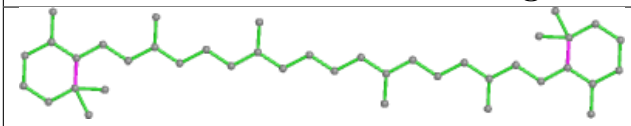


Torsions



Rings

Ligand BCR C 518



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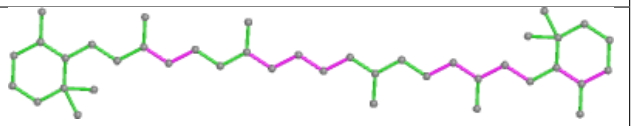

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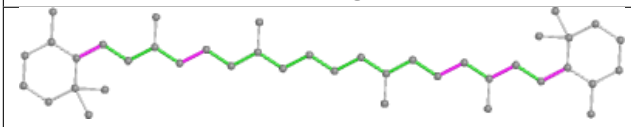
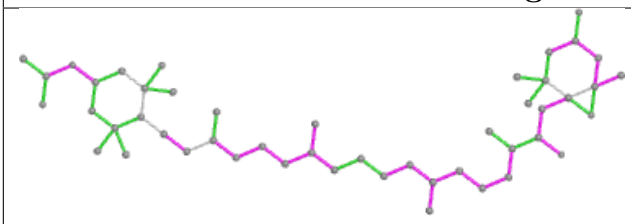


Torsions

Rings

Ligand A86 21 313



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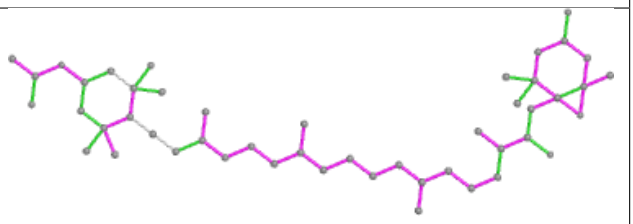

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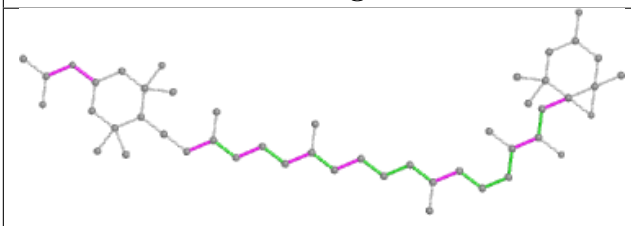

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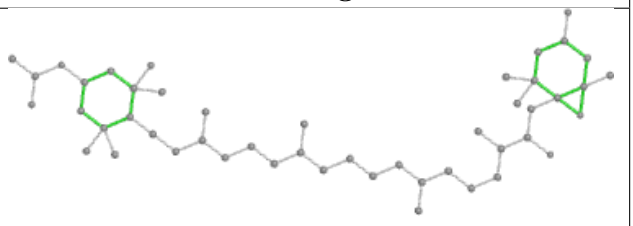
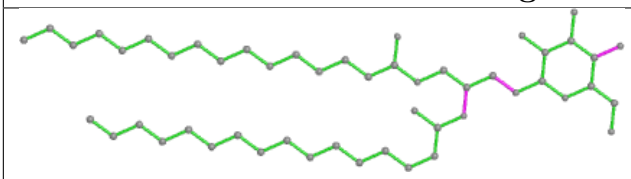


Rings

Ligand LMG D 408



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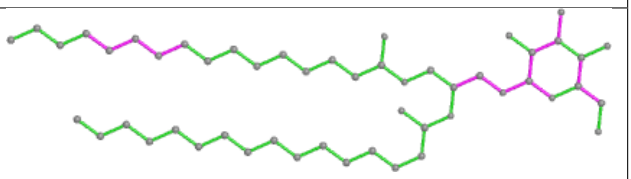

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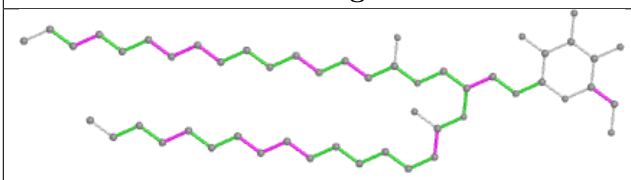

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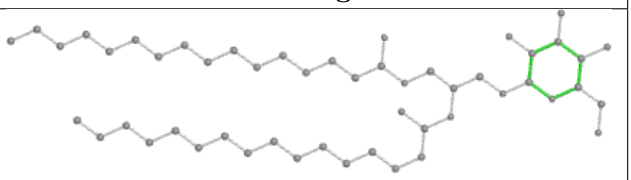
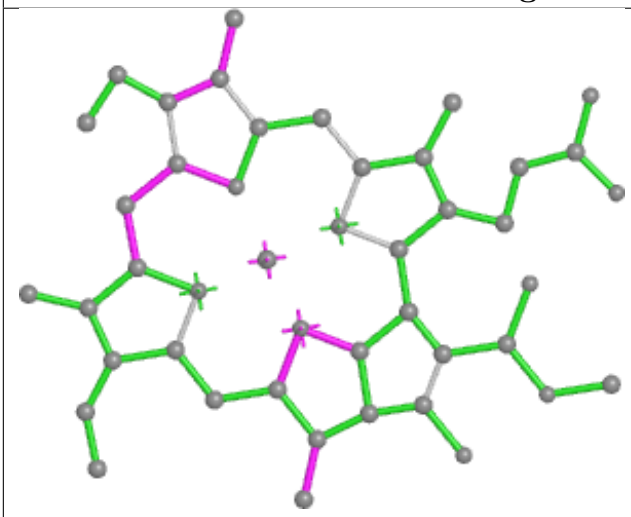


Rings

Ligand CLA 20 206



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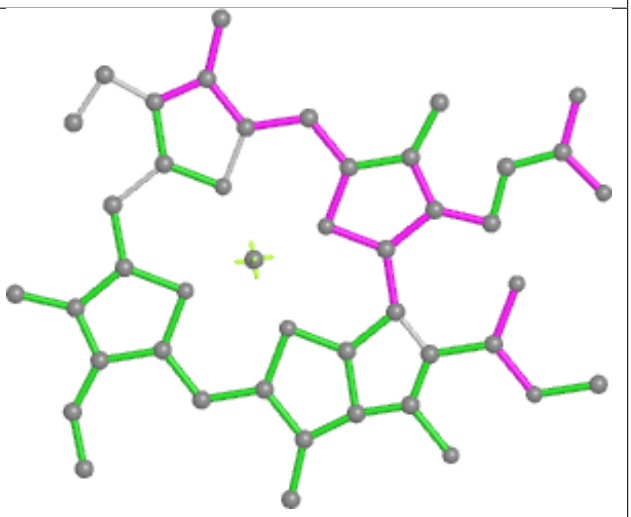

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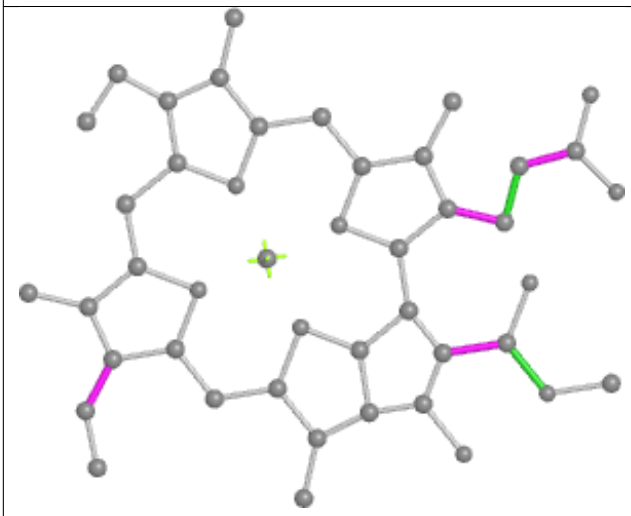

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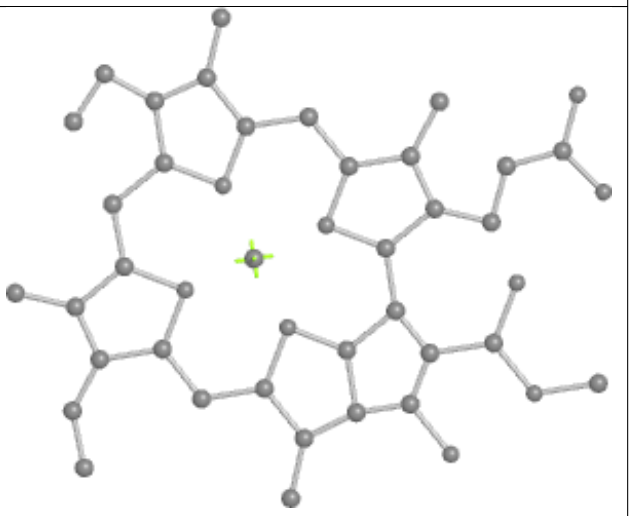
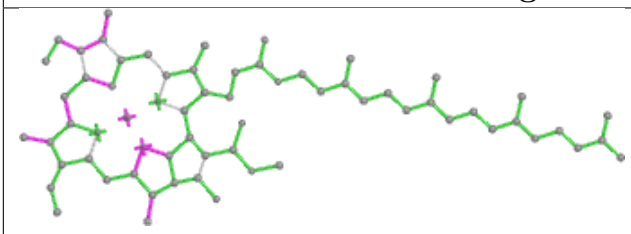


Rings

Ligand CLA 35 307



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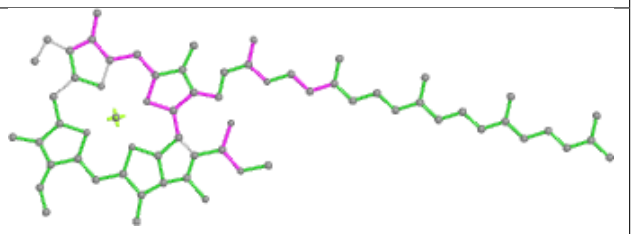

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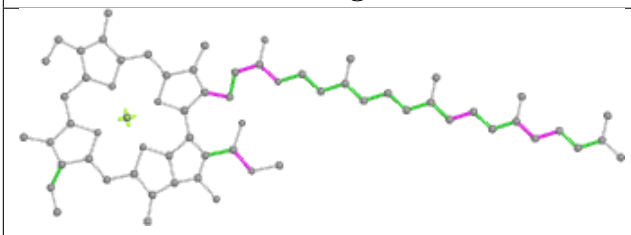

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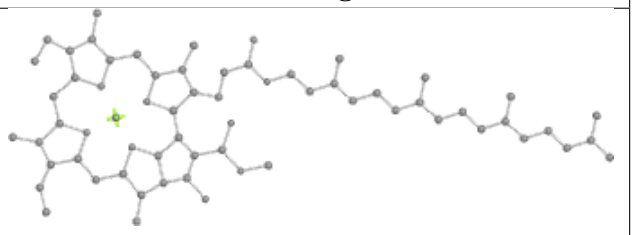
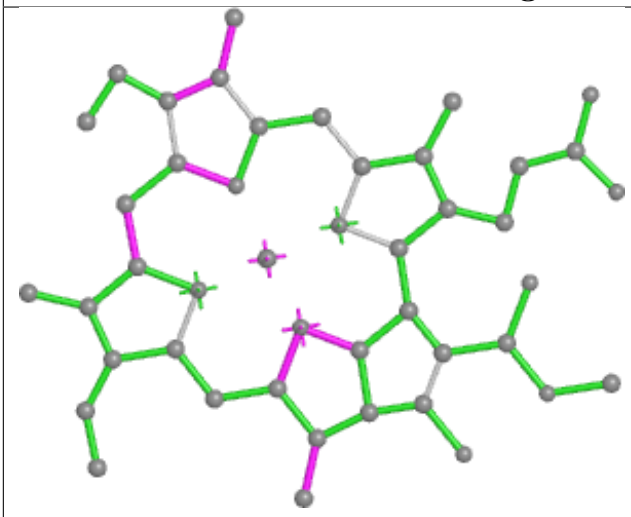


Rings

Ligand CLA 19 304



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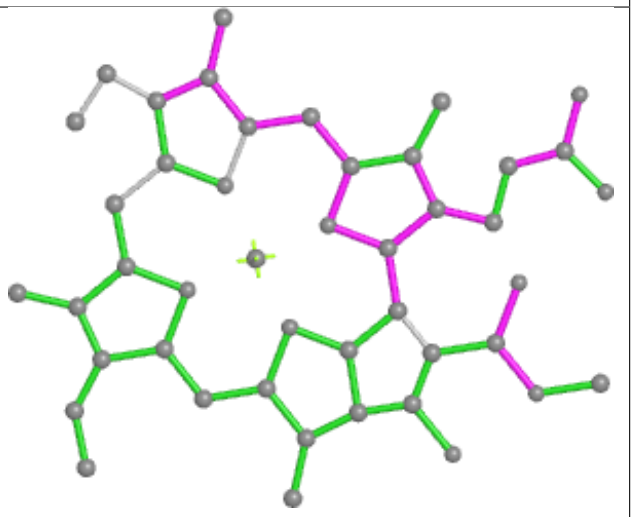

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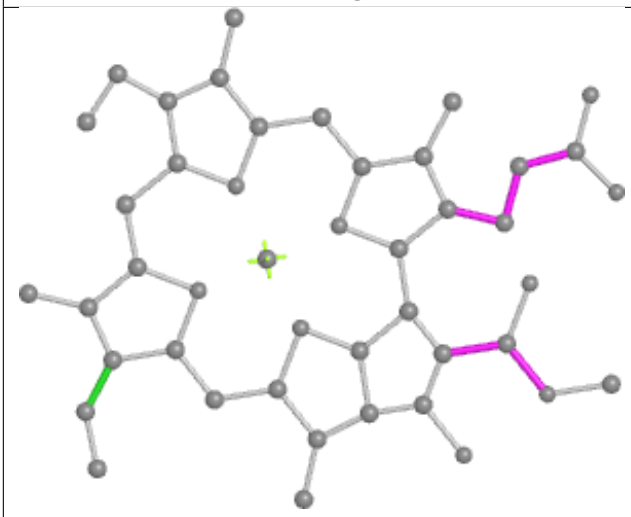

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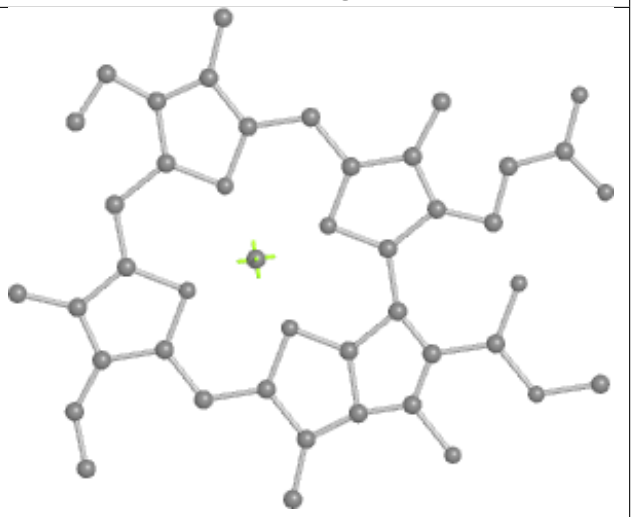
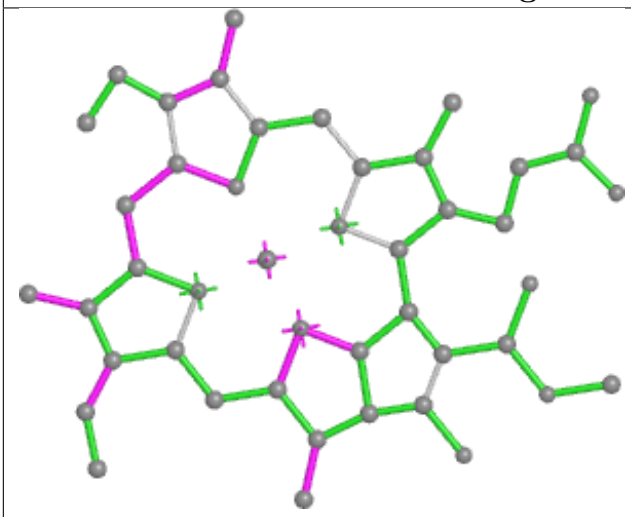


Rings

Ligand CLA 37 304



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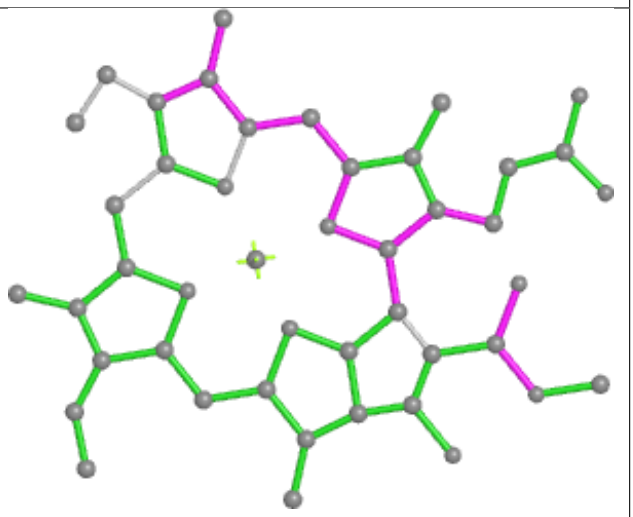

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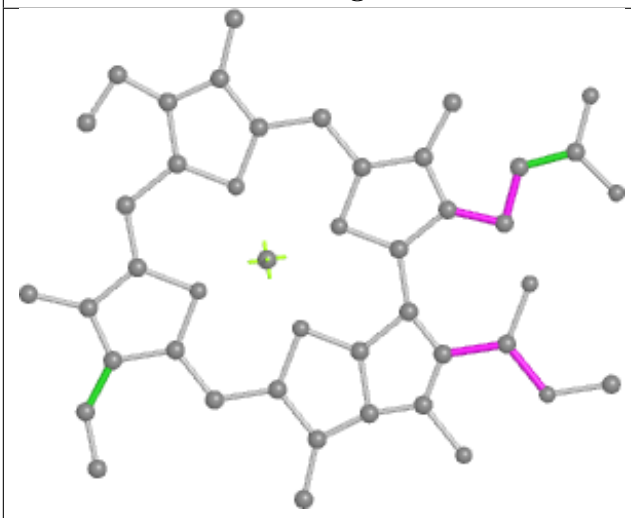

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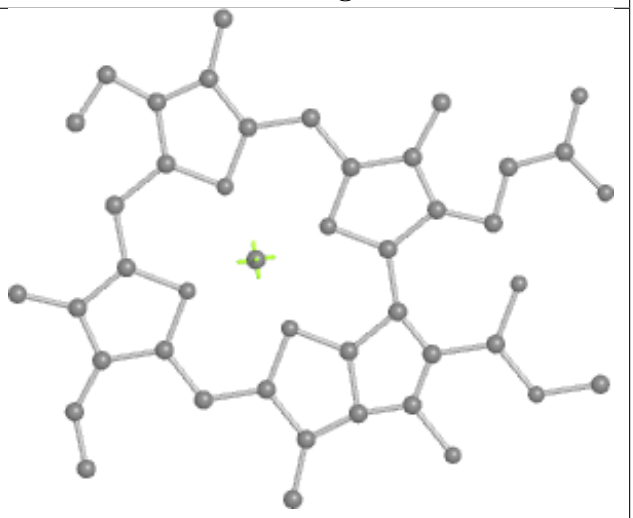
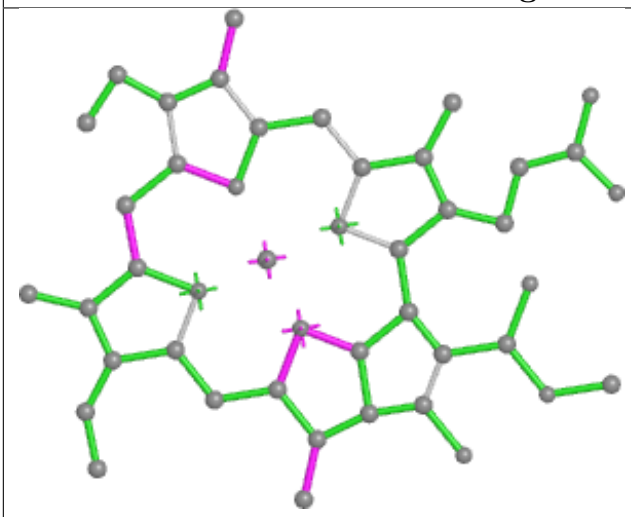


Rings

Ligand CLA 39 308



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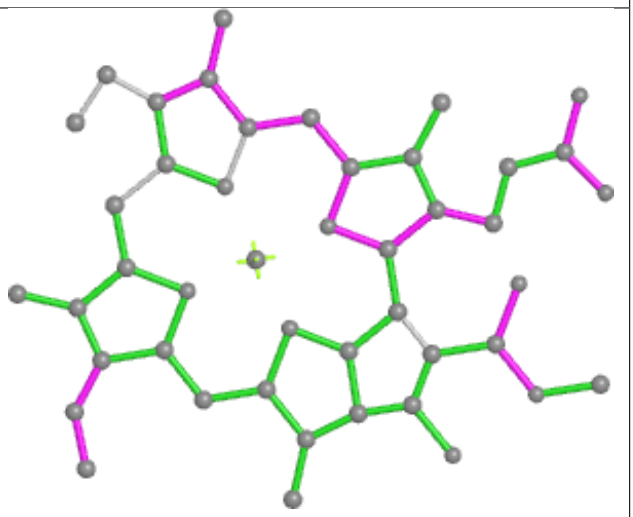

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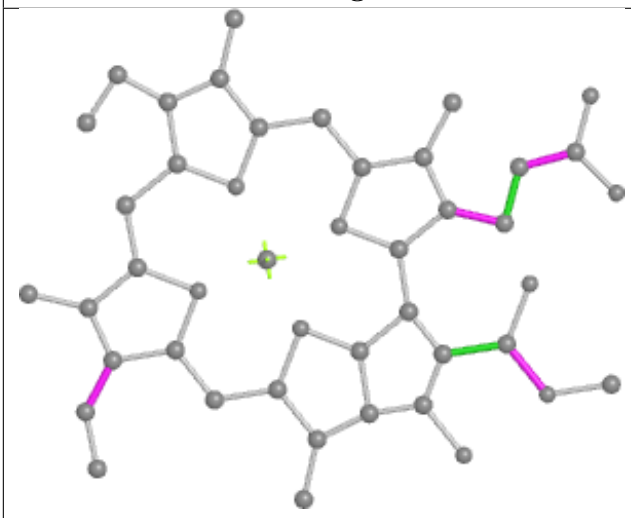

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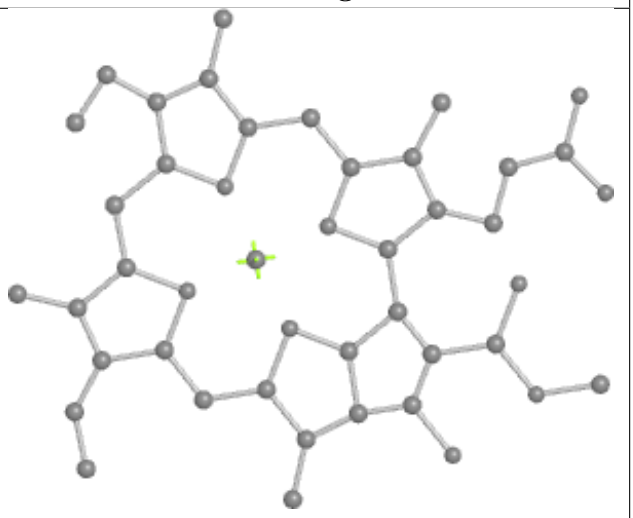
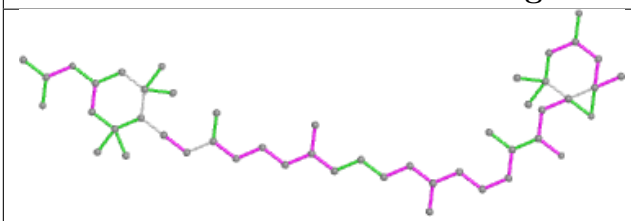


Rings

Ligand A86 31 312



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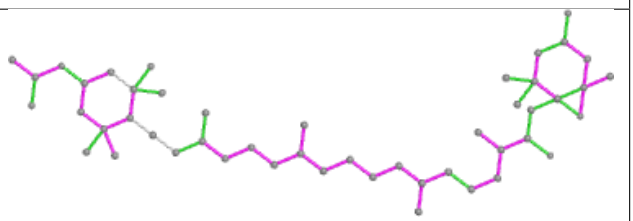

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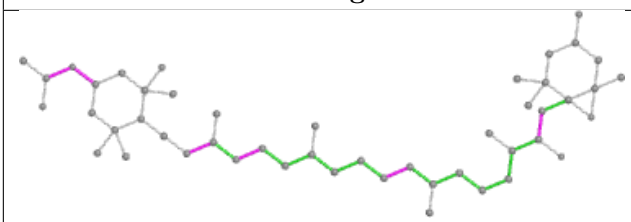

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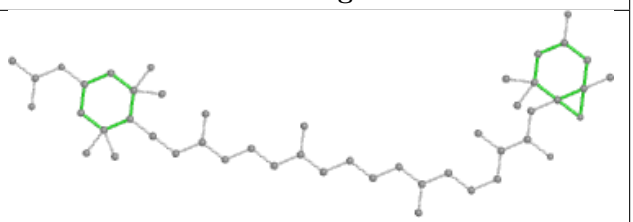
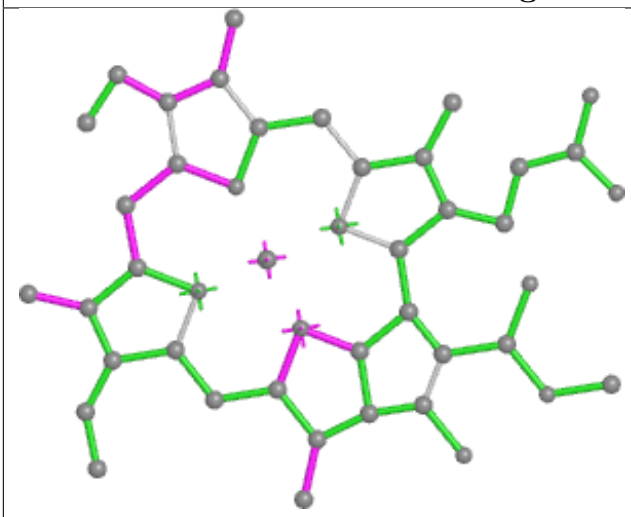


Rings

Ligand CLA 34 303



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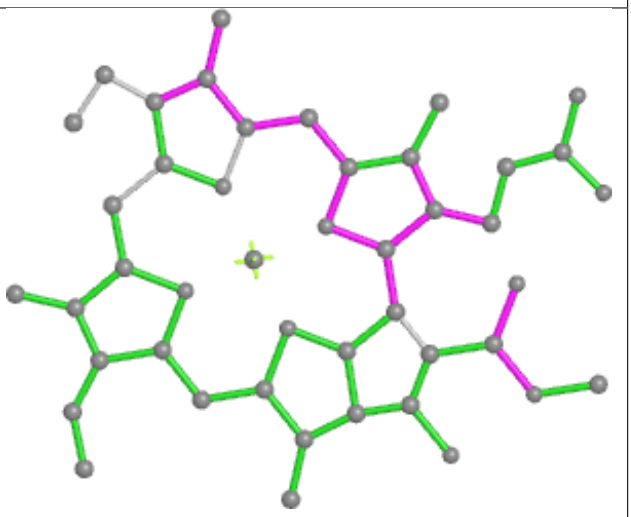

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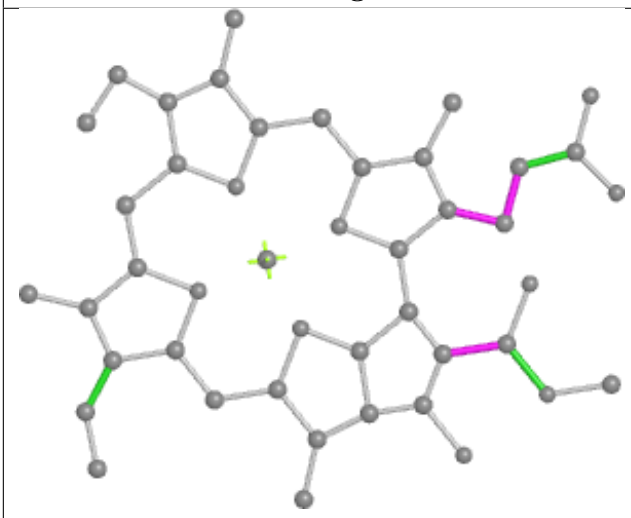

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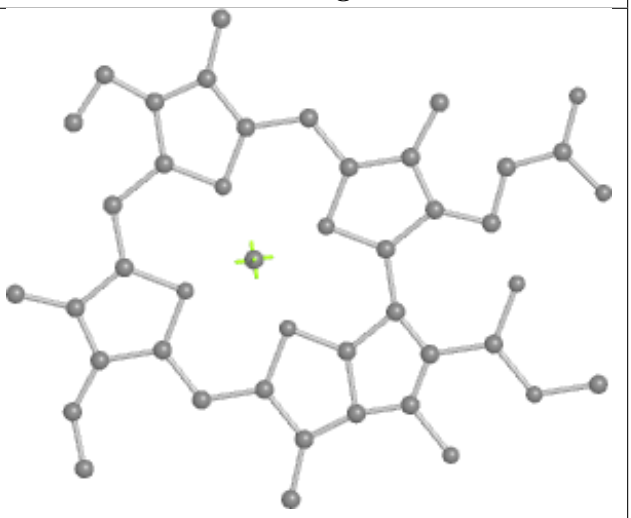
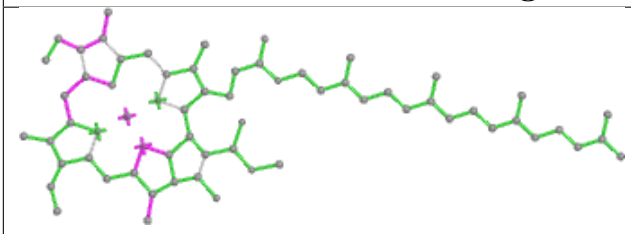


Rings

Ligand CLA 17 308



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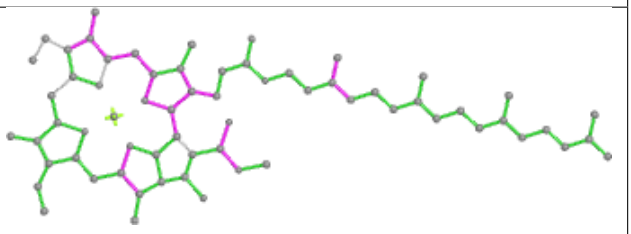

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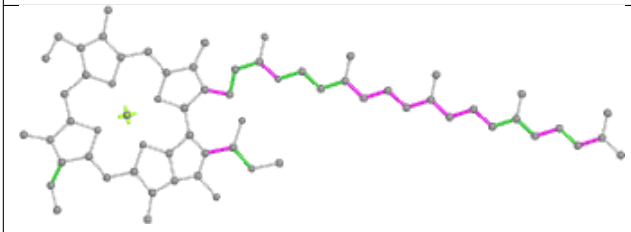

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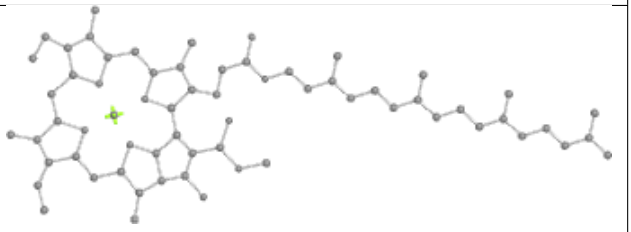
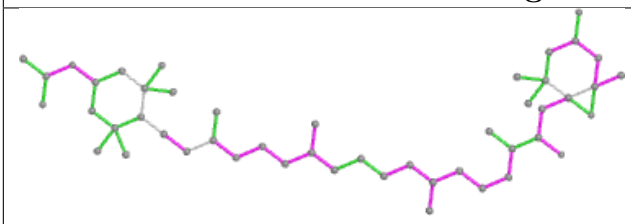


Rings

Ligand A86 16 310



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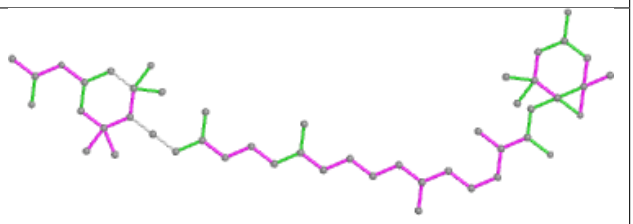
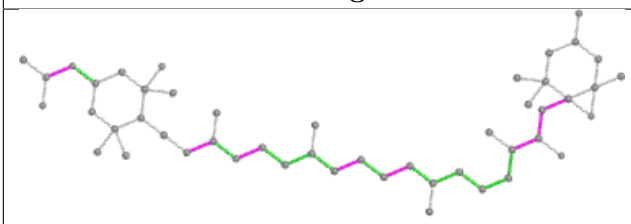


Bond angles



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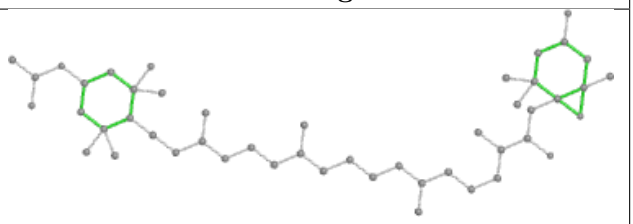
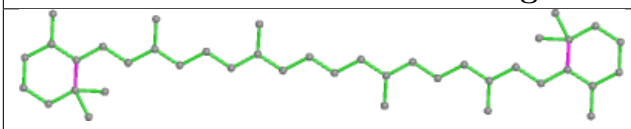


Rings

Ligand BCR m 103



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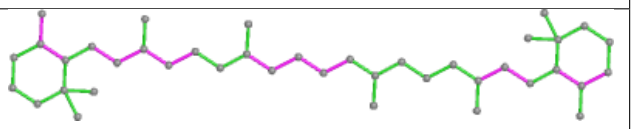

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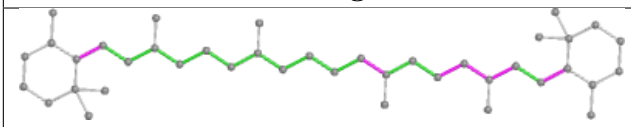

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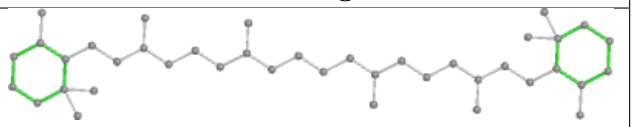
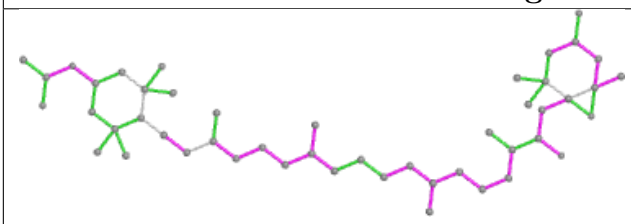


Rings

Ligand A86 12 318



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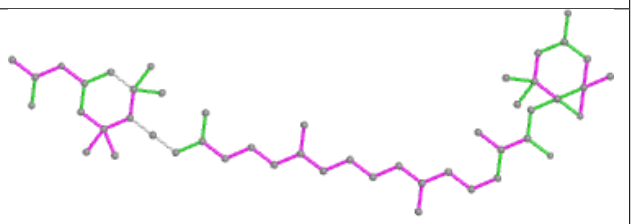
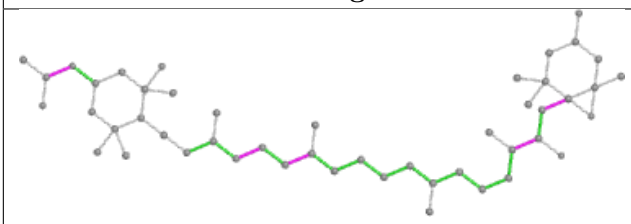
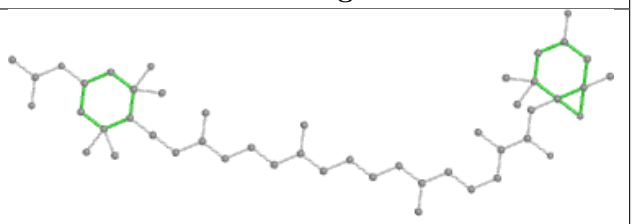


Bond angles

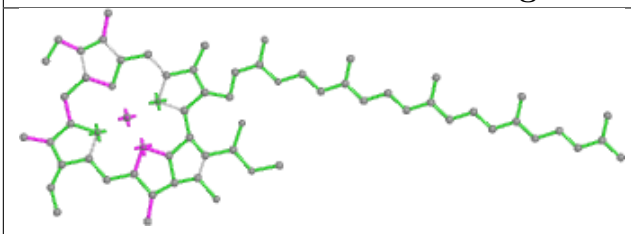


Torsions



Rings

Ligand CLA 15 301



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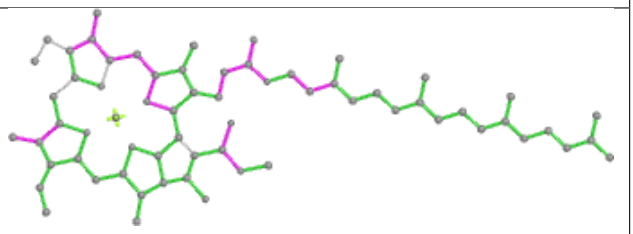

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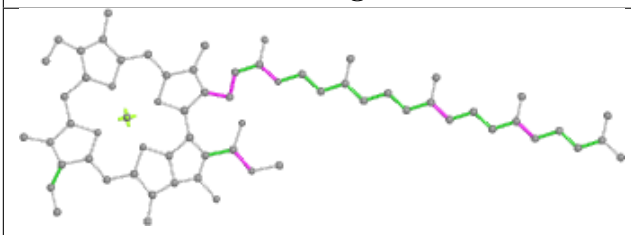

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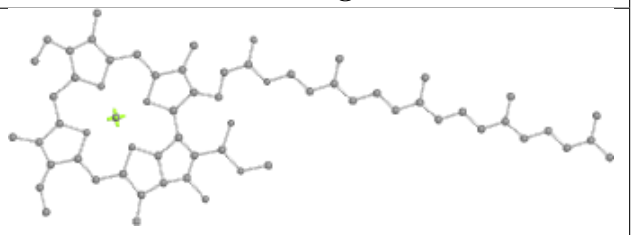

Rings

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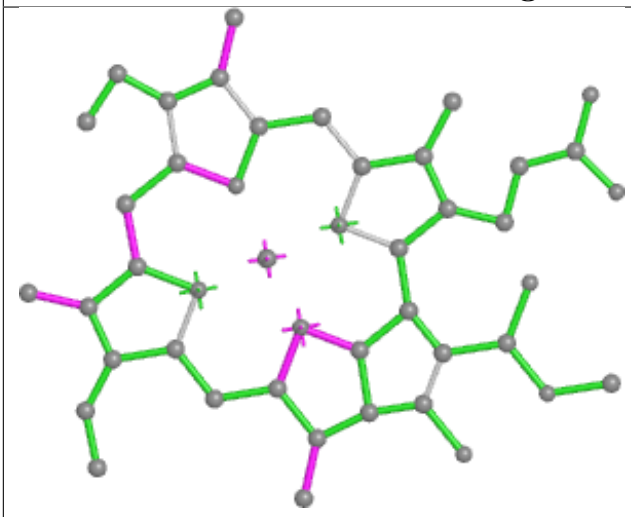

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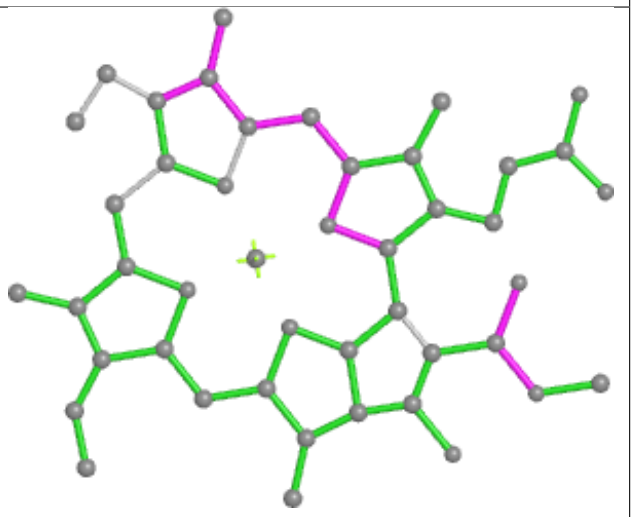

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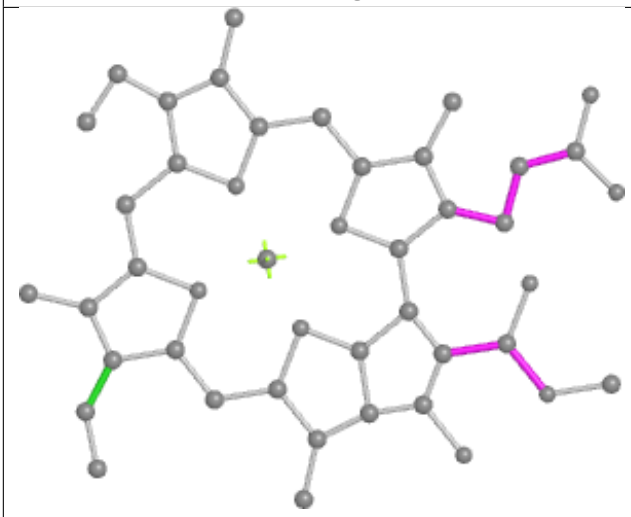

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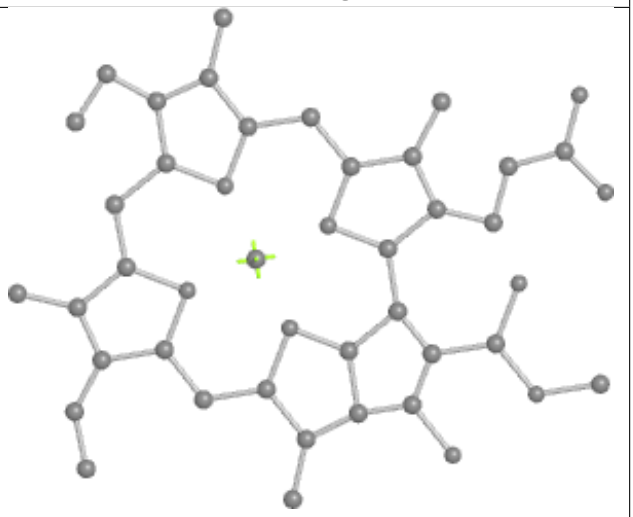

Rings

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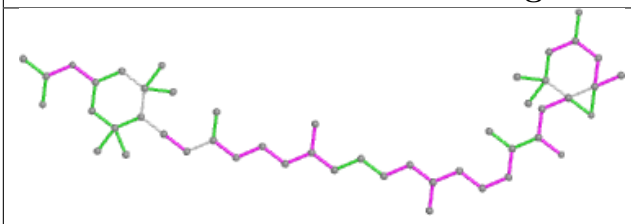

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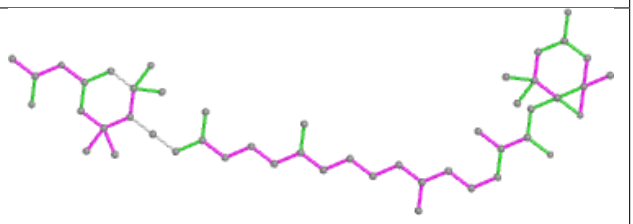

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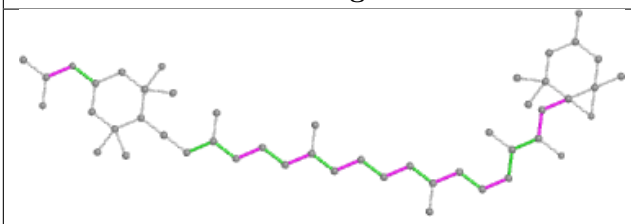

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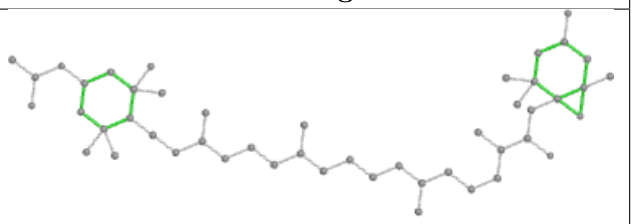

Rings

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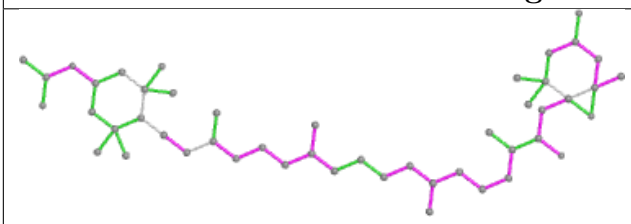

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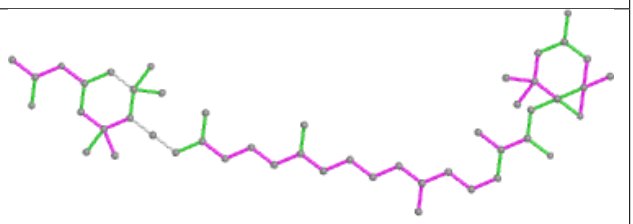

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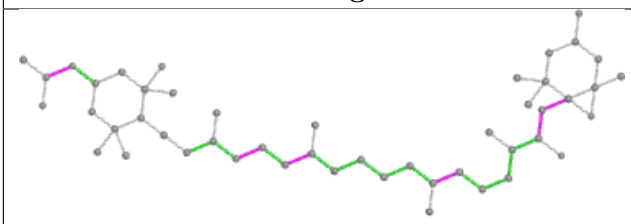

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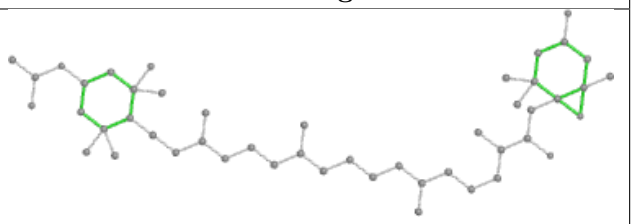

Rings

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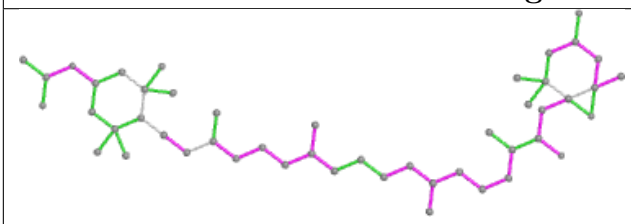

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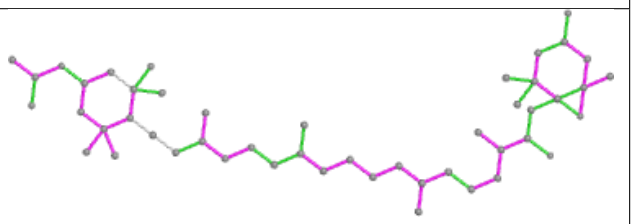

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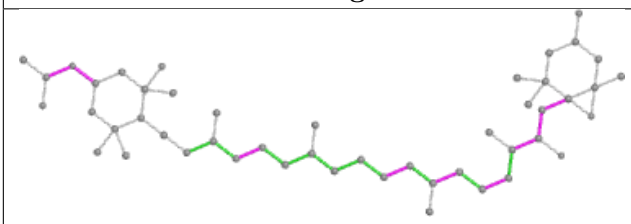

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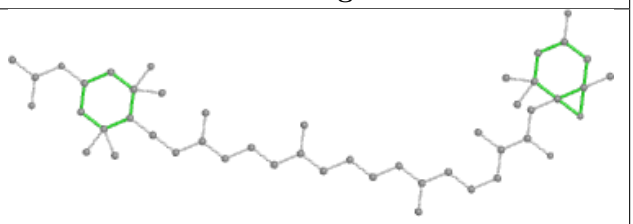

Rings

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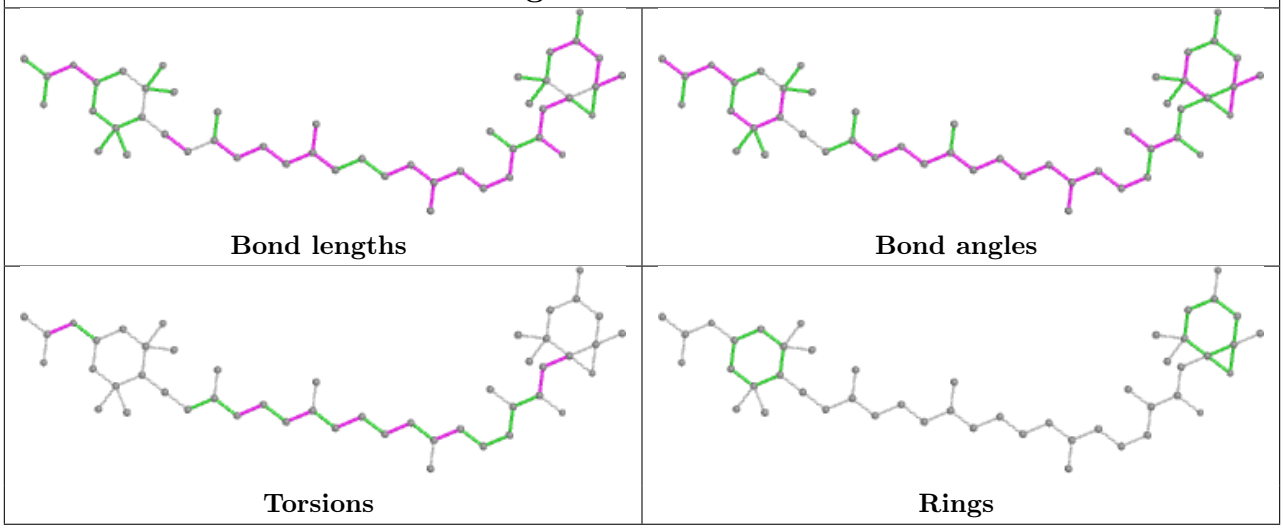

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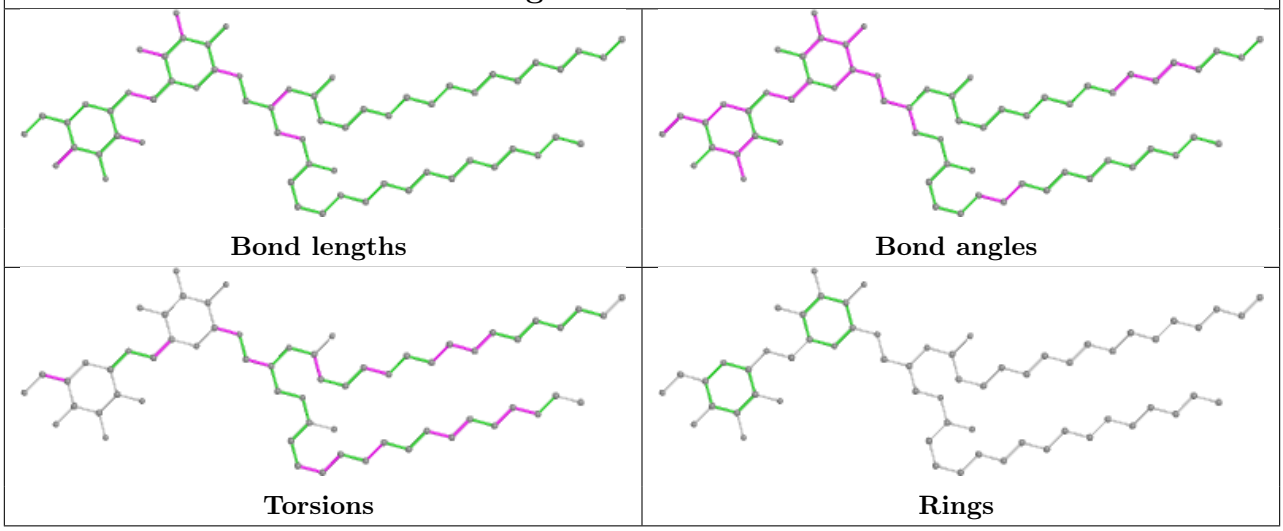

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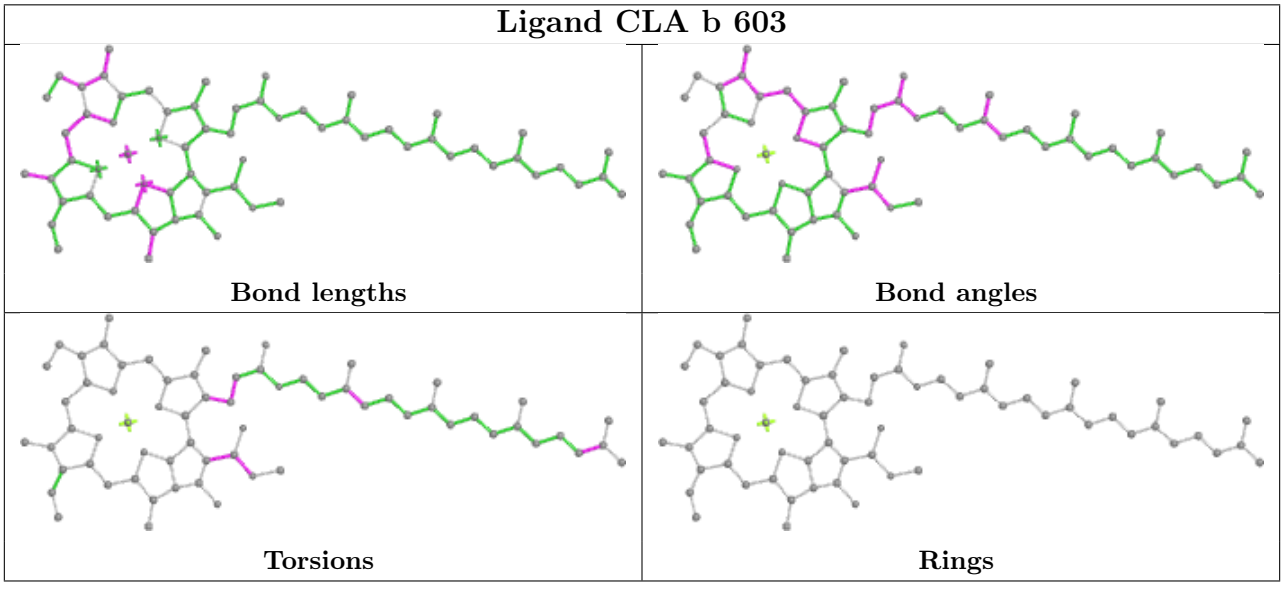

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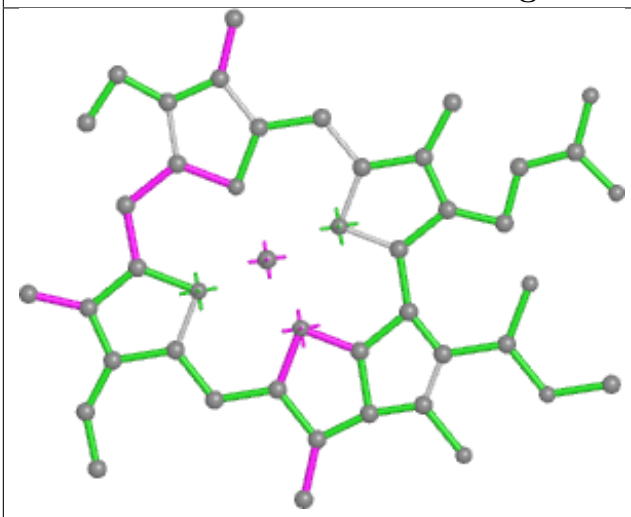

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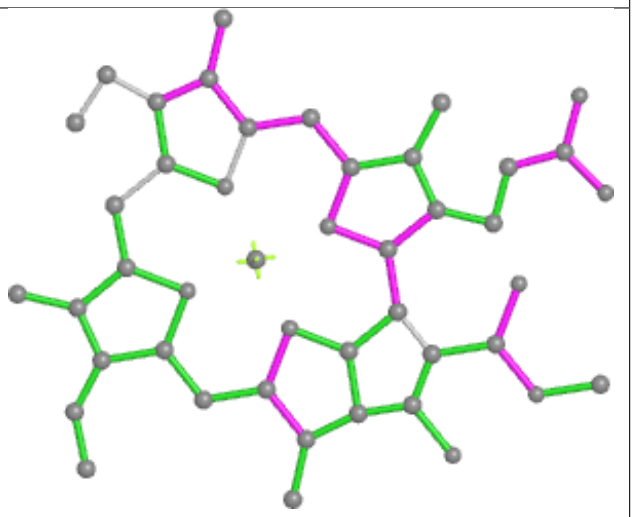
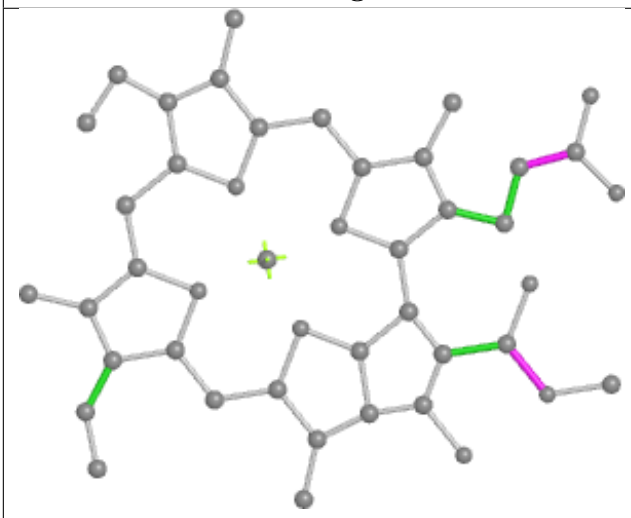


Bond angles



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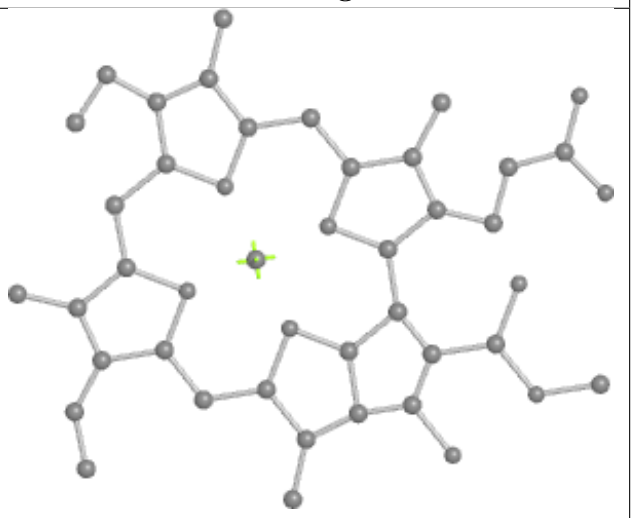
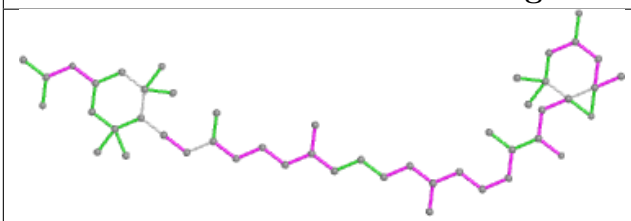


Rings

Ligand A86 41 311



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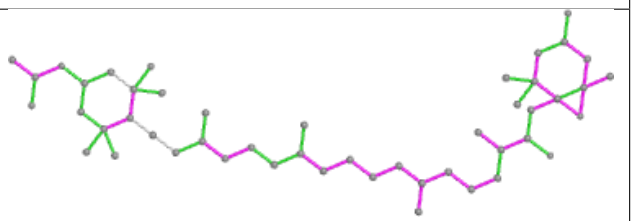

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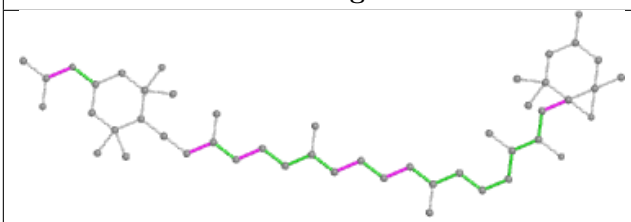

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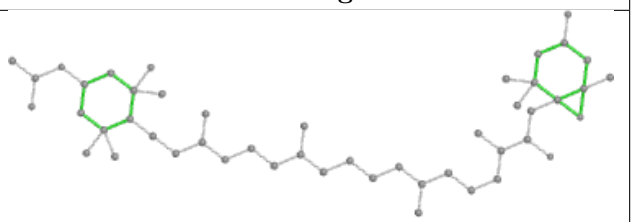

Rings

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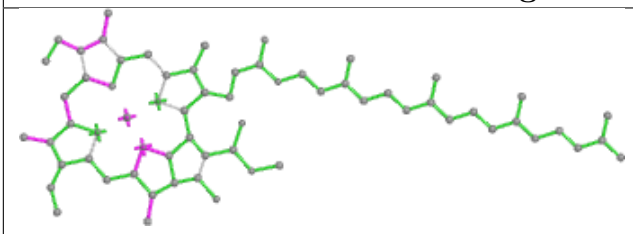

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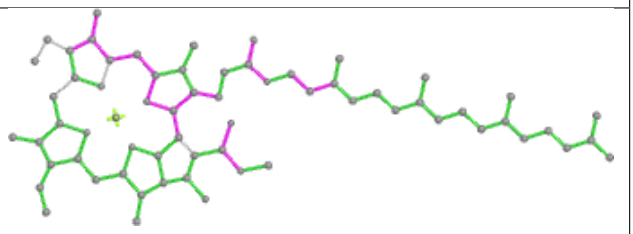

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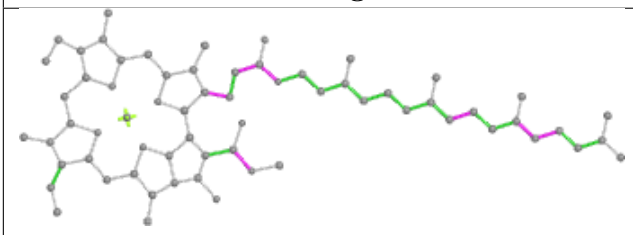

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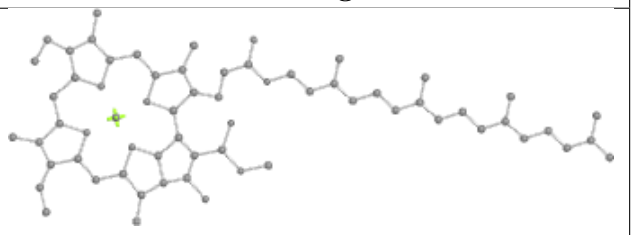

Rings

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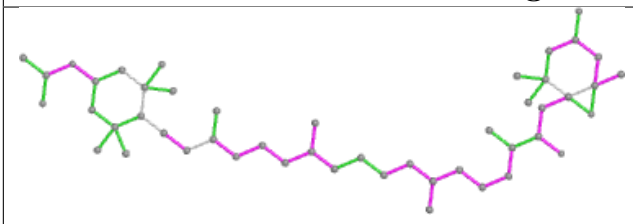

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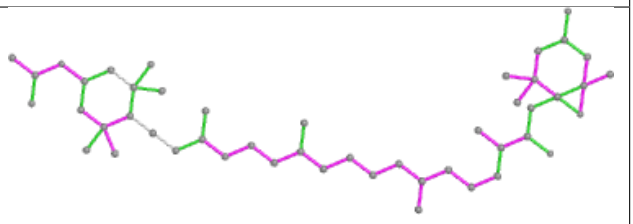

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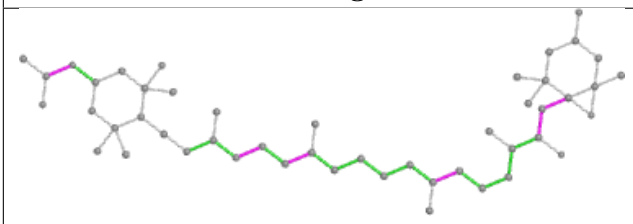

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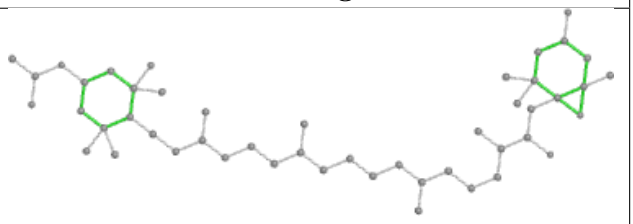
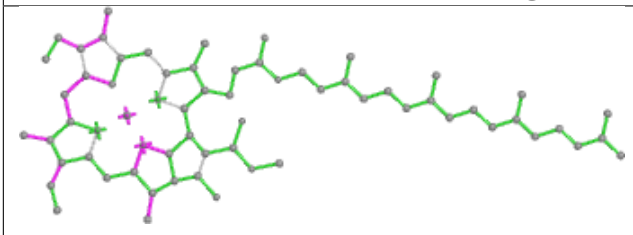


Rings

Ligand CLA D 401



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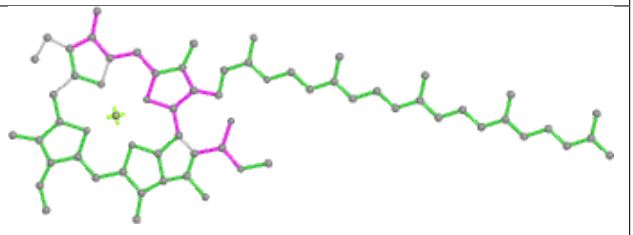

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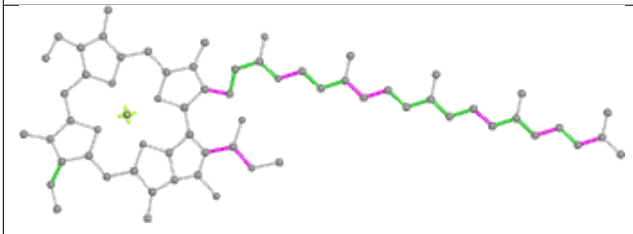

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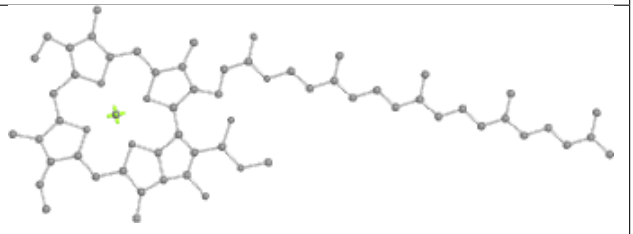
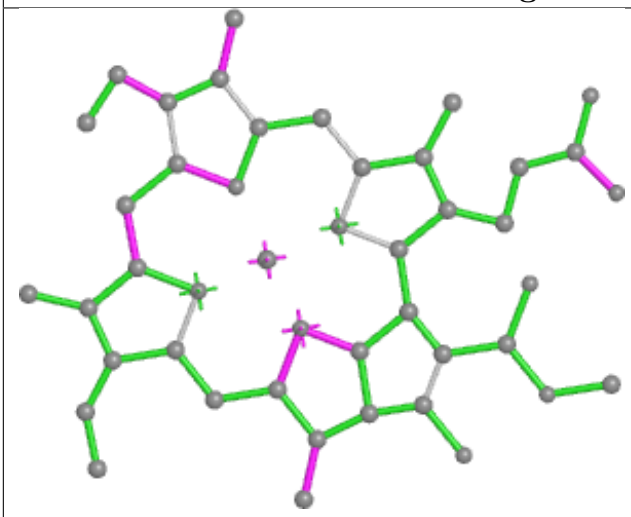


Rings

Ligand CLA 15 309



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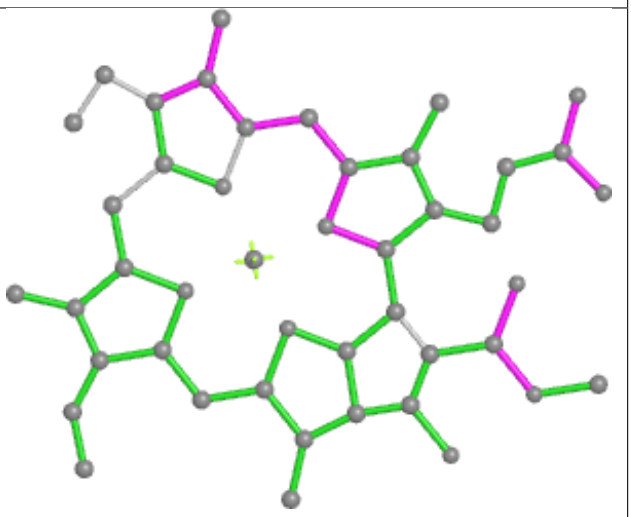

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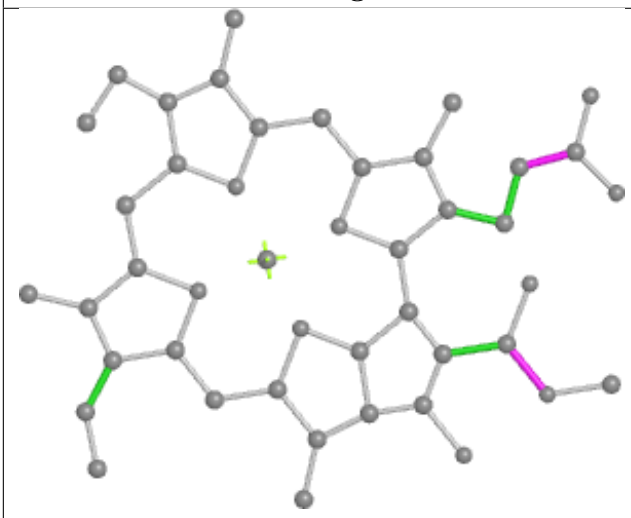

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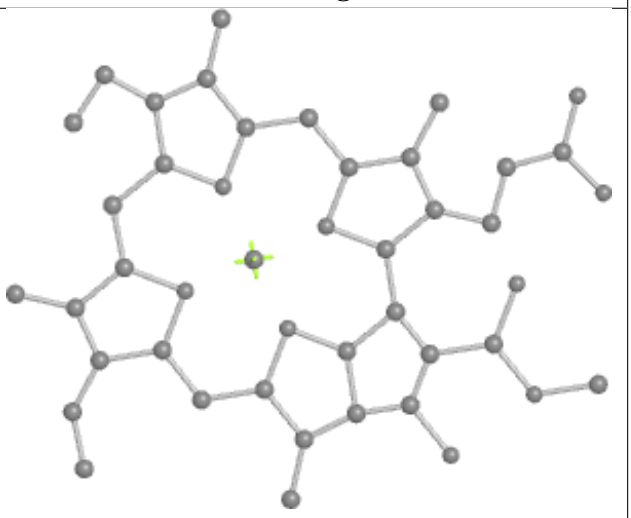

Rings

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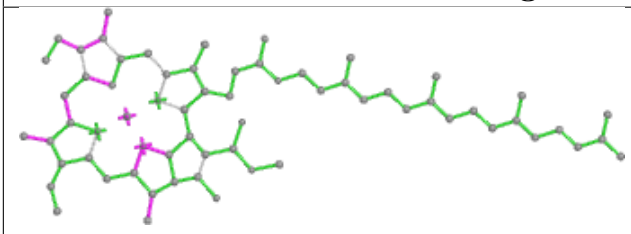

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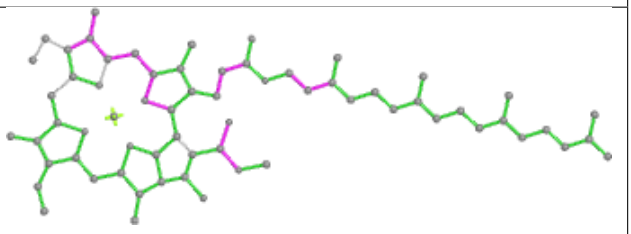

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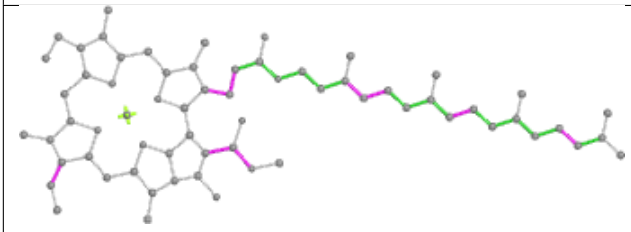

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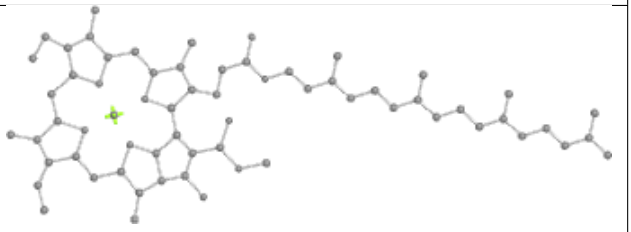
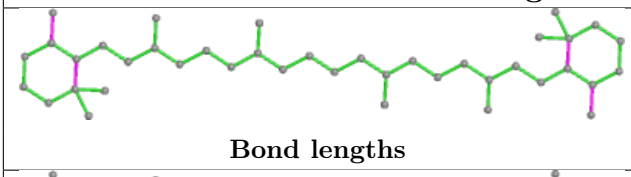


Rings

Ligand BCR h 101



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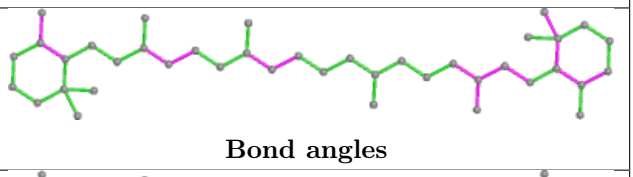

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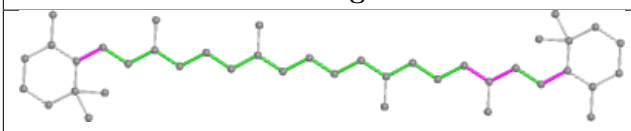

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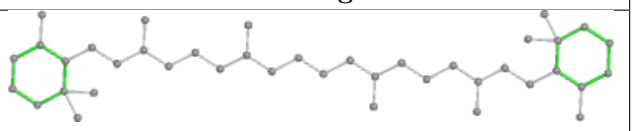
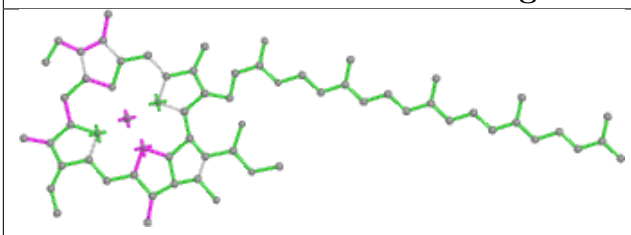


Rings

Ligand CLA 11 303



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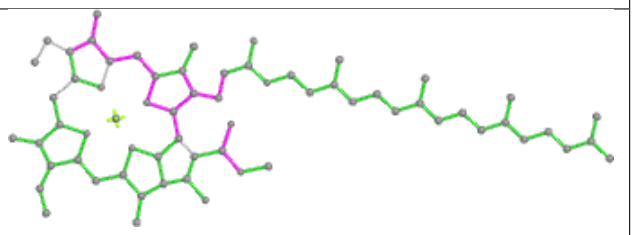

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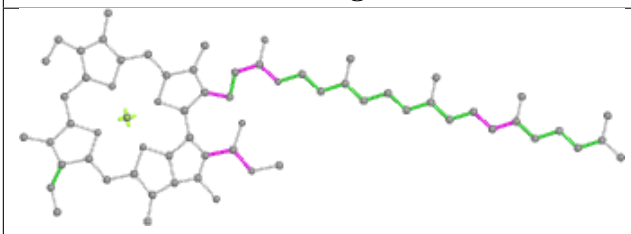
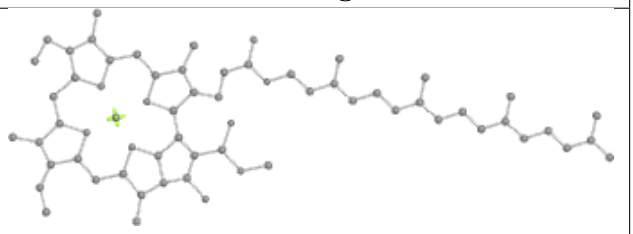
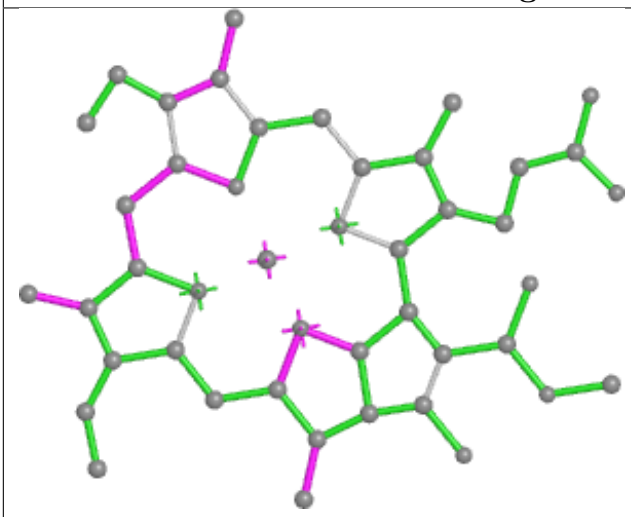


Torsions



Rings

Ligand CLA 20 205



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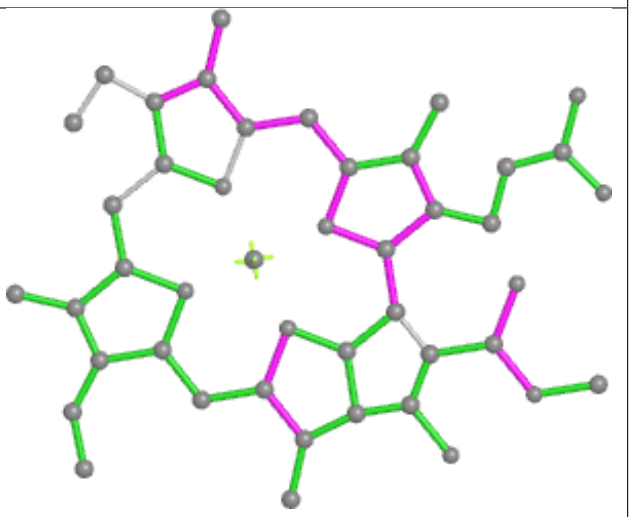

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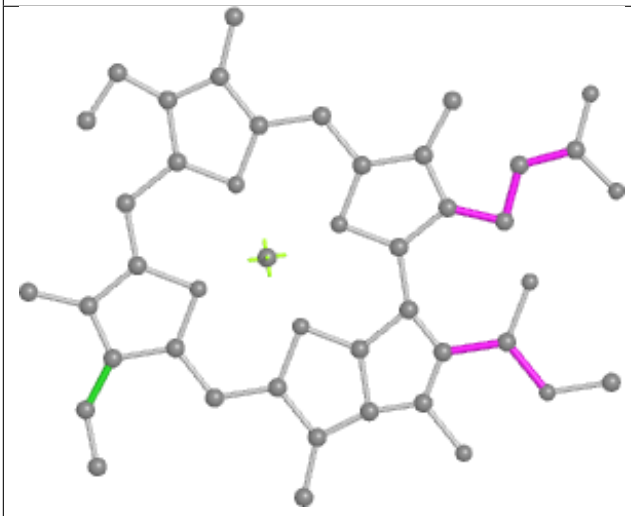

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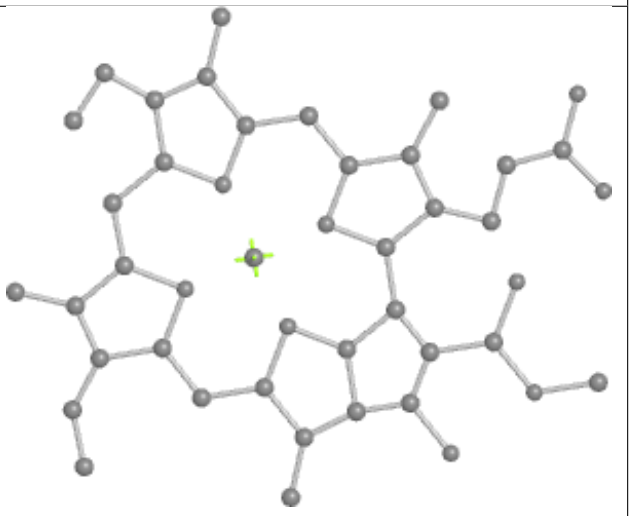
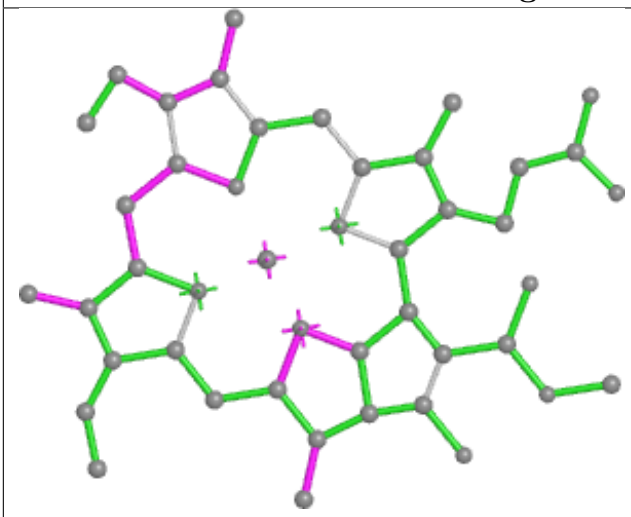


Rings

Ligand CLA 12 313



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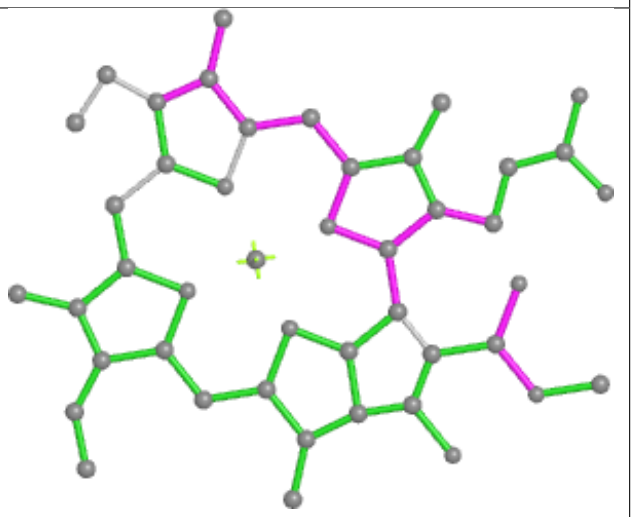

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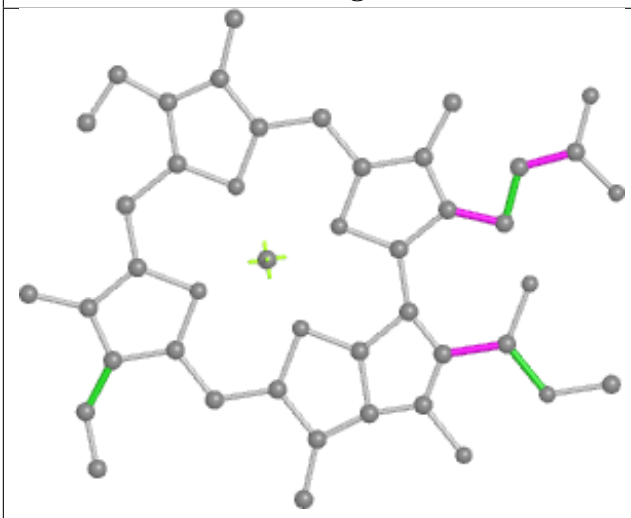

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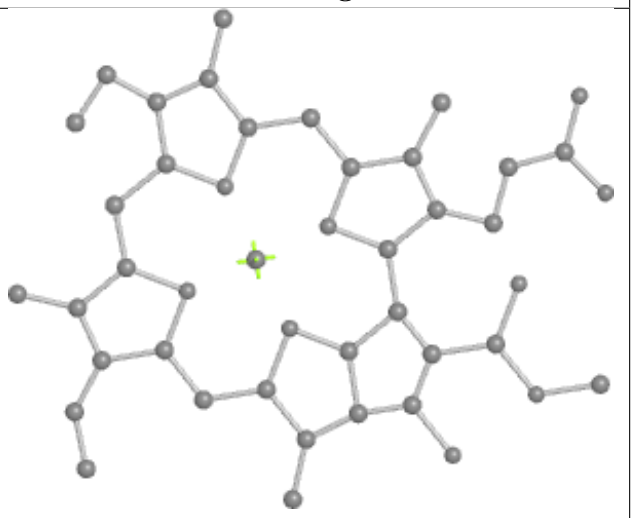
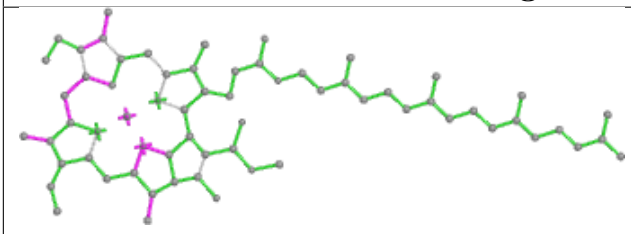


Rings

Ligand CLA 18 310



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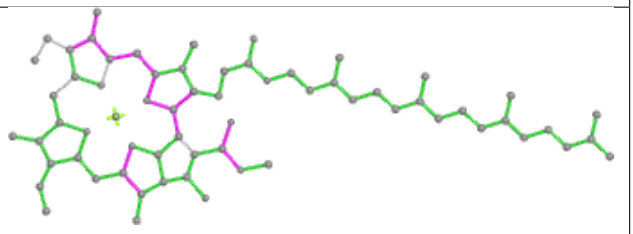

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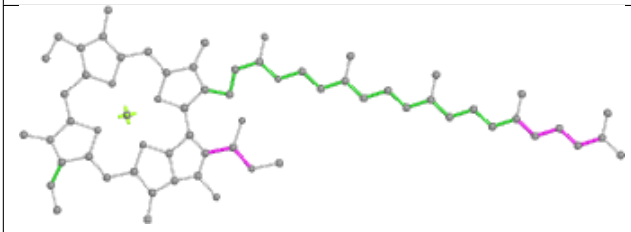

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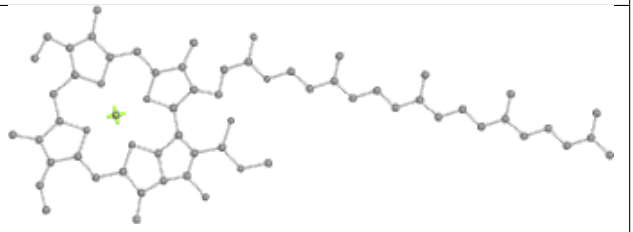
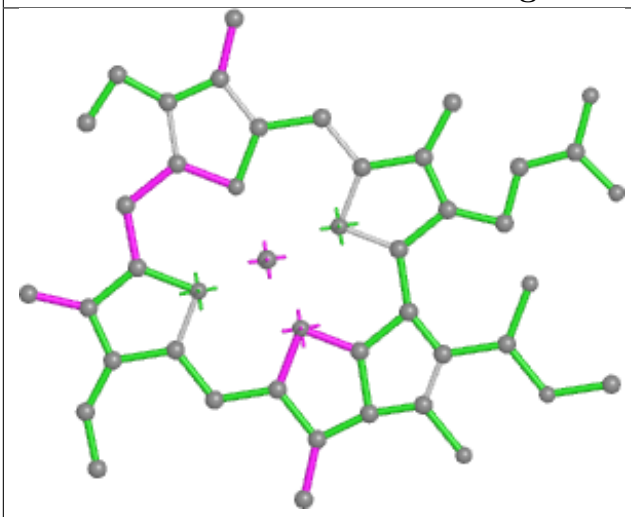


Rings

Ligand CLA 39 302



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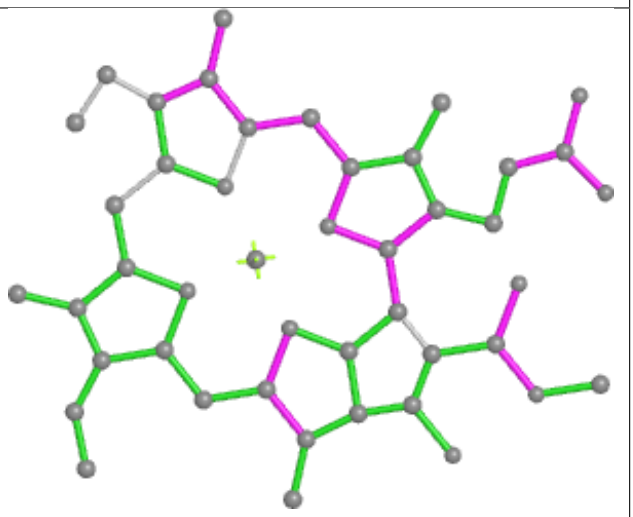

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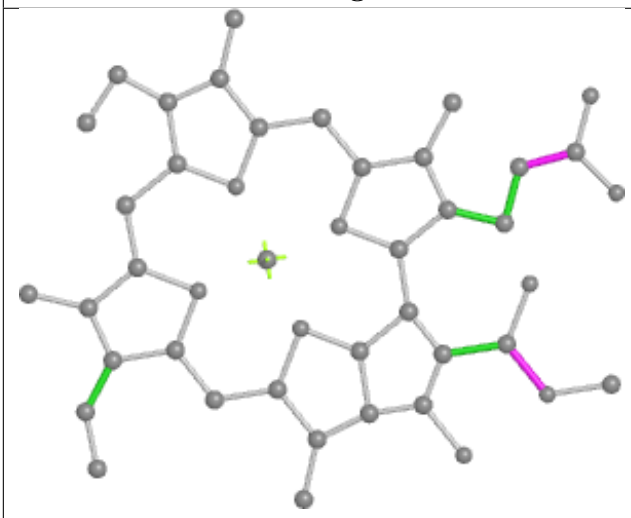

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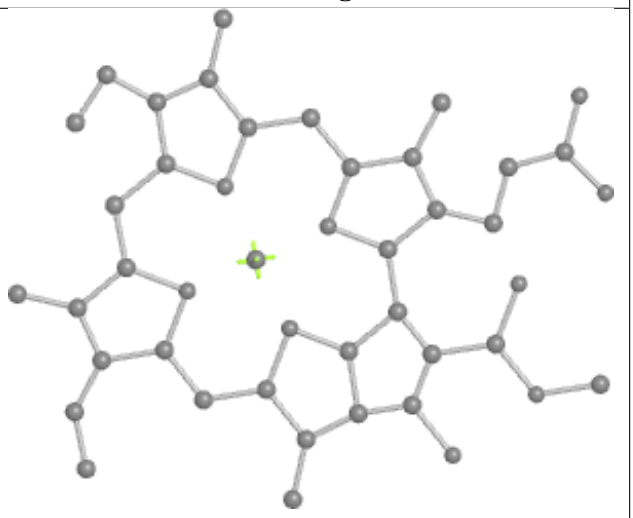
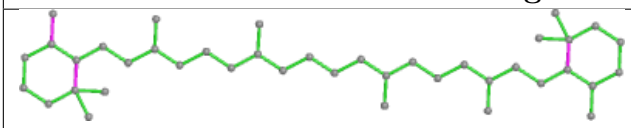


Rings

Ligand BCR F 101



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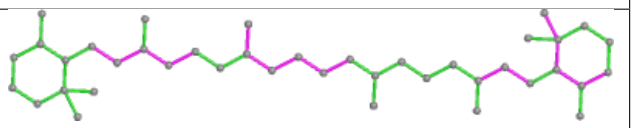

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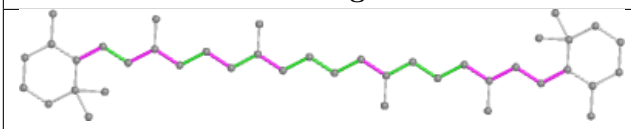

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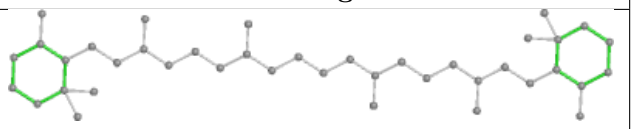
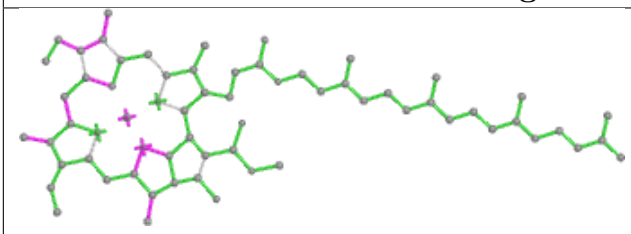


Rings

Ligand CLA 13 302



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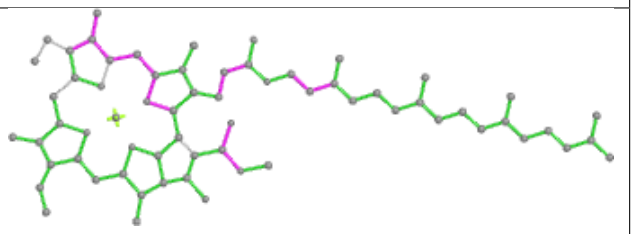

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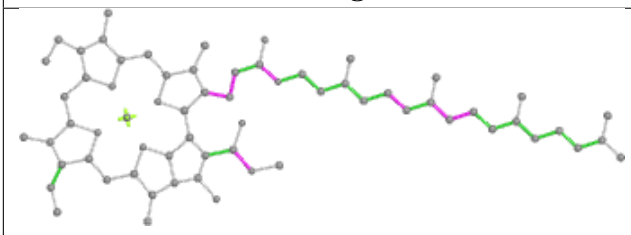

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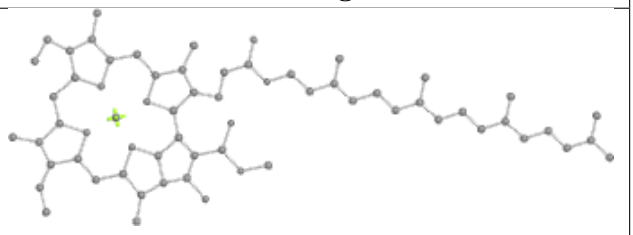
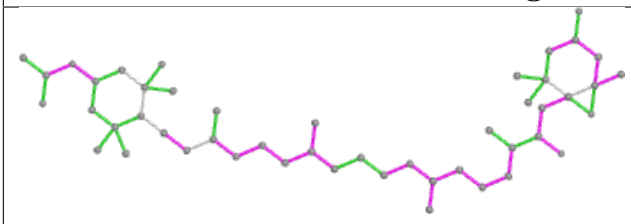


Rings

Ligand A86 32 315



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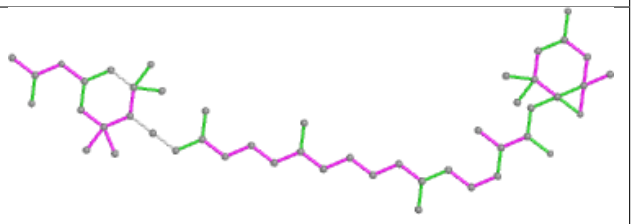

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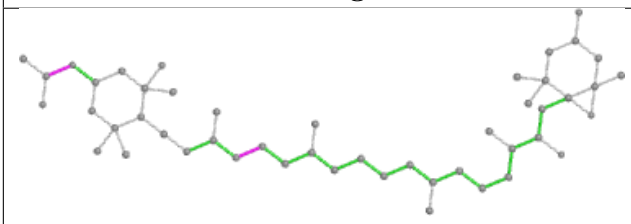

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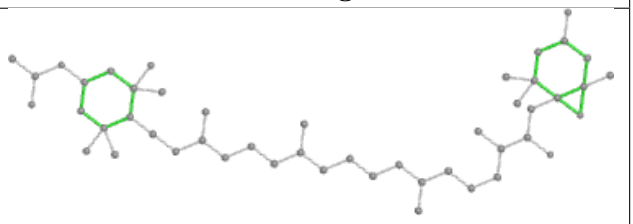
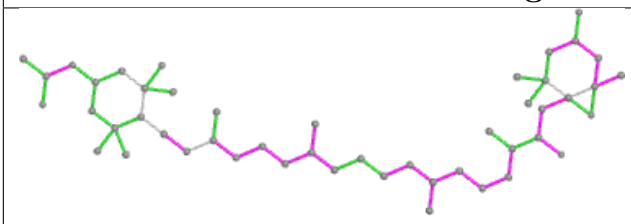


Rings

Ligand A86 21 312



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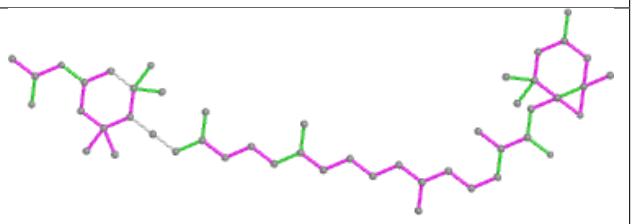

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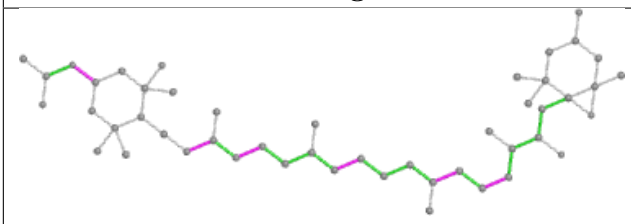

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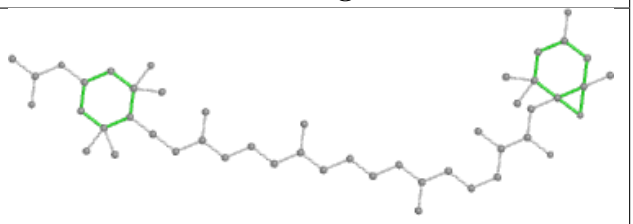
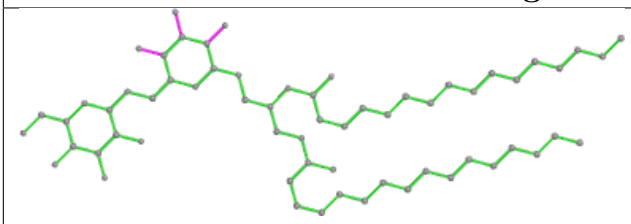


Rings

Ligand DGD h 102



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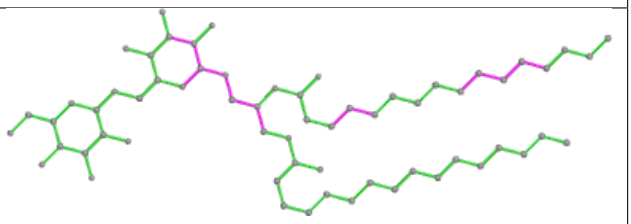

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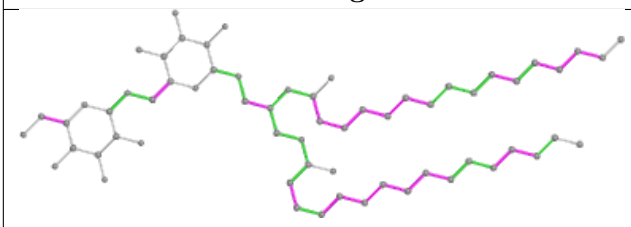

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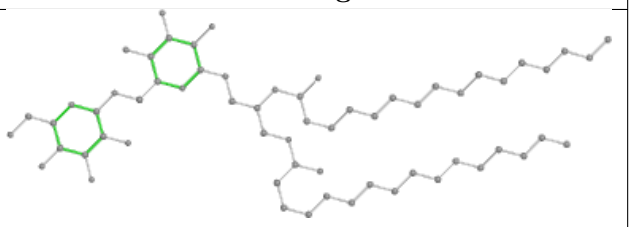
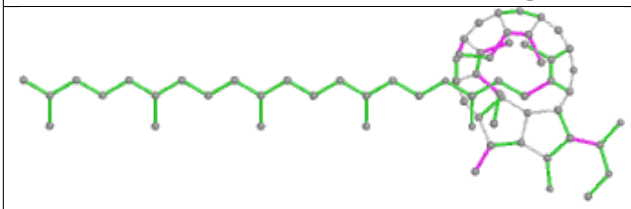


Rings

Ligand PHO A 403



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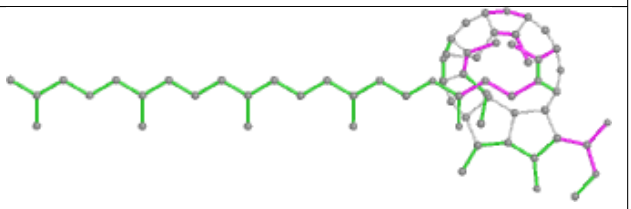

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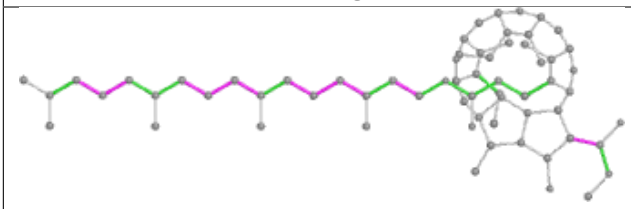

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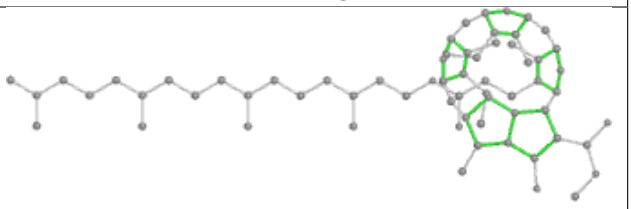
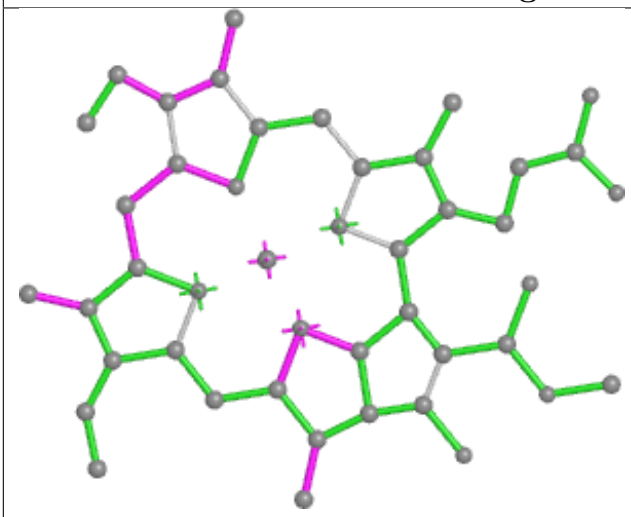


Rings

Ligand CLA 14 309



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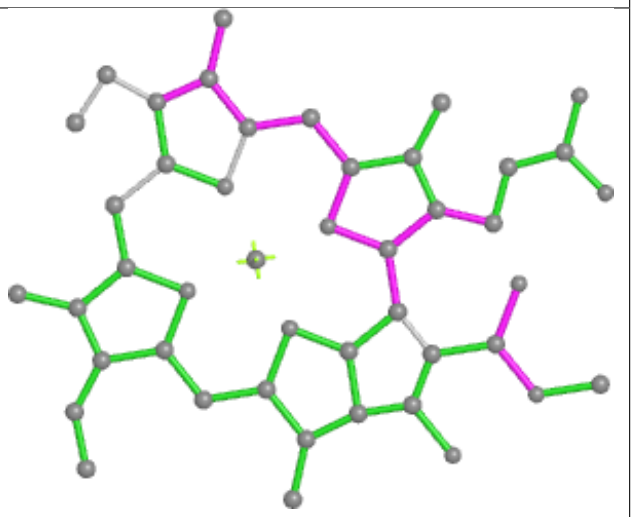
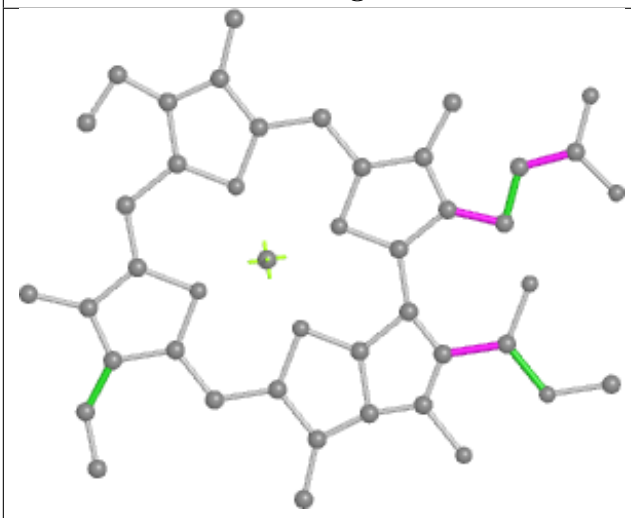


Bond angles



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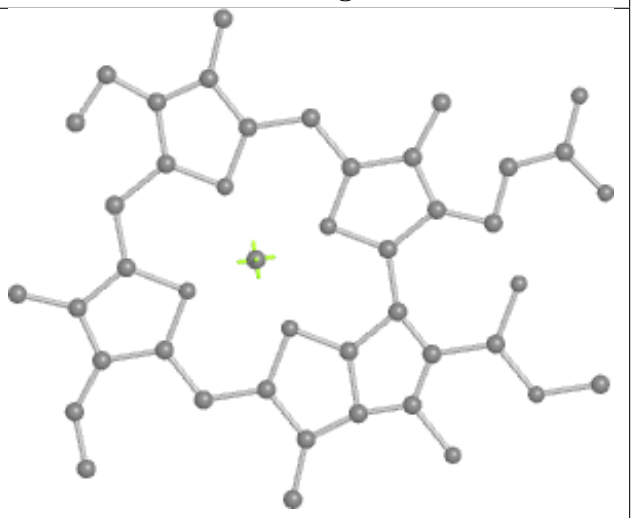
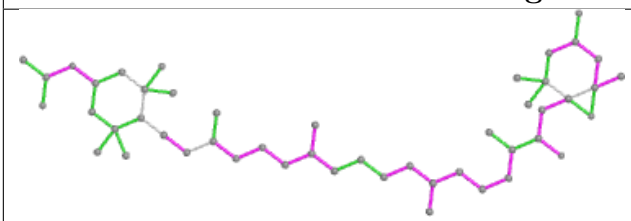


Rings

Ligand A86 17 314



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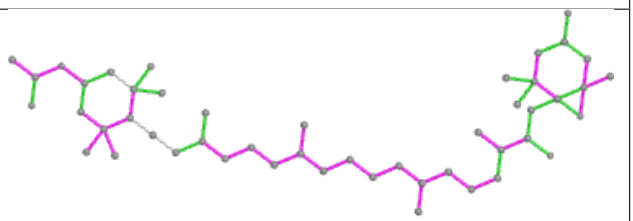
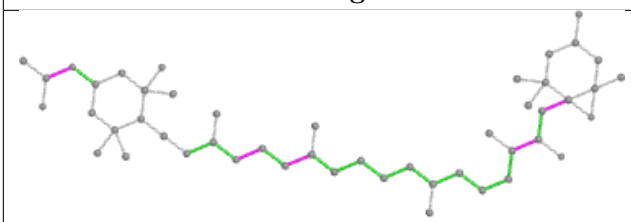


Bond angles



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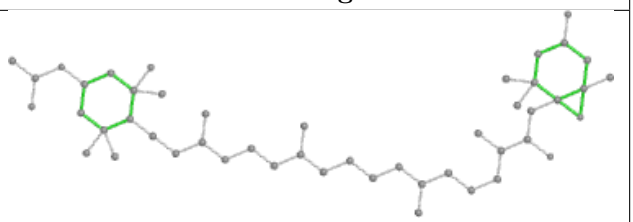
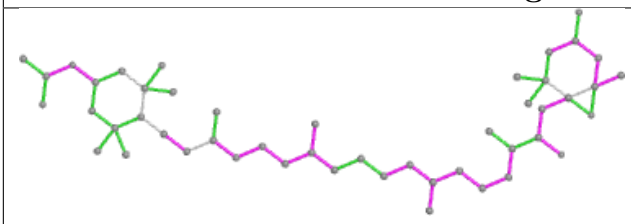


Rings

Ligand A86 37 314



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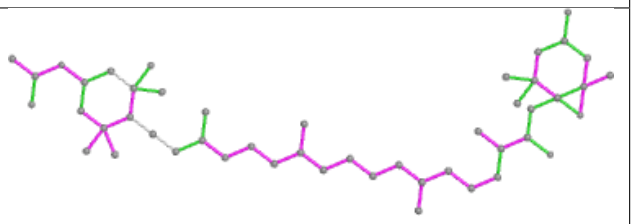

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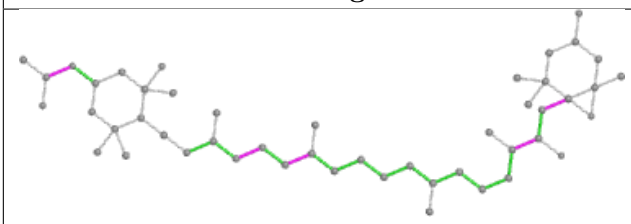

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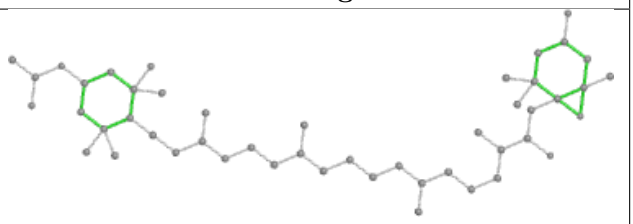
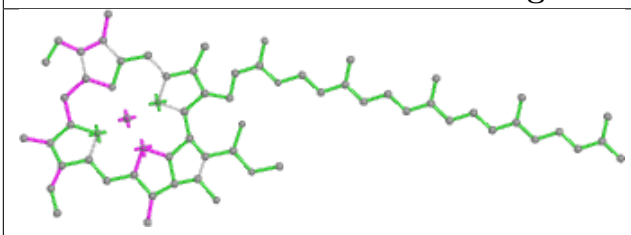
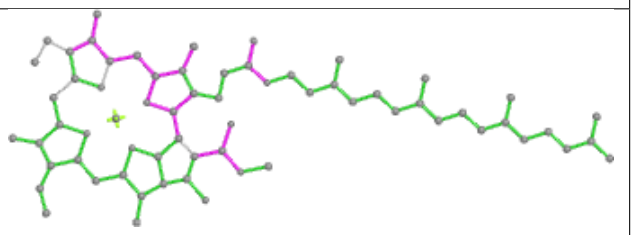


Rings

Ligand CLA b 615



Bond lengths



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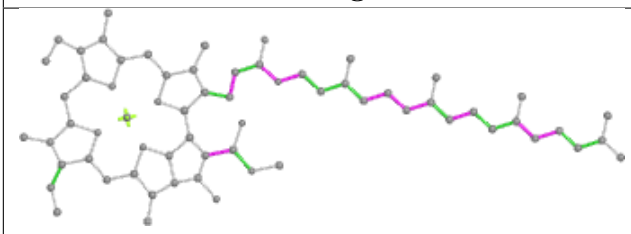
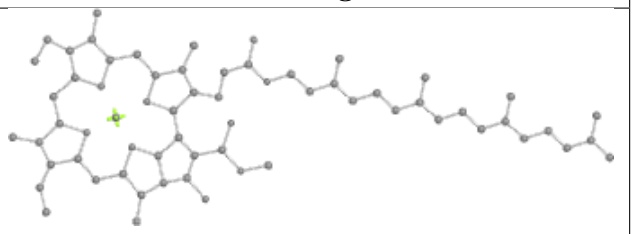
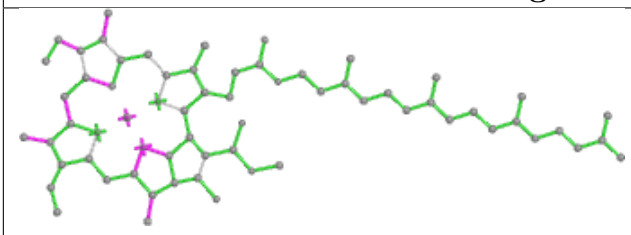


Torsions



Rings

Ligand CLA z 101



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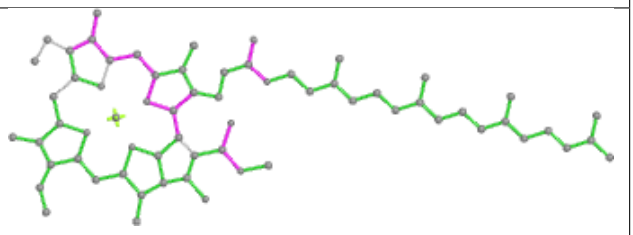

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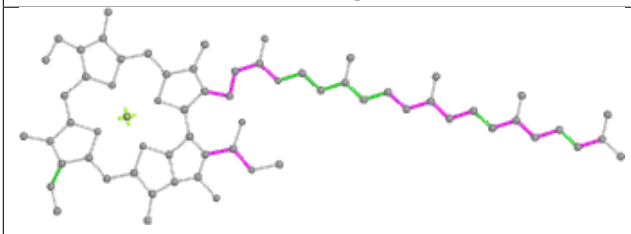

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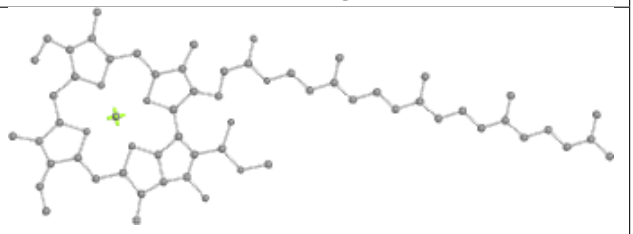
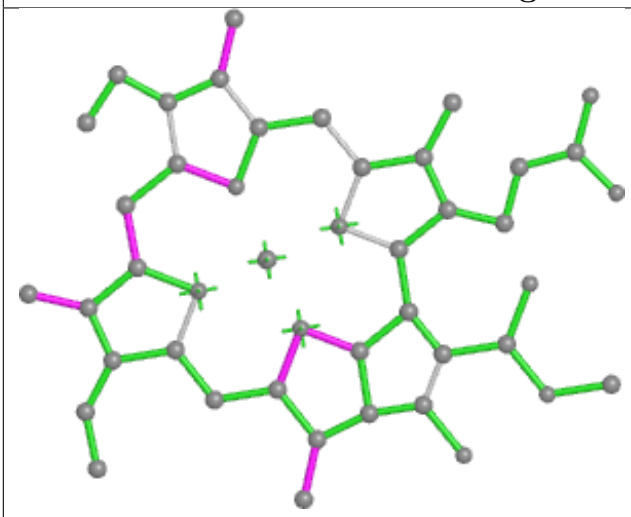


Rings

Ligand CLA 35 306



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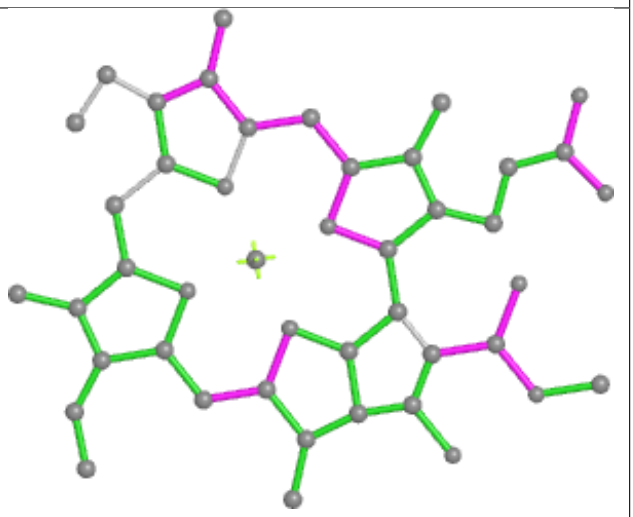

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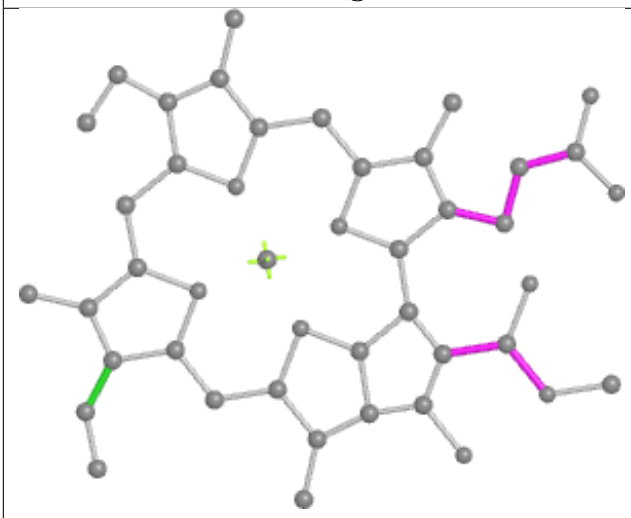

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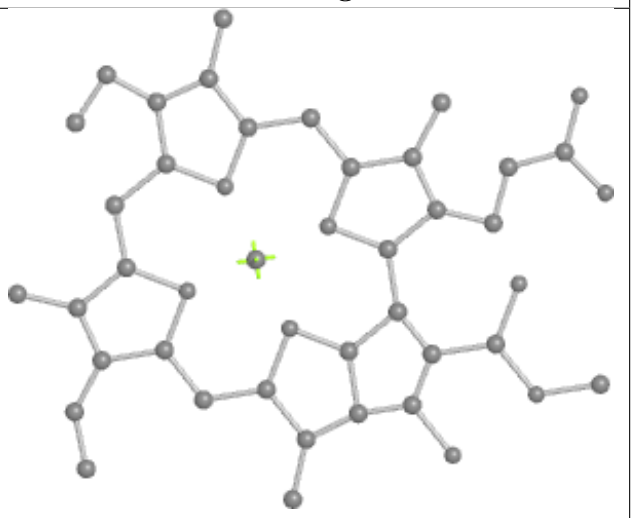
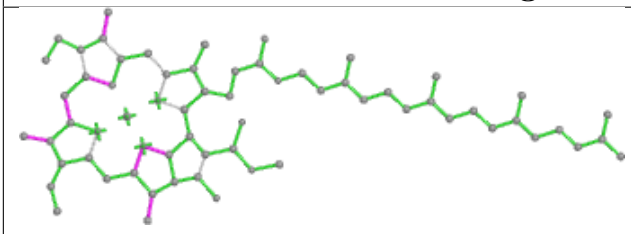


Rings

Ligand CLA 40 202



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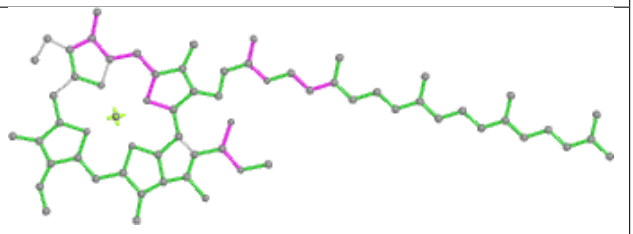

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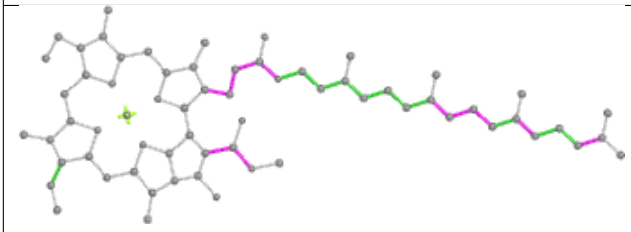

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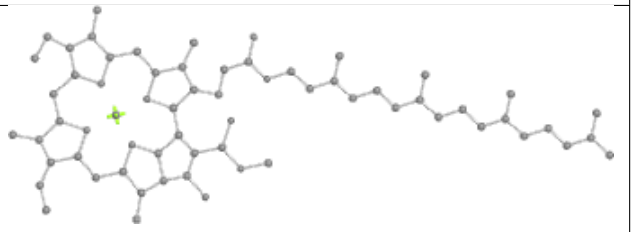
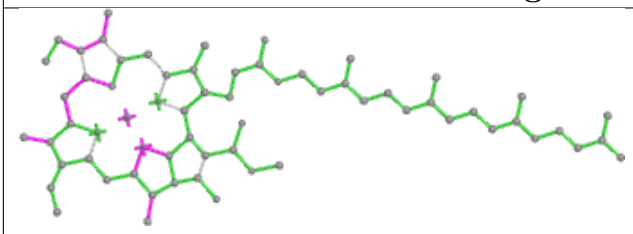


Rings

Ligand CLA C 520



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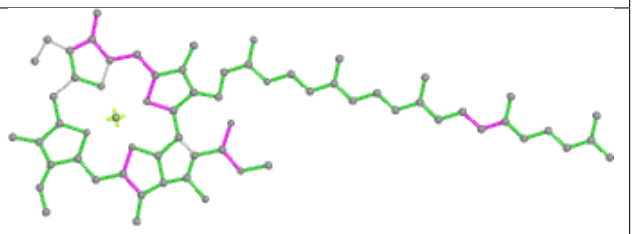

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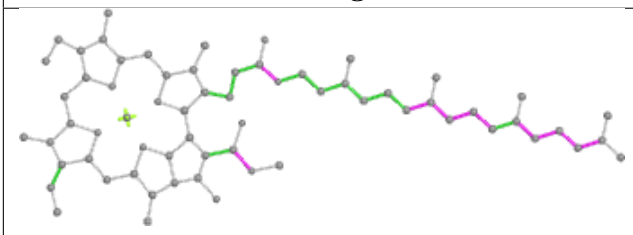

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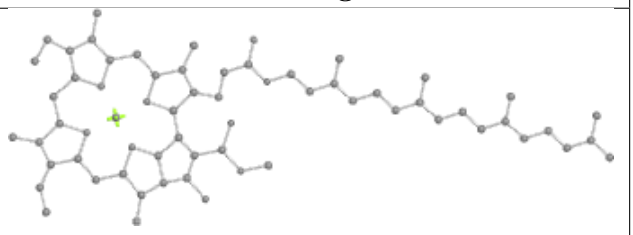
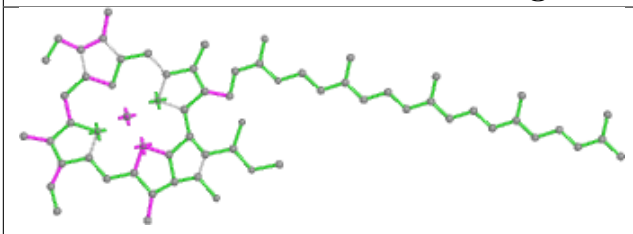


Rings

Ligand CLA c 511



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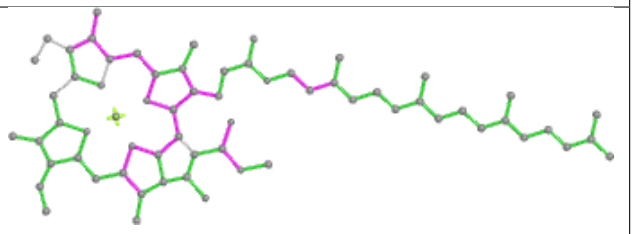

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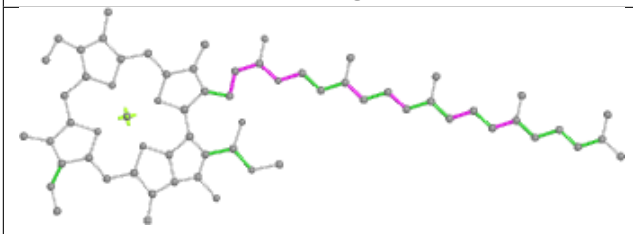

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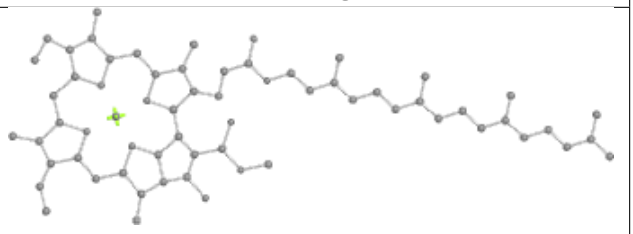
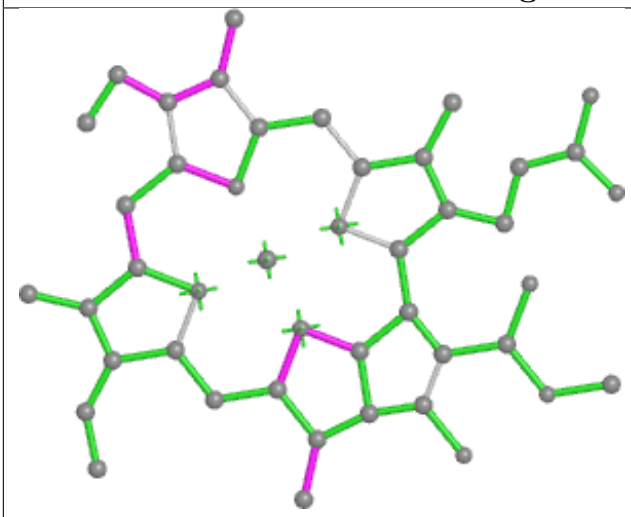


Rings

Ligand CLA 14 307



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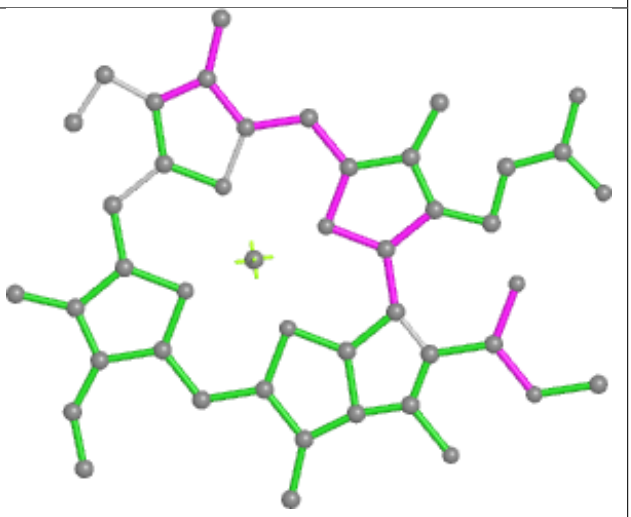

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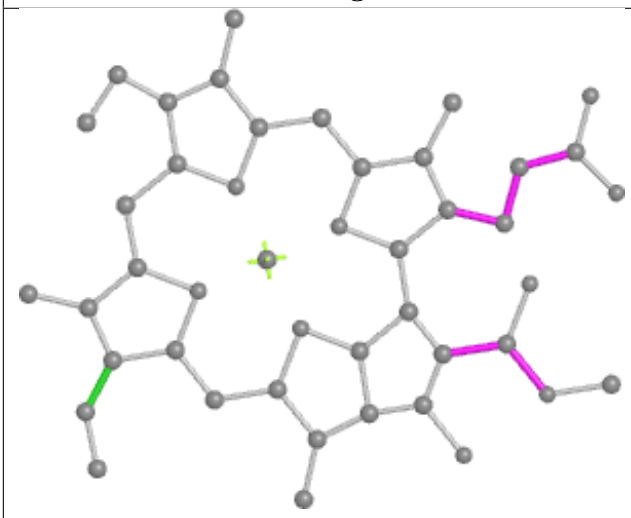

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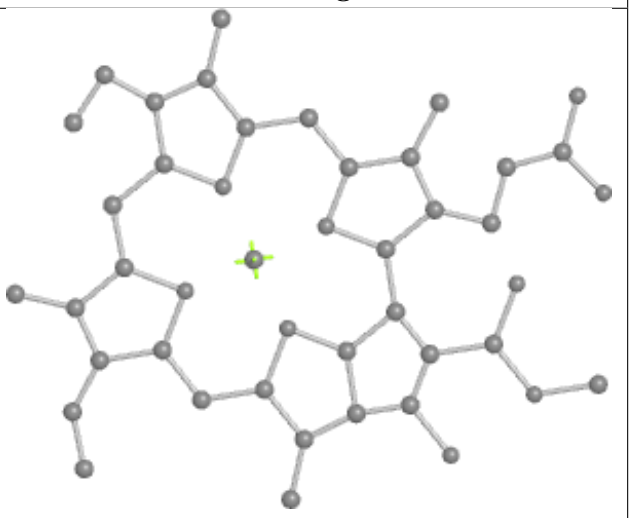
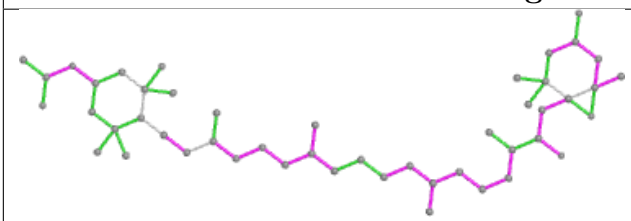


Rings

Ligand A86 13 317



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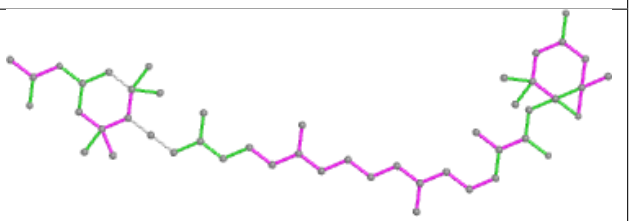

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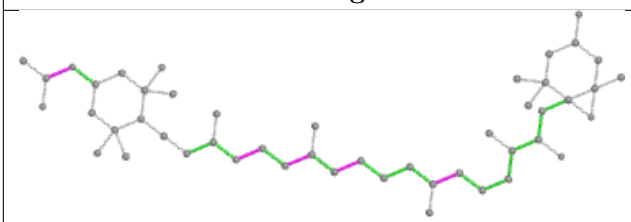

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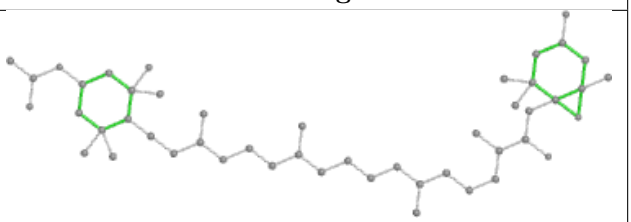
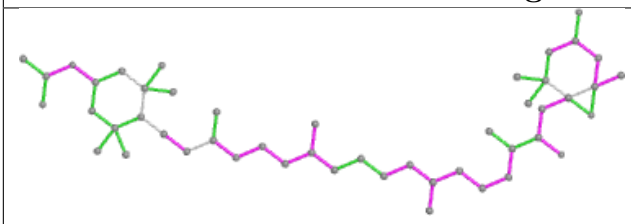


Rings

Ligand A86 17 315



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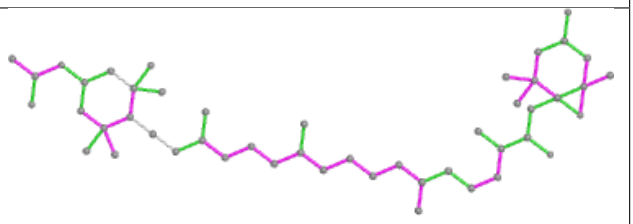

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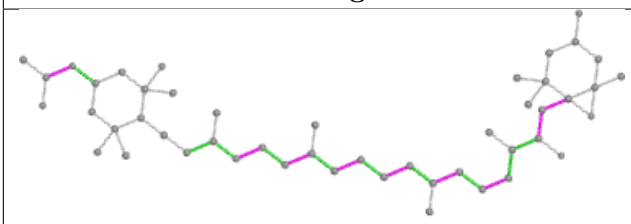

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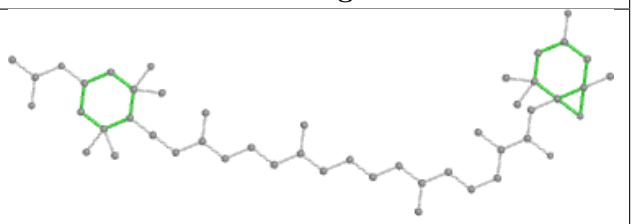
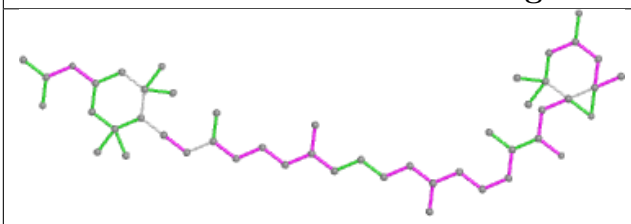


Rings

Ligand A86 13 314



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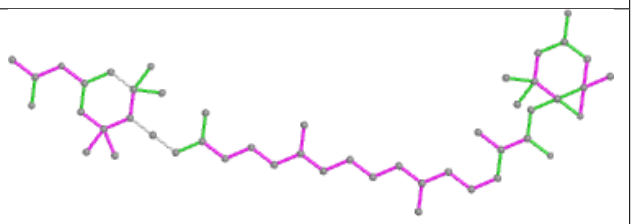

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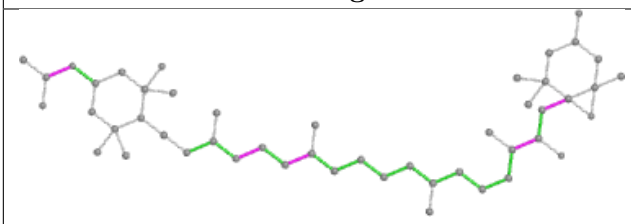

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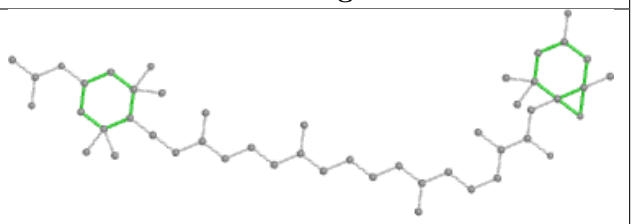
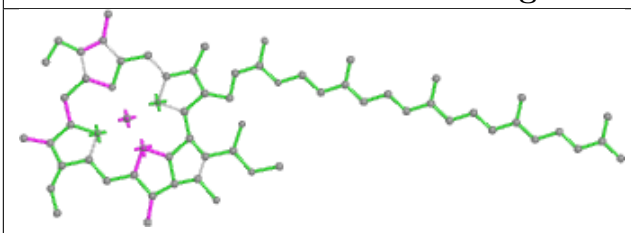


Rings

Ligand CLA 12 303



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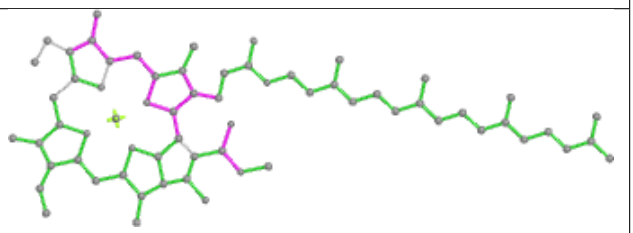

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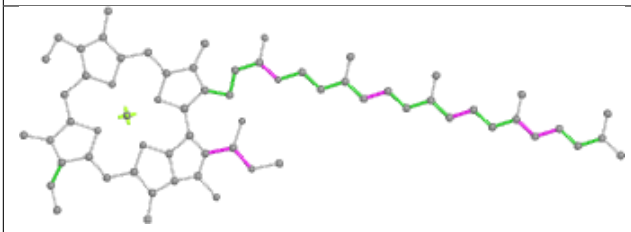

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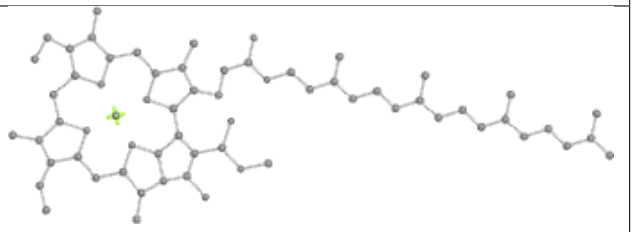
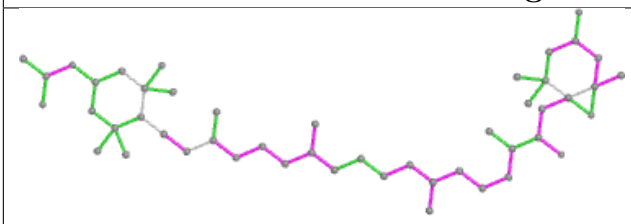


Rings

Ligand A86 12 317



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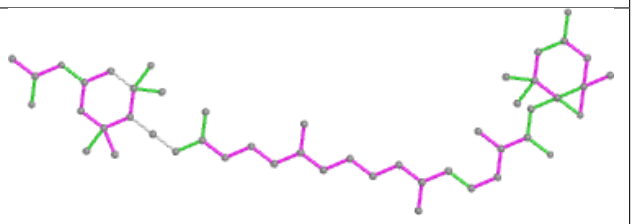
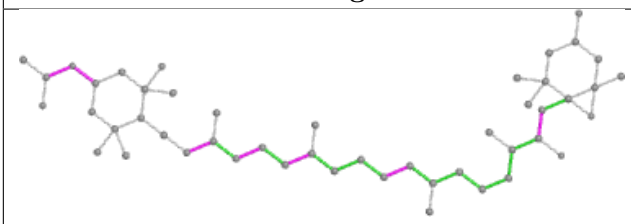


Bond angles



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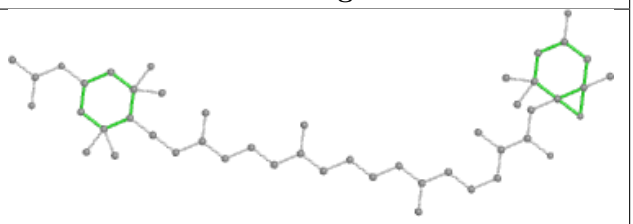
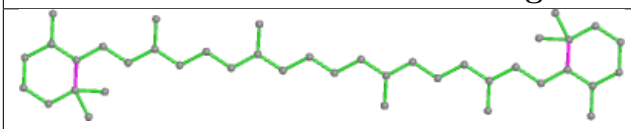


Rings

Ligand BCR b 617



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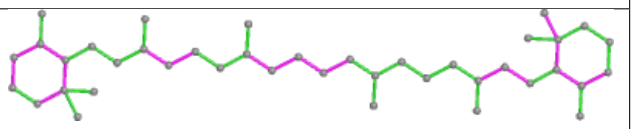
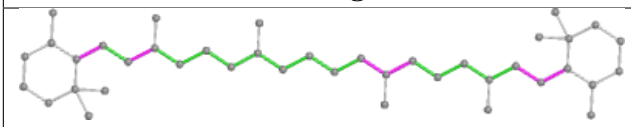
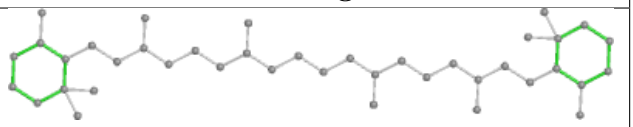


Bond angles

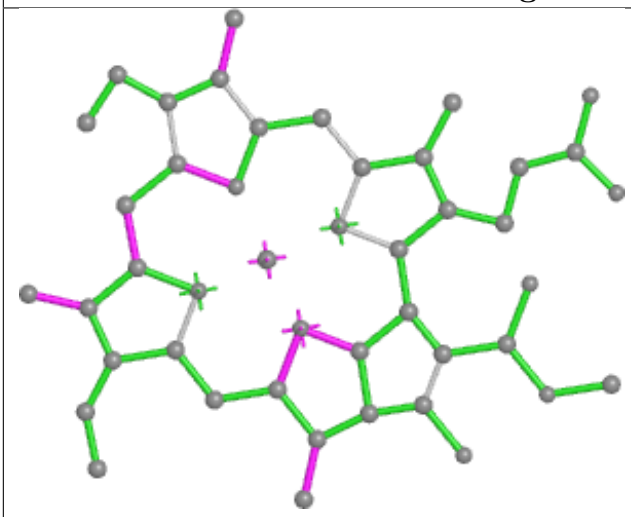


Torsions



Rings

Ligand CLA 11 309



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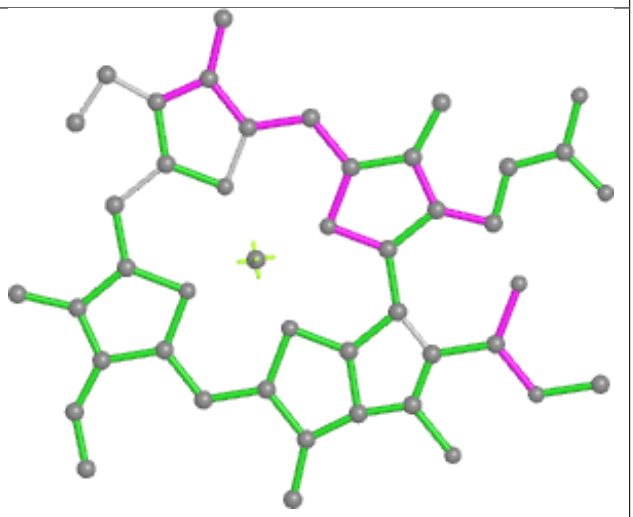
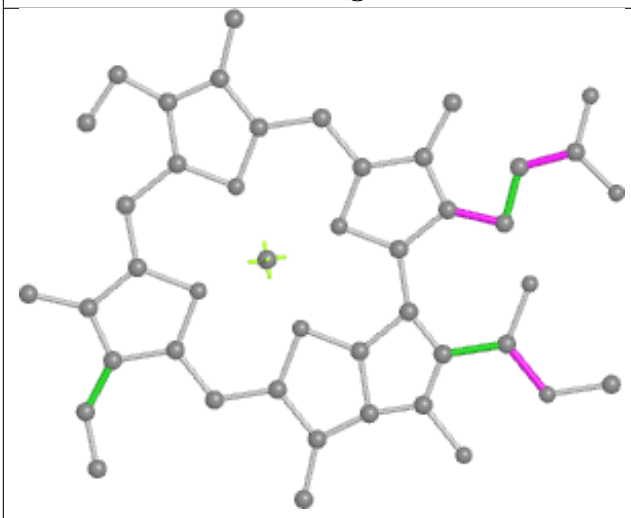


Bond angles



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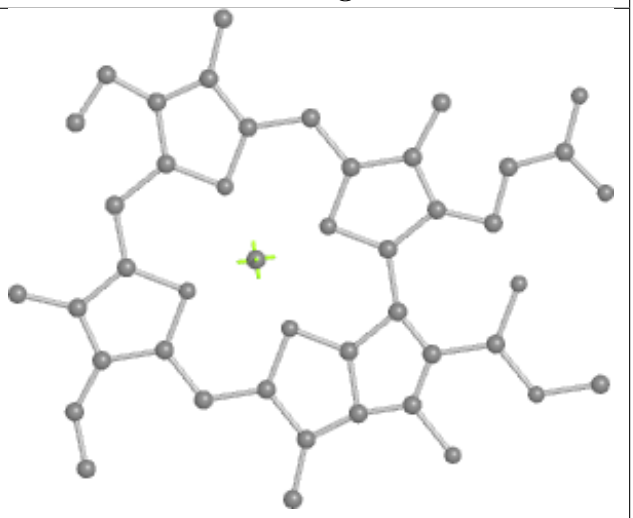
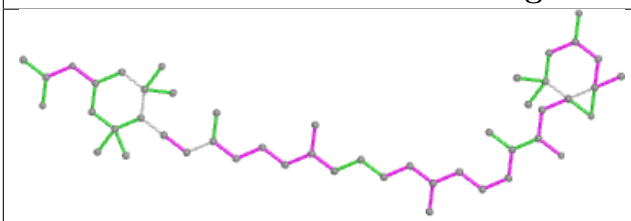
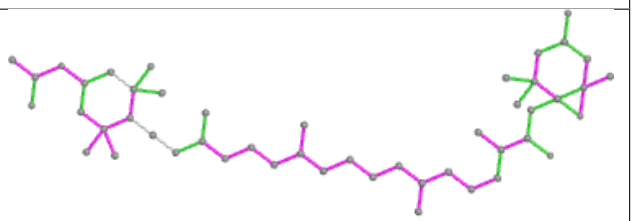


Rings

Ligand A86 34 314



Bond lengths



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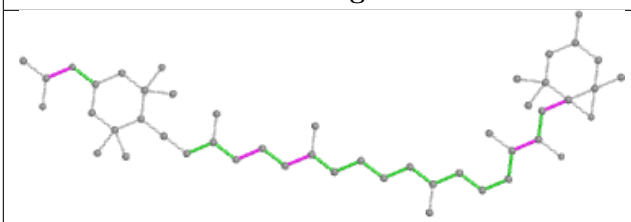
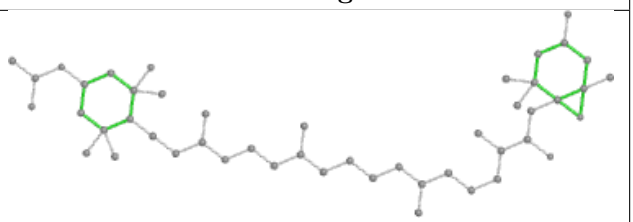
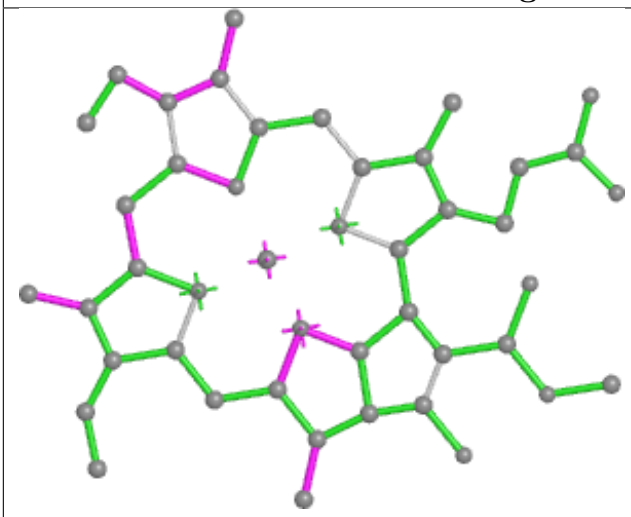


Torsions



Rings

Ligand CLA 31 306



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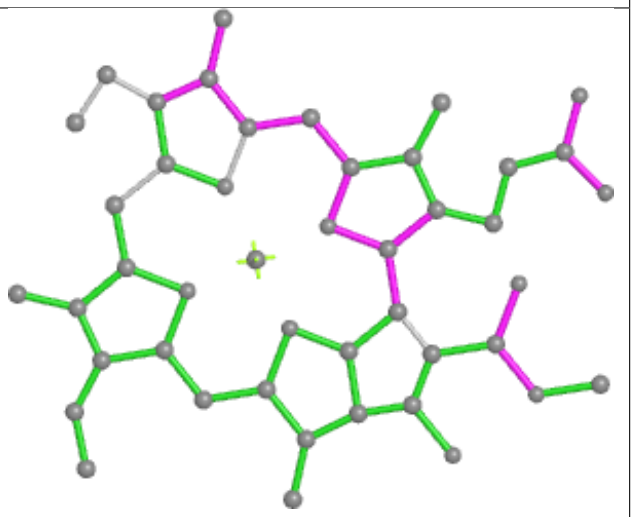

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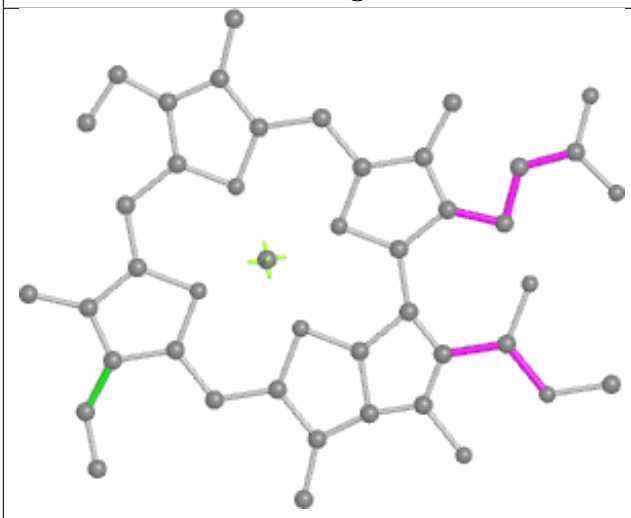

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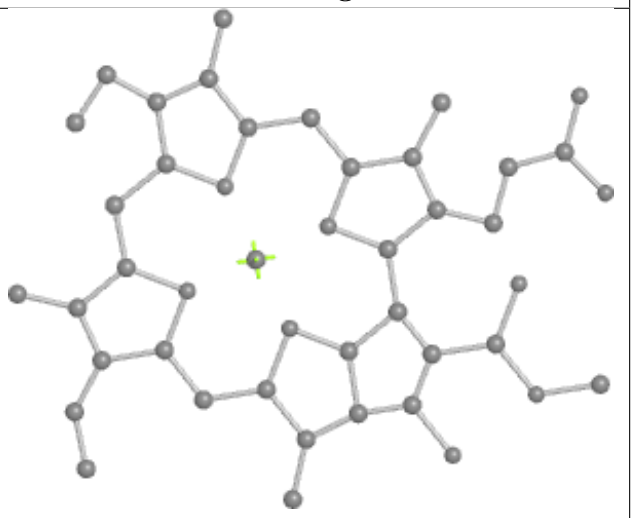
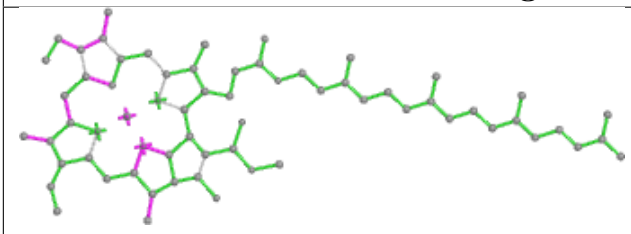


Rings

Ligand CLA 18 303



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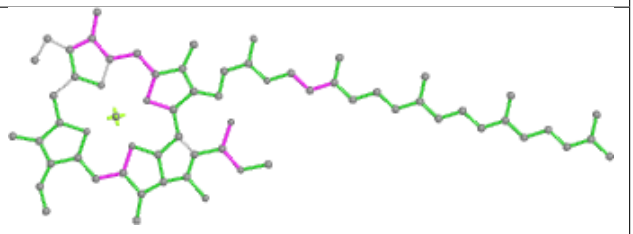

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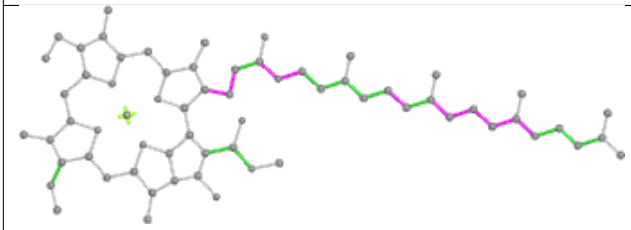

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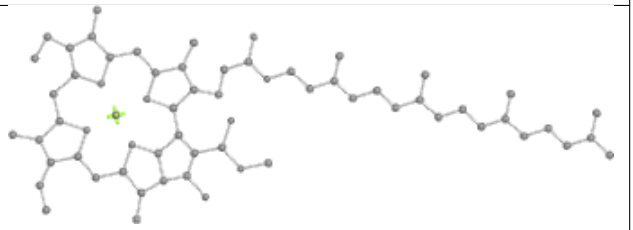
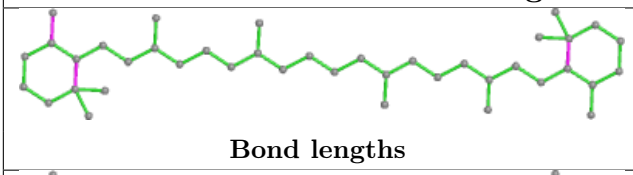


Rings

Ligand BCR b 623



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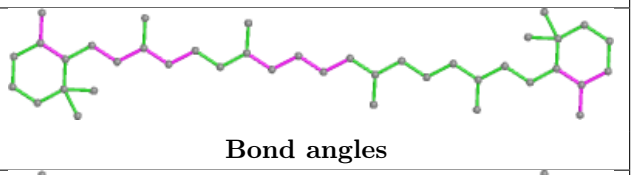

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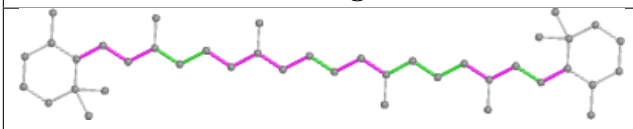

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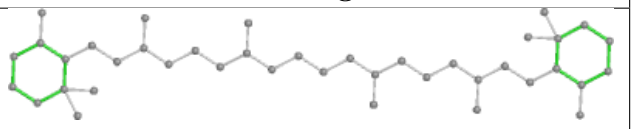
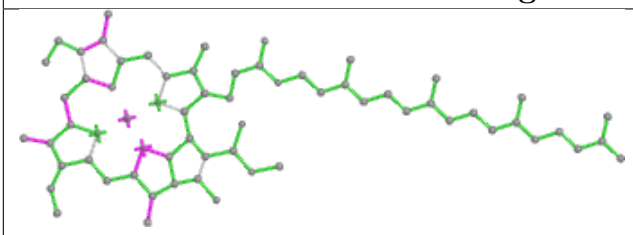


Rings

Ligand CLA W 102



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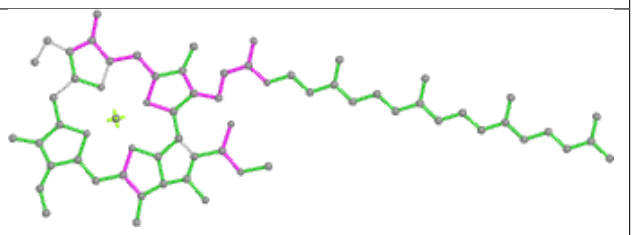
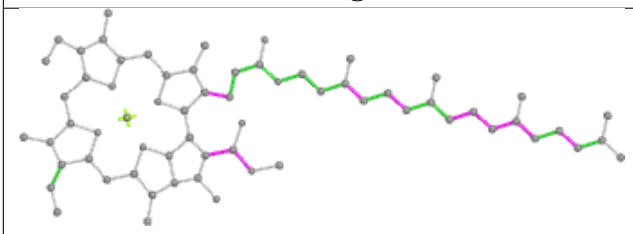


Bond angles



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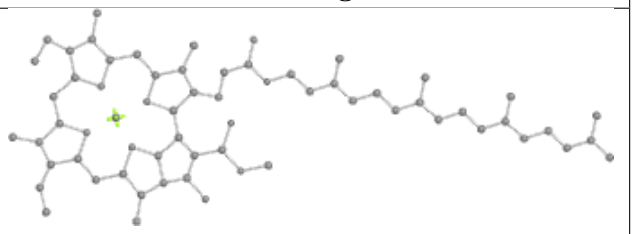
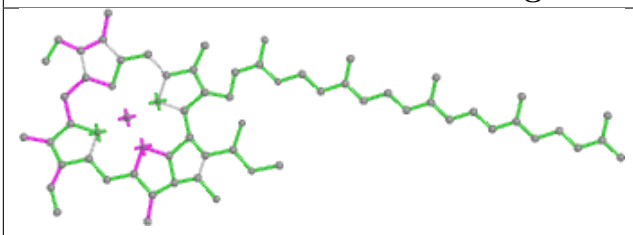


Rings

Ligand CLA C 508



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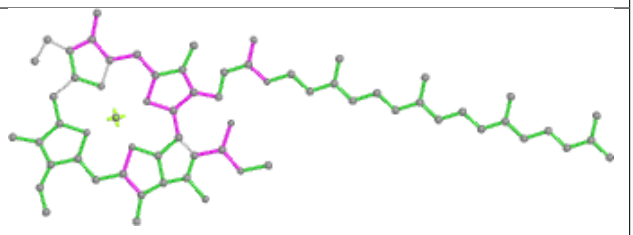
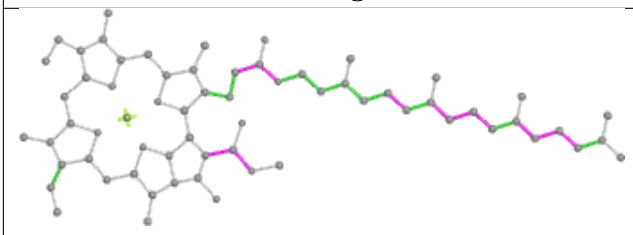


Bond angles



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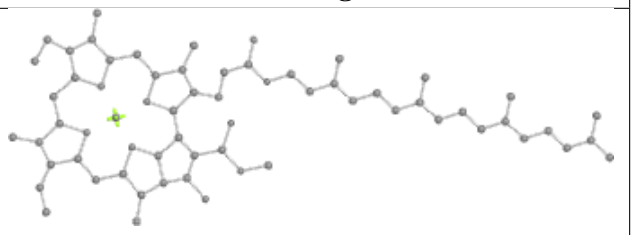
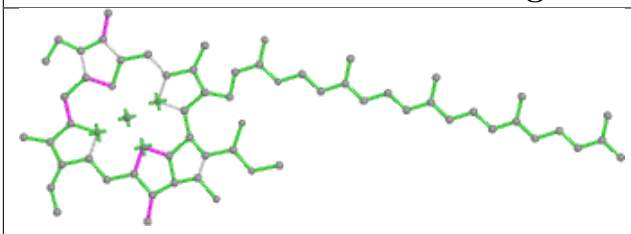


Rings

Ligand CLA Z 102



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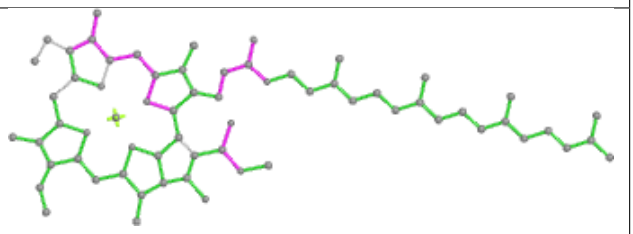

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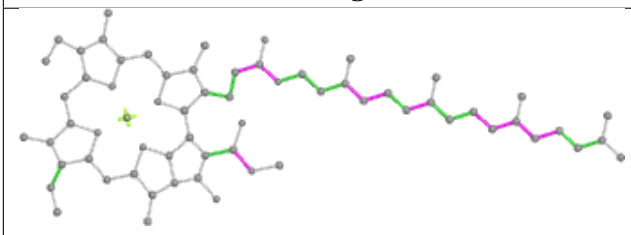

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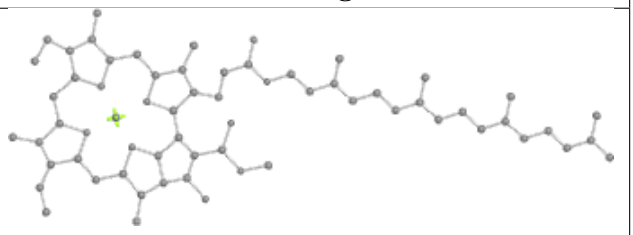
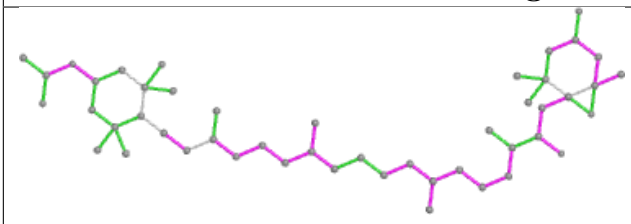


Rings

Ligand A86 15 311



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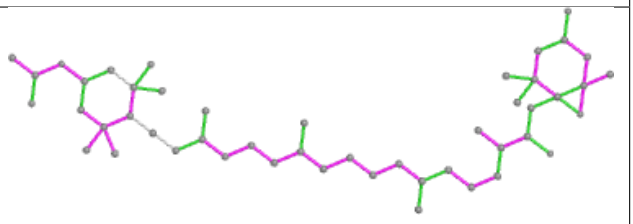

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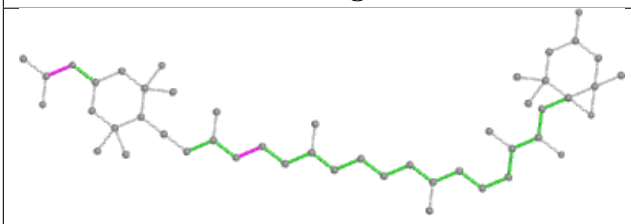

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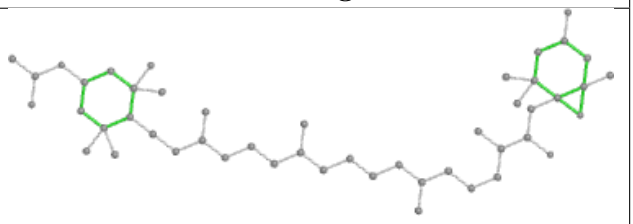
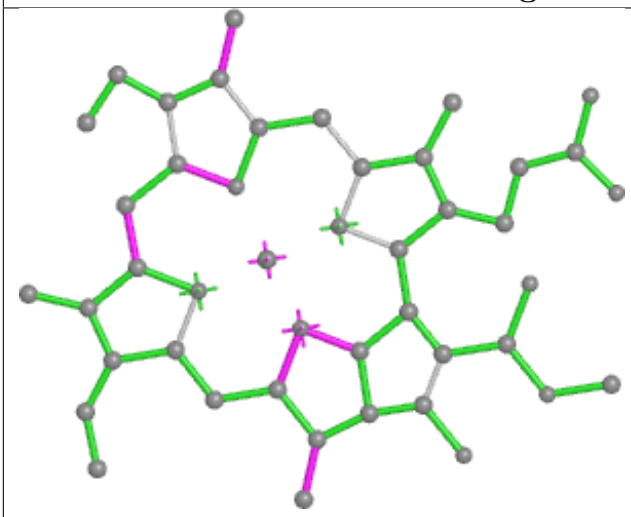


Rings

Ligand CLA 17 306



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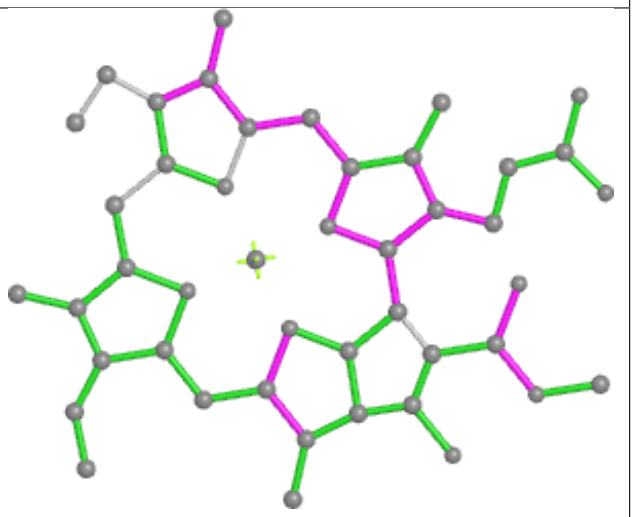

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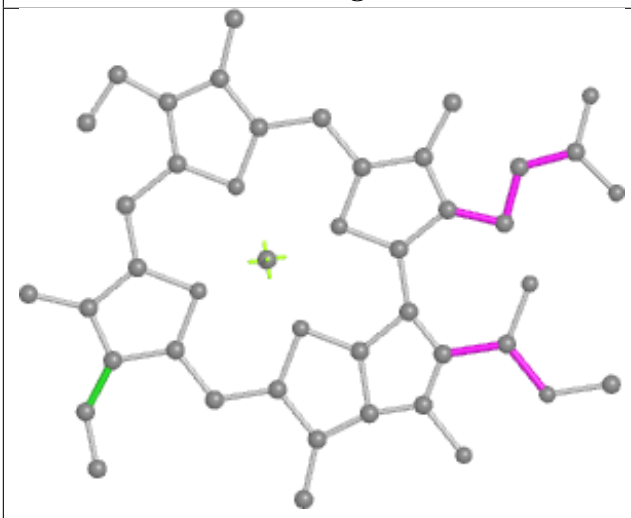

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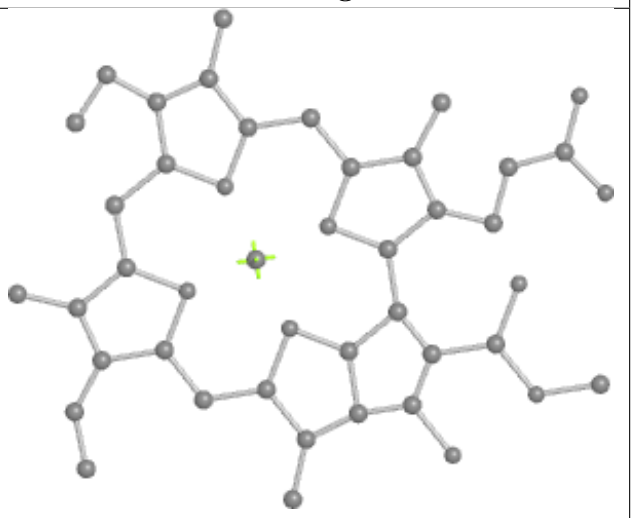
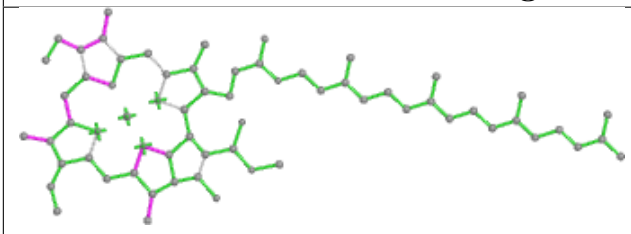


Rings

Ligand CLA 16 302



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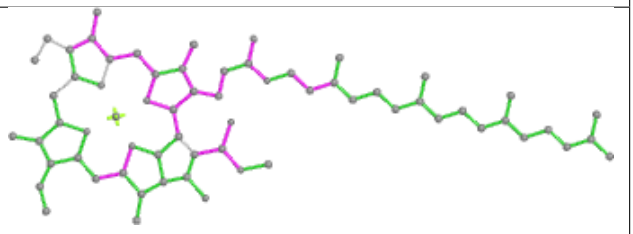

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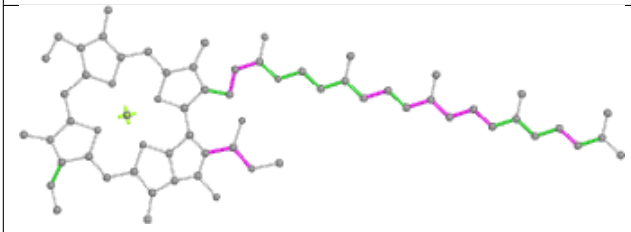

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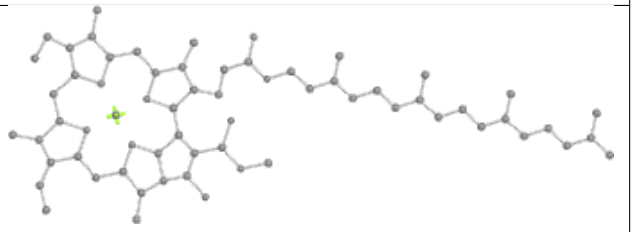
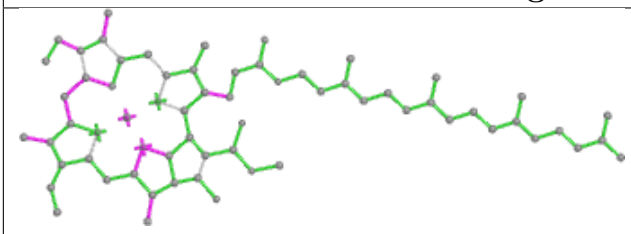


Rings

Ligand CLA b 613



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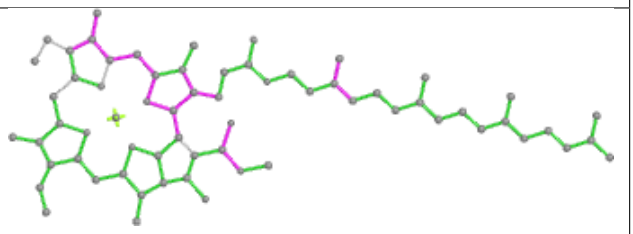

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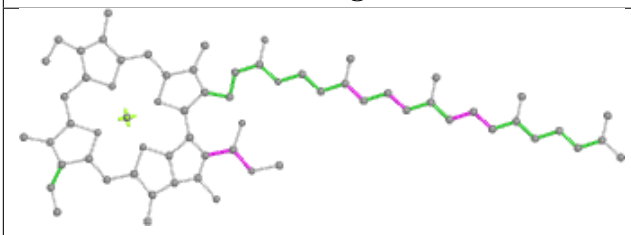

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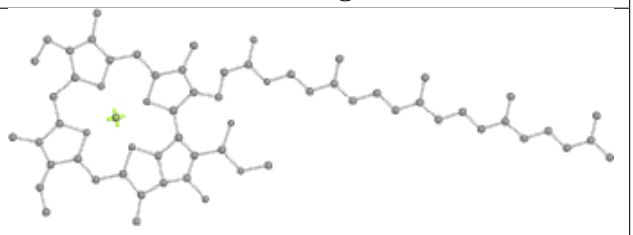
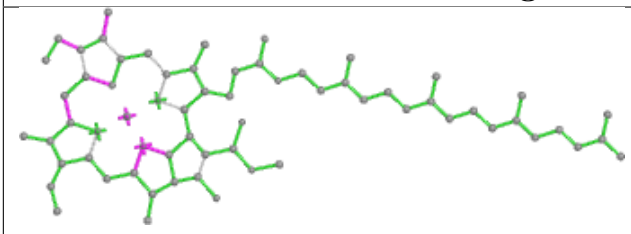


Rings

Ligand CLA 41 303



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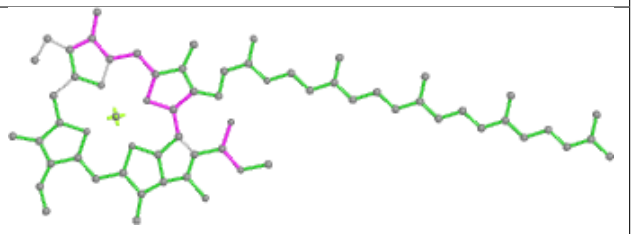
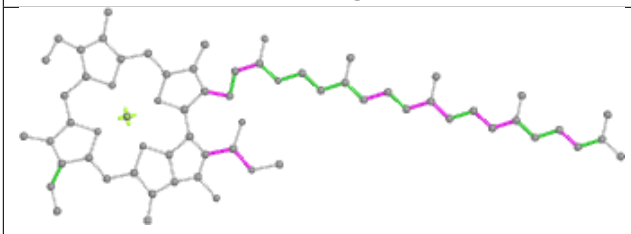


Bond angles



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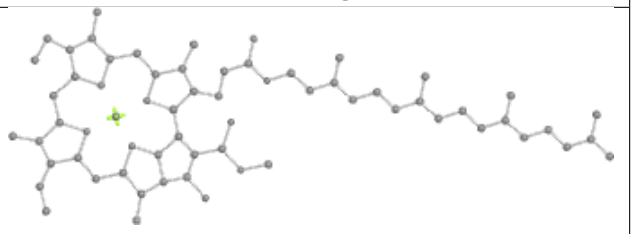
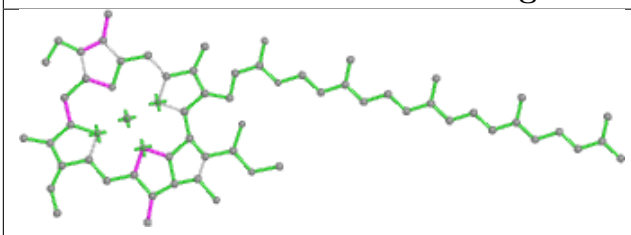


Rings

Ligand CLA 21 306



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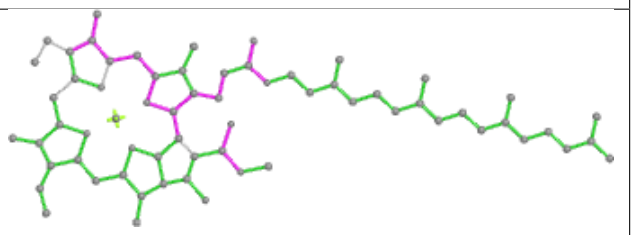
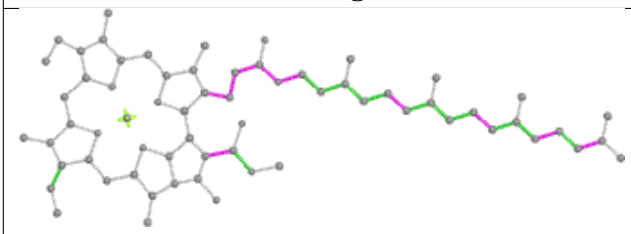


Bond angles



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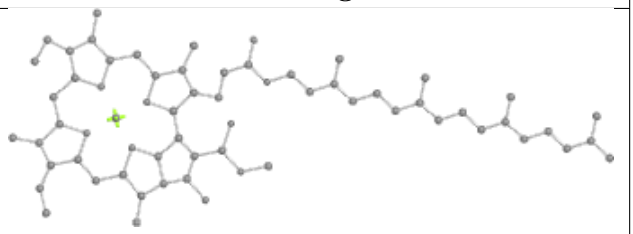
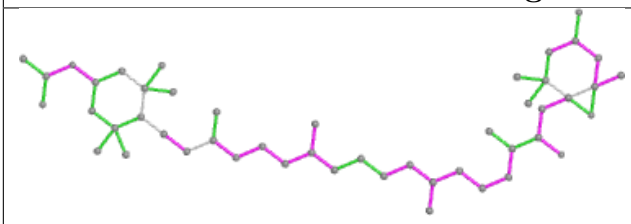


Rings

Ligand A86 18 314



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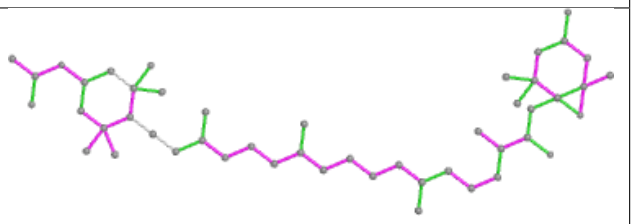
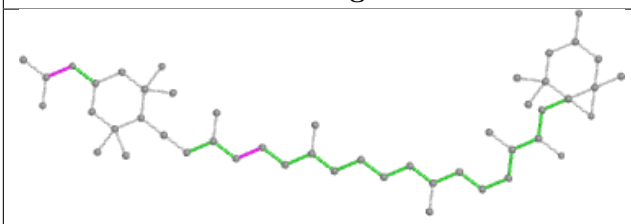


Bond angles



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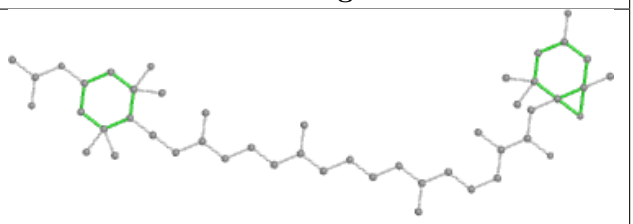
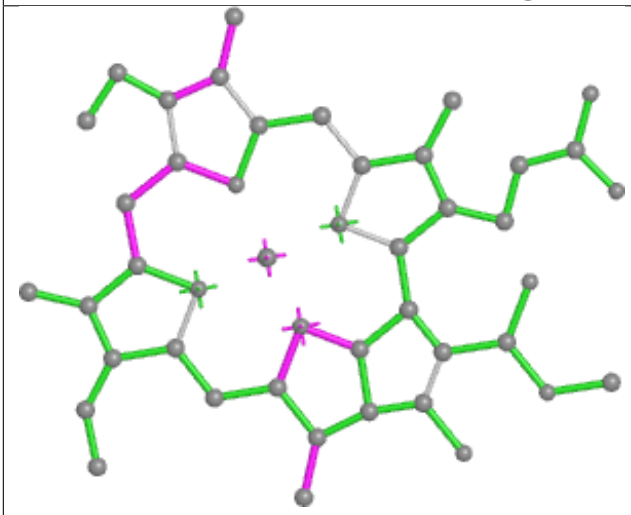
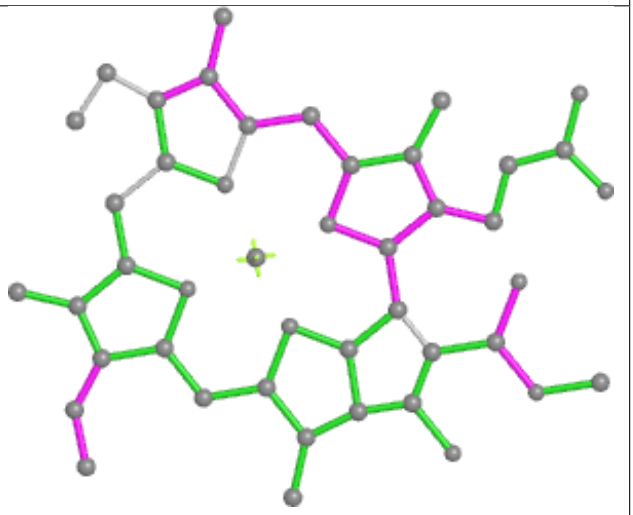


Rings

Ligand CLA 40 203



Bond lengths



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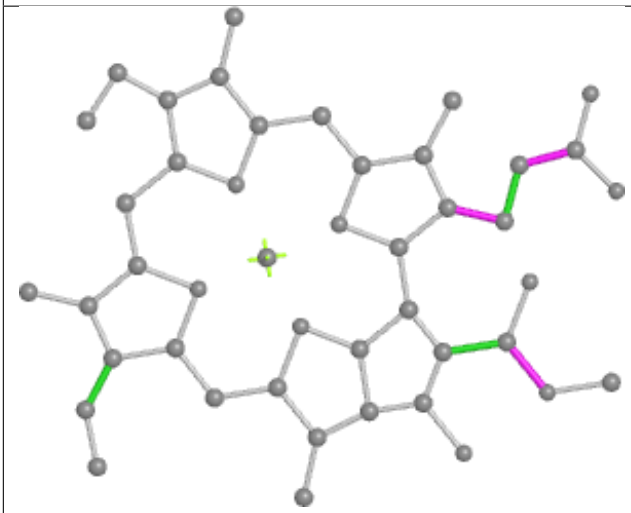
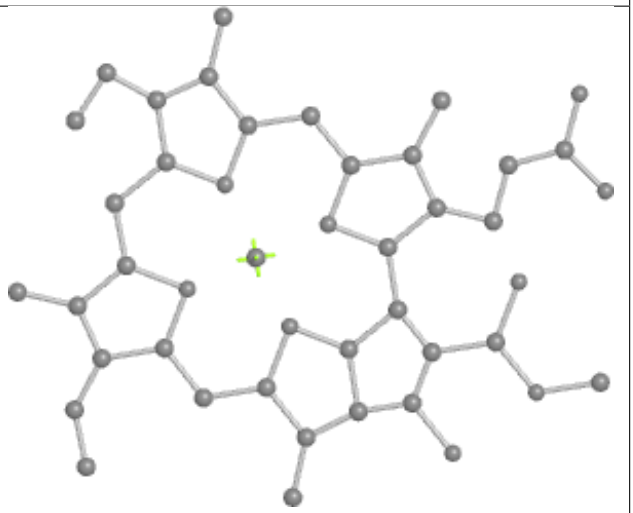
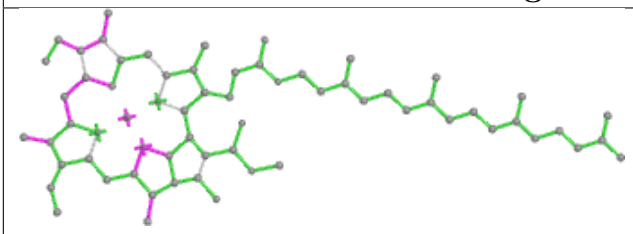


Torsions



Rings

Ligand CLA C 519



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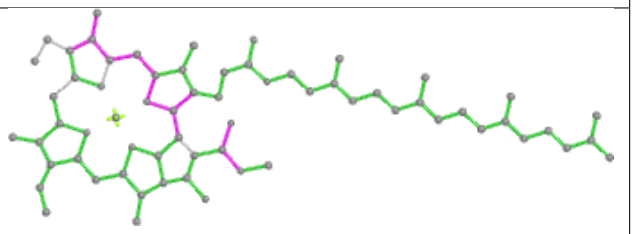

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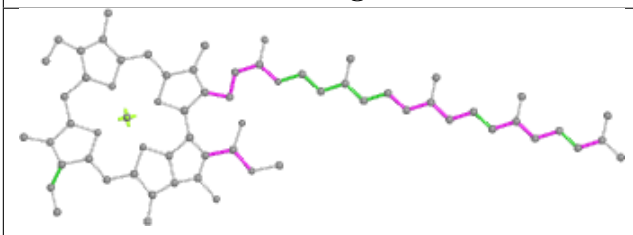

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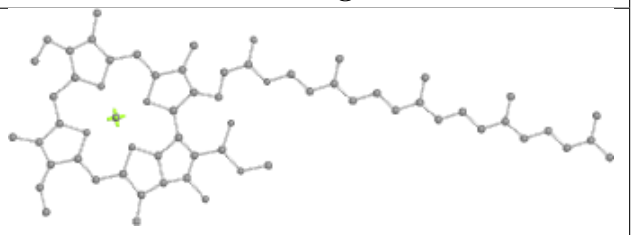
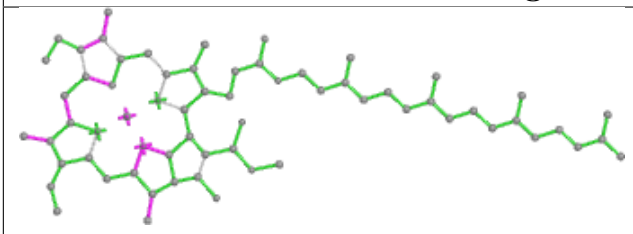


Rings

Ligand CLA C 513



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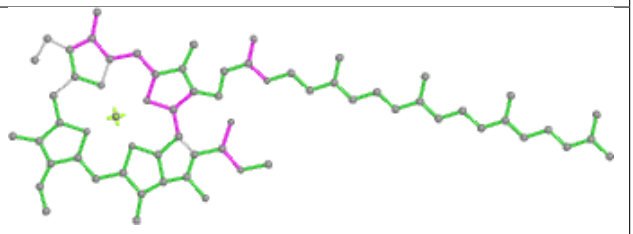

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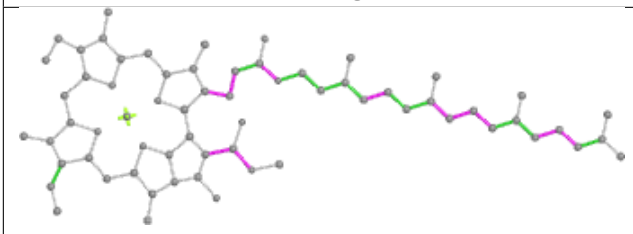

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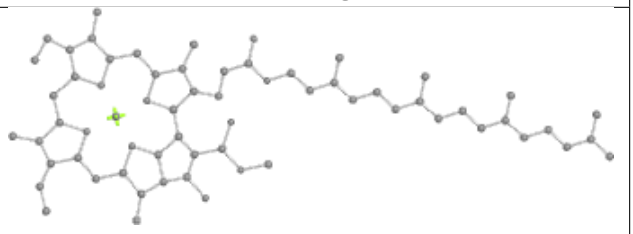
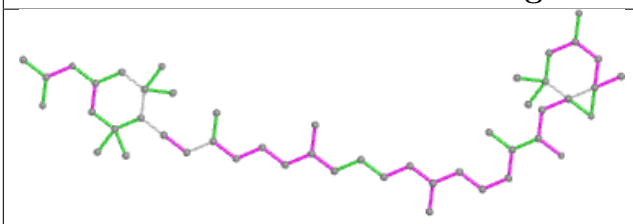


Rings

Ligand A86 11 312



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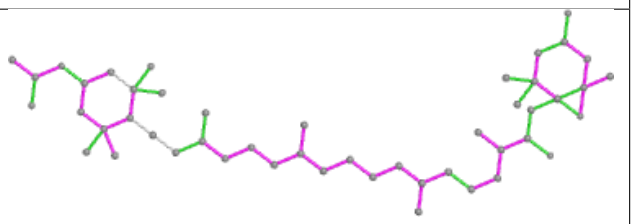

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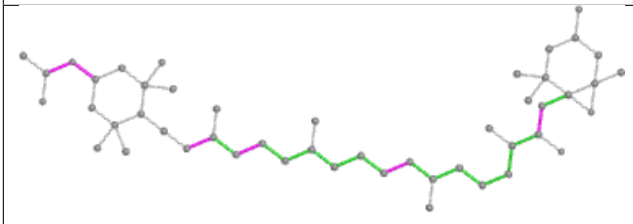

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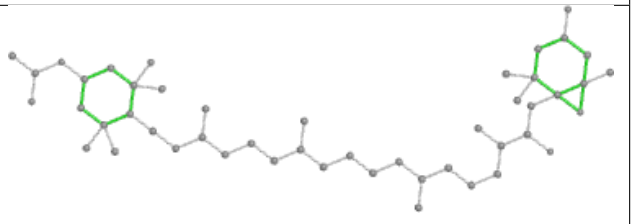
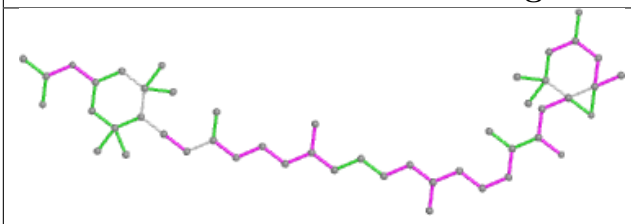


Rings

Ligand A86 35 314



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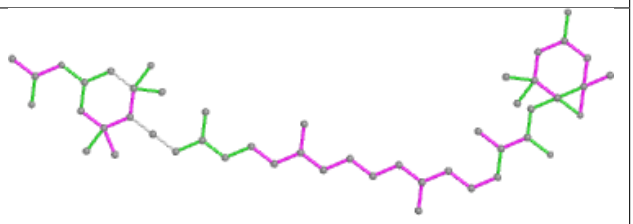

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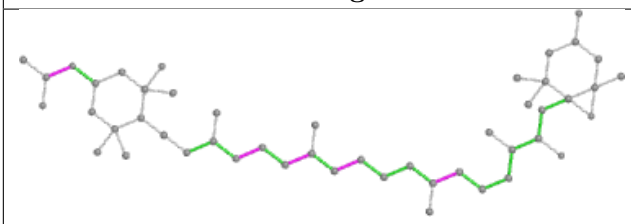

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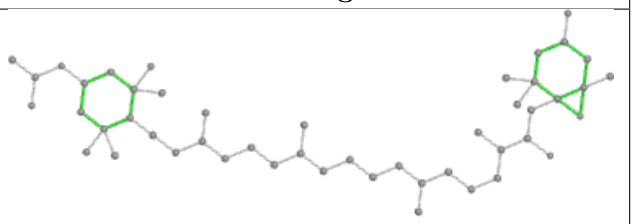
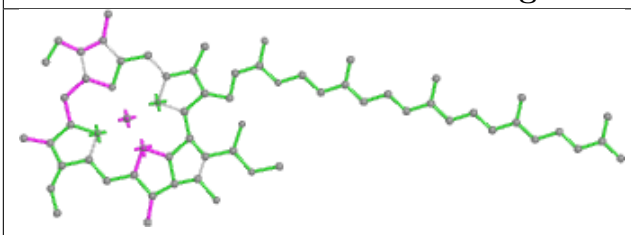


Rings

Ligand CLA 33 305



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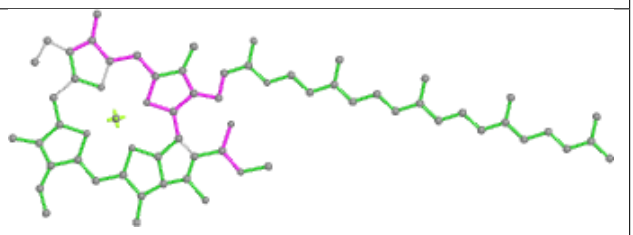

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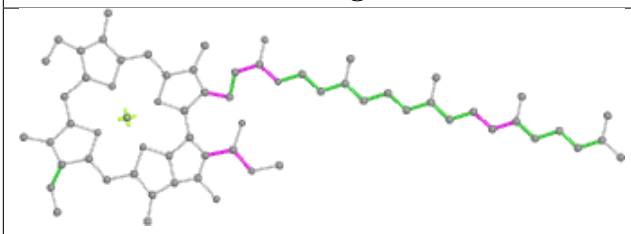

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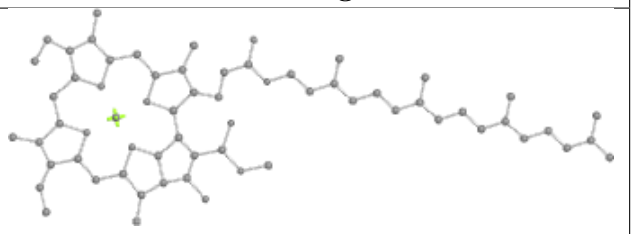
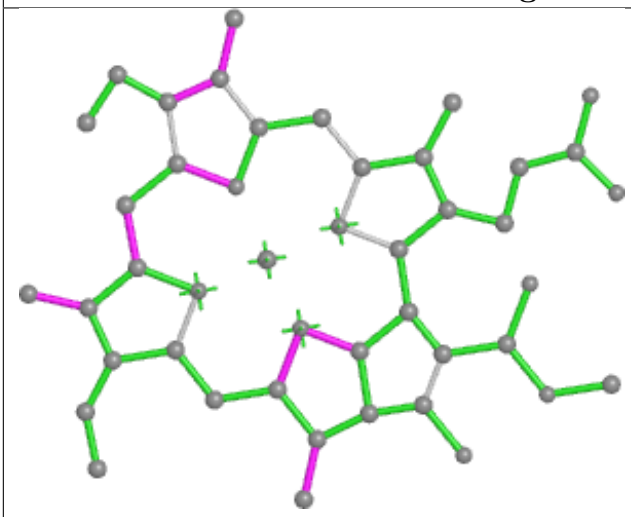


Rings

Ligand CLA 15 306



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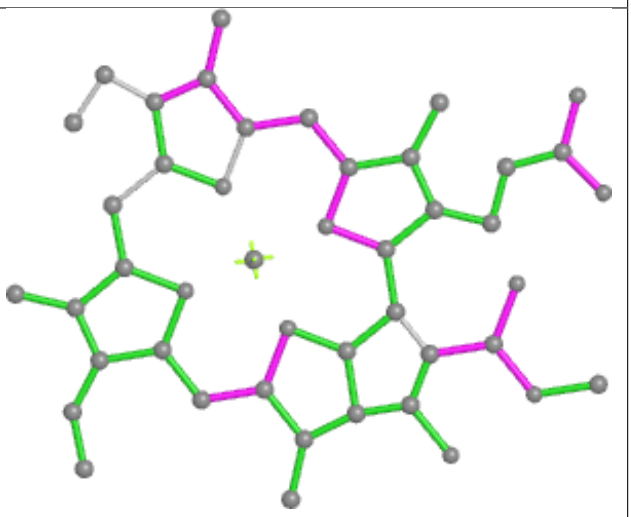

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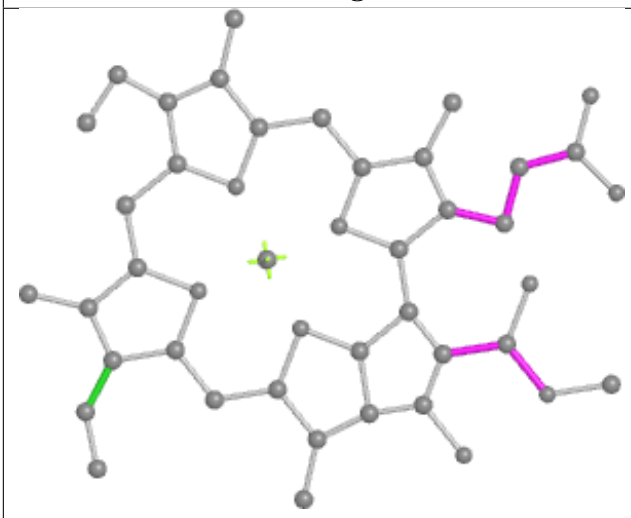

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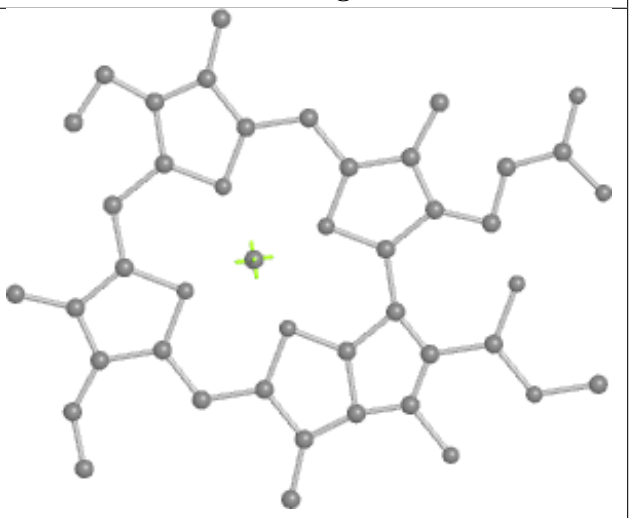
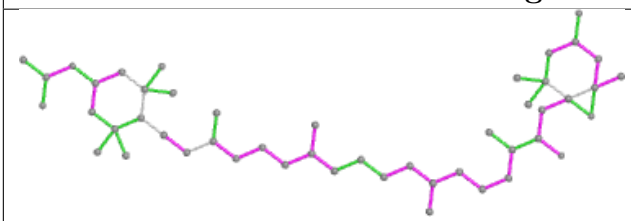


Rings

Ligand A86 13 313



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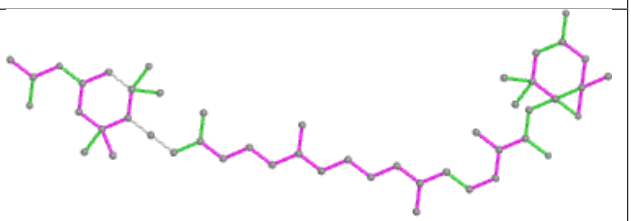

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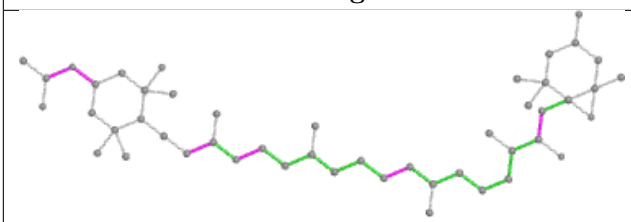

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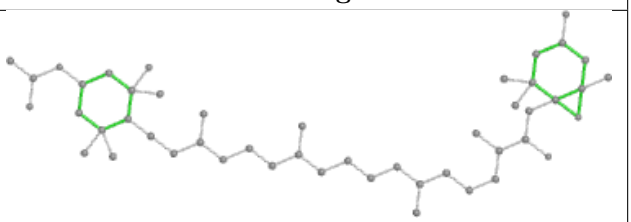
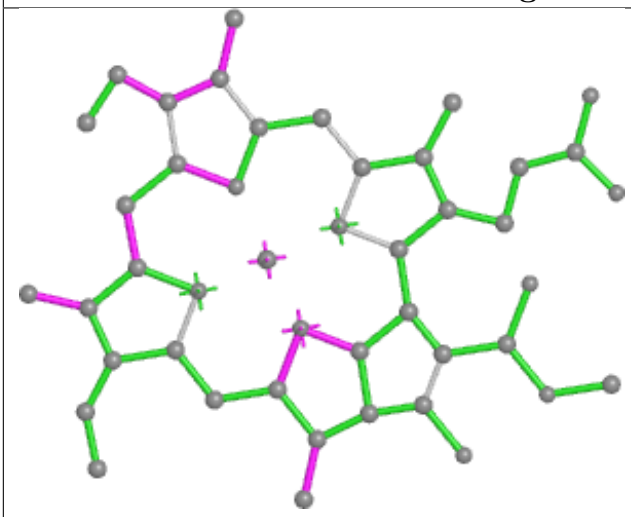


Rings

Ligand CLA 16 307



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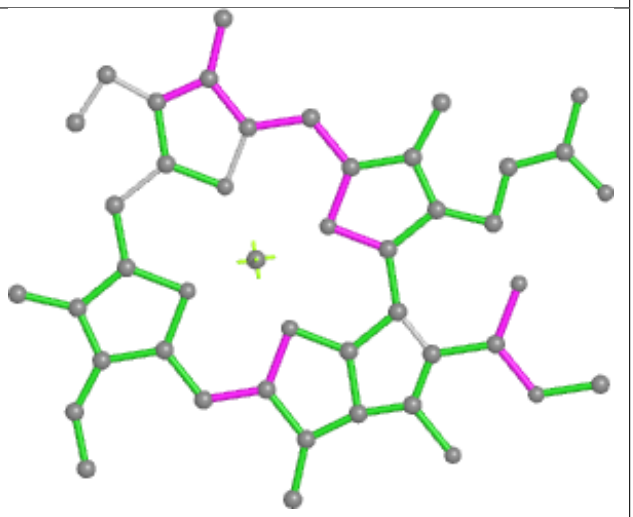

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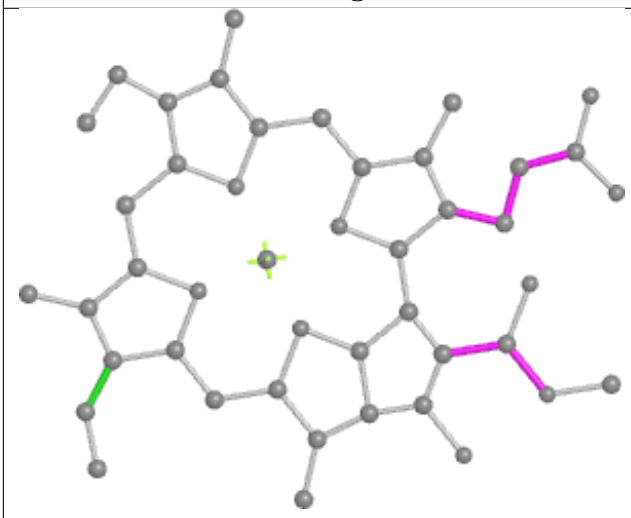

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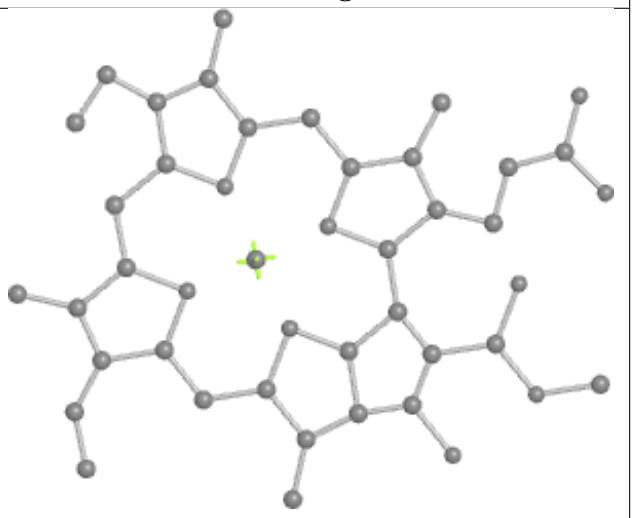
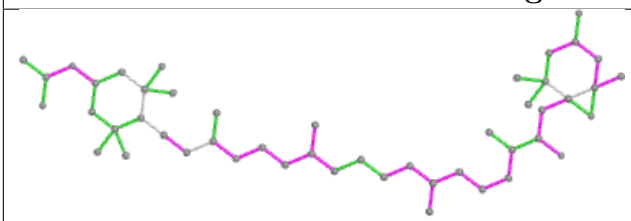


Rings

Ligand A86 12 304



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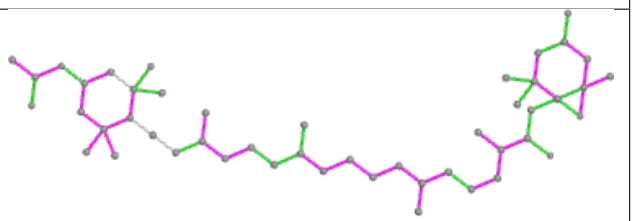

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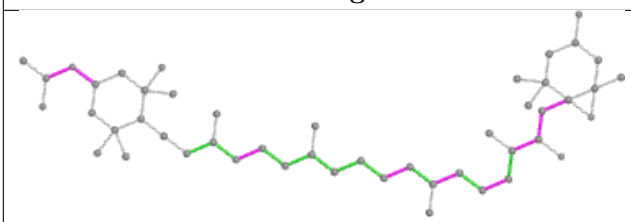

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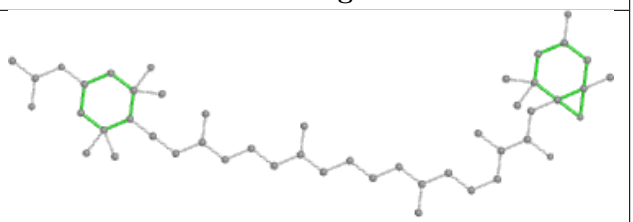
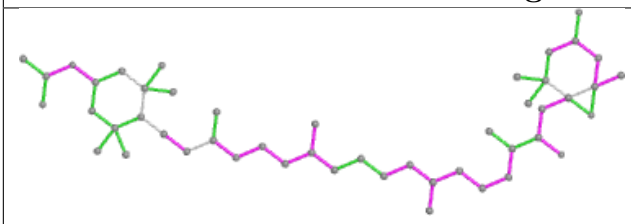


Rings

Ligand A86 41 314



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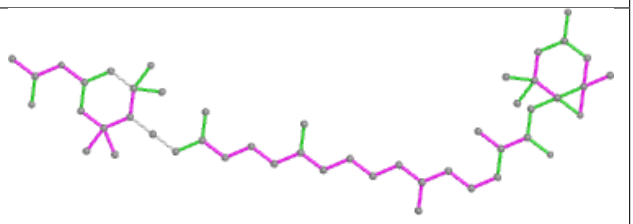

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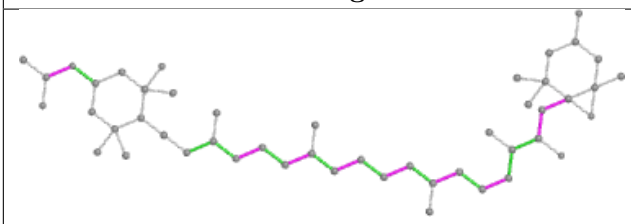

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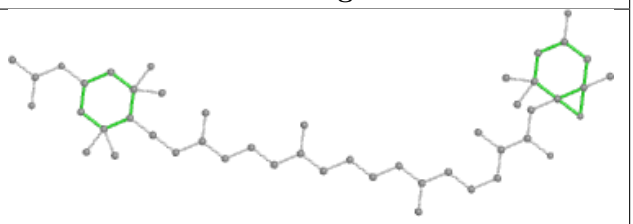
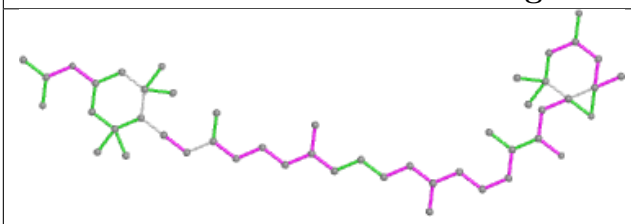


Rings

Ligand A86 13 312



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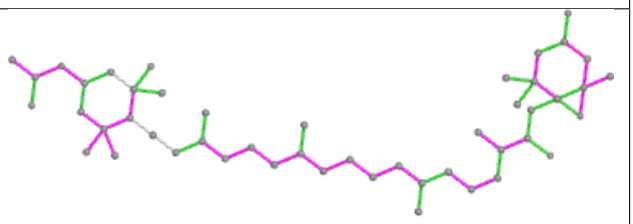
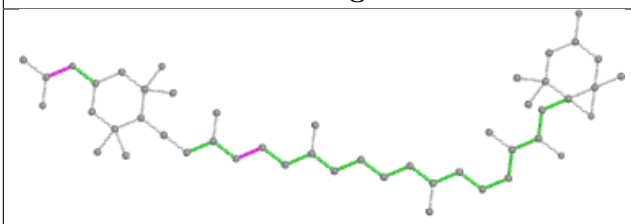


Bond angles



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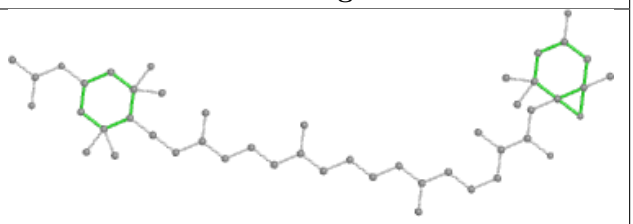
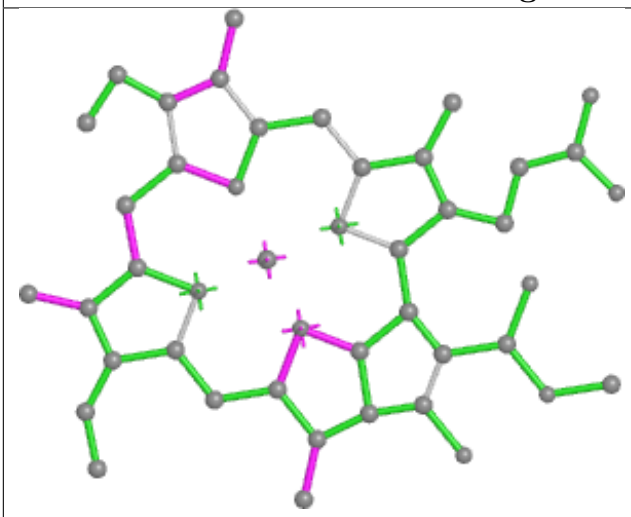


Rings

Ligand CLA 40 207



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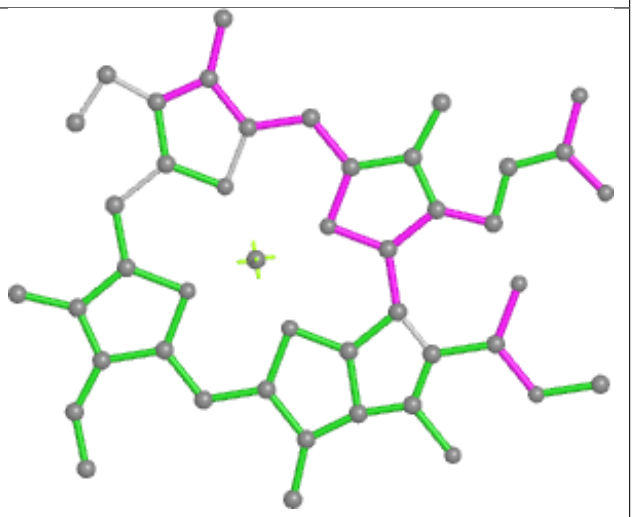
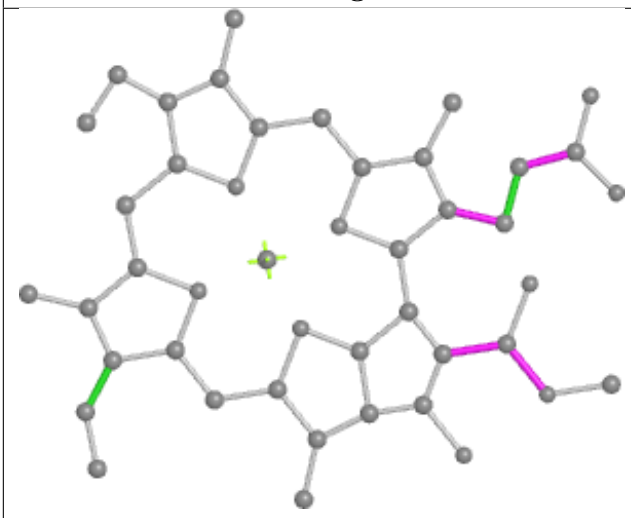
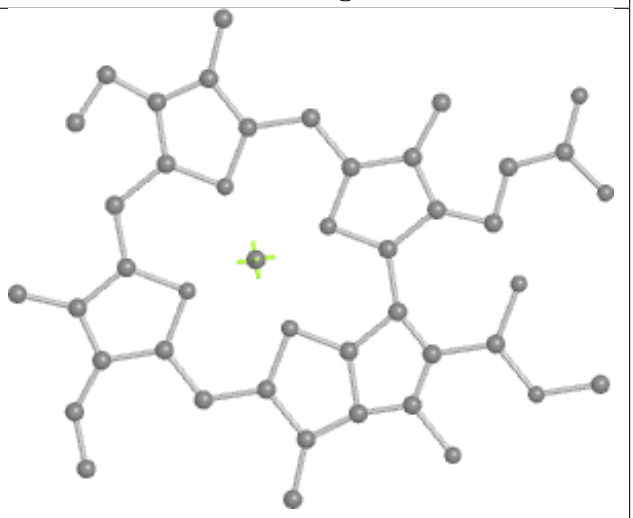


Bond angles

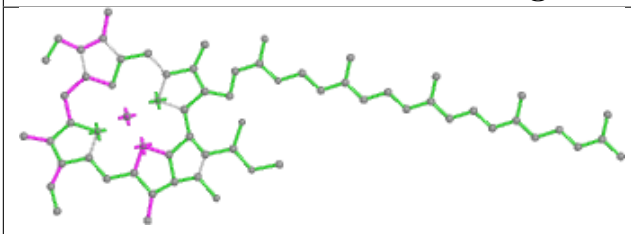


Torsions



Rings

Ligand CLA c 505



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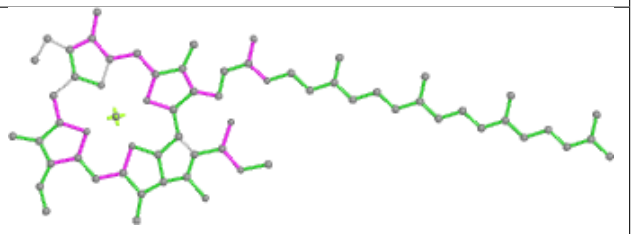
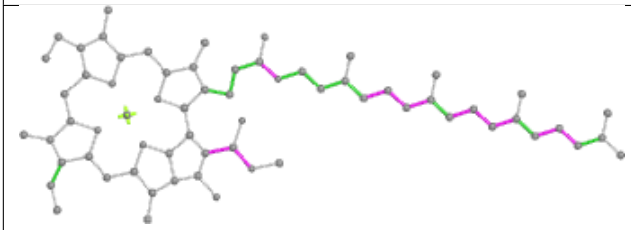


Bond angles



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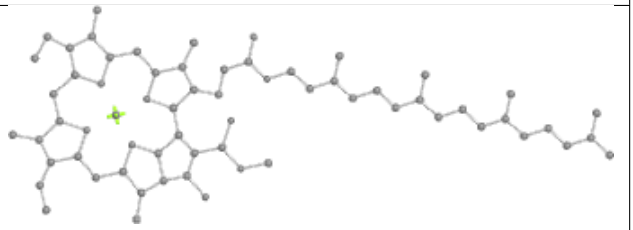
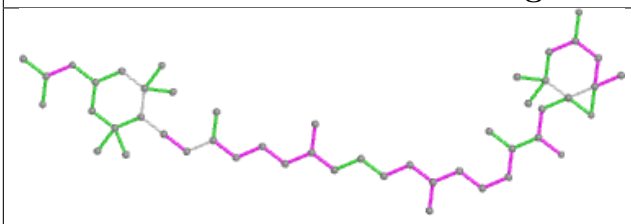
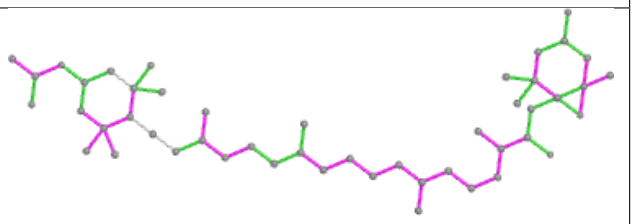


Rings

Ligand A86 39 311



Bond lengths



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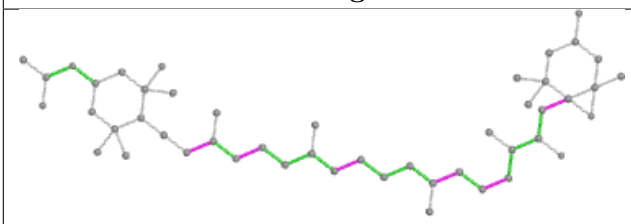
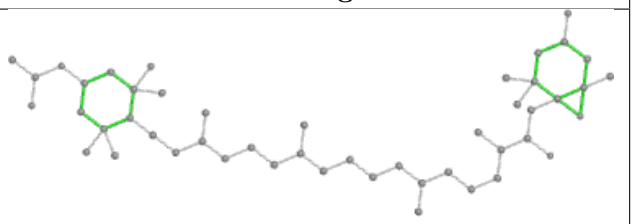
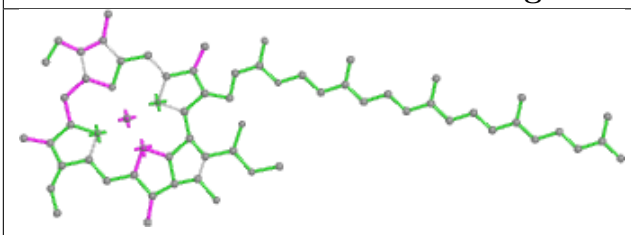


Torsions



Rings

Ligand CLA C 510



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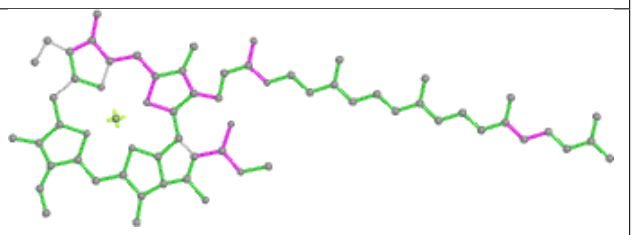

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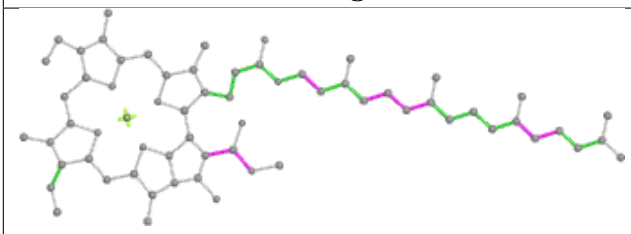

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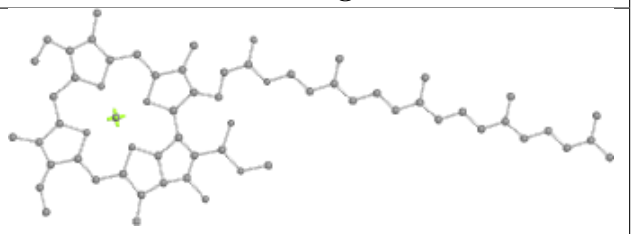
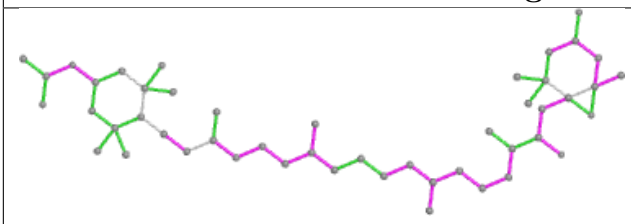


Rings

Ligand A86 32 304



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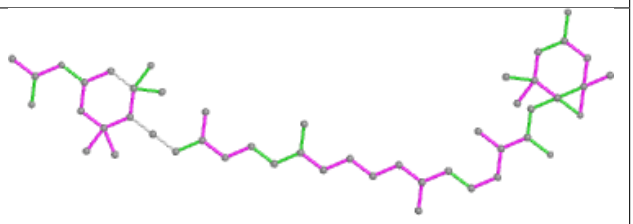

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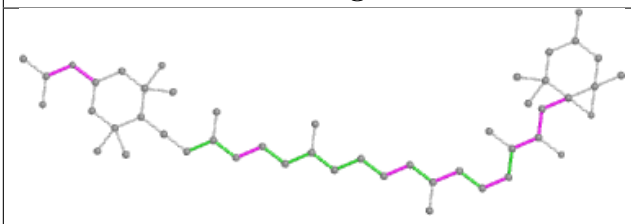

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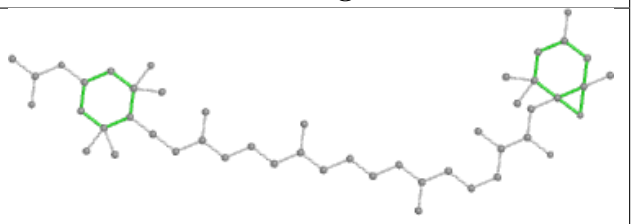
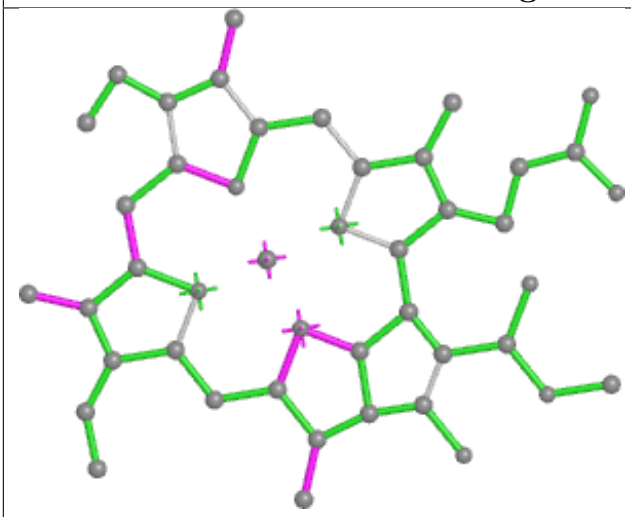


Rings

Ligand CLA 32 308



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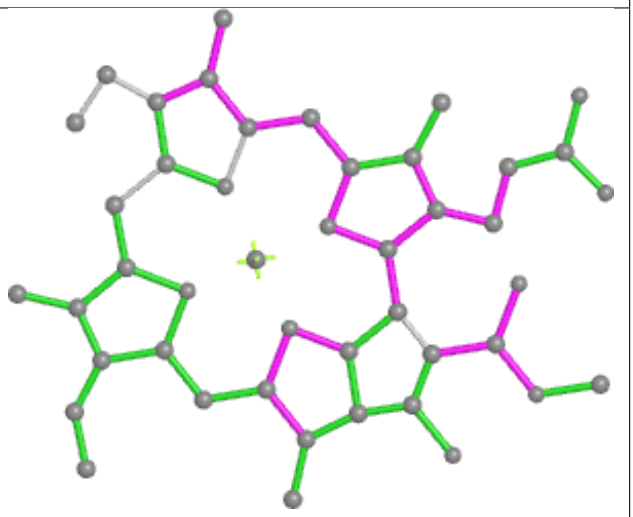

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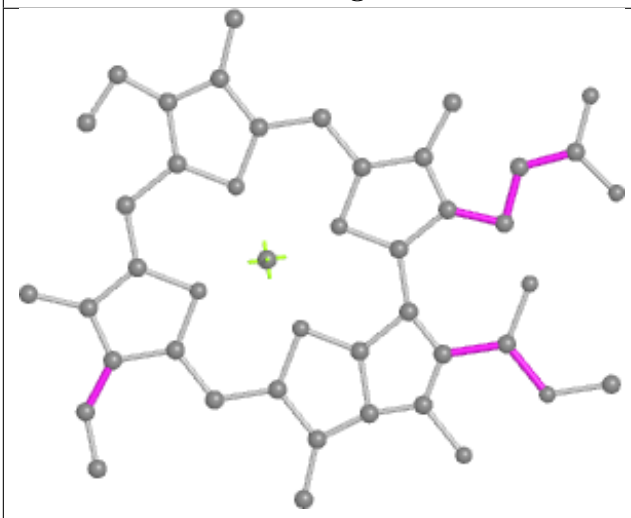

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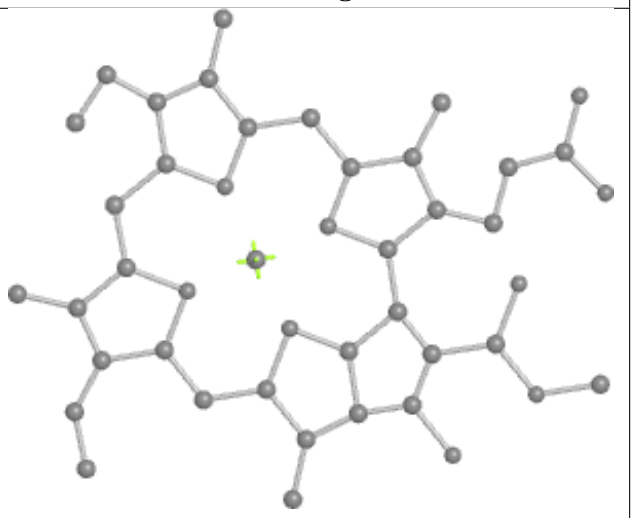
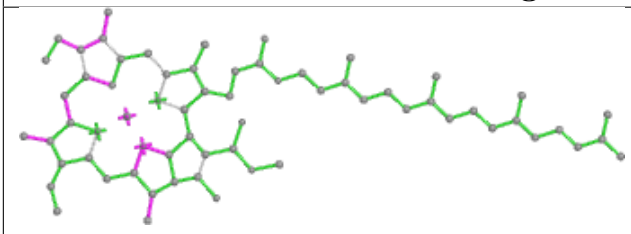


Rings

Ligand CLA M 101



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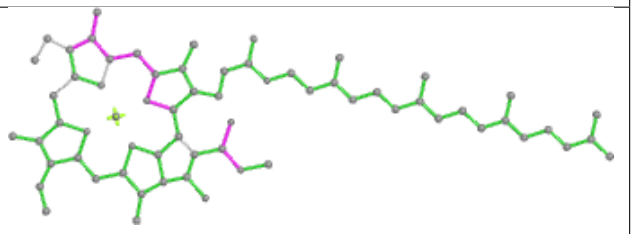

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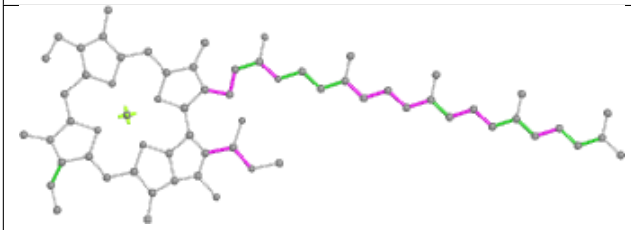

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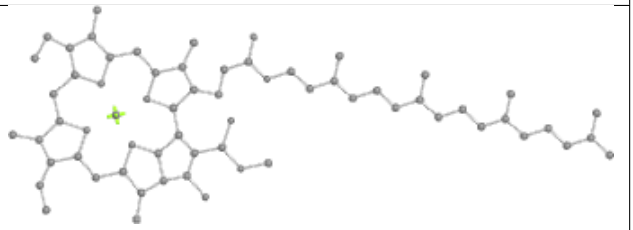
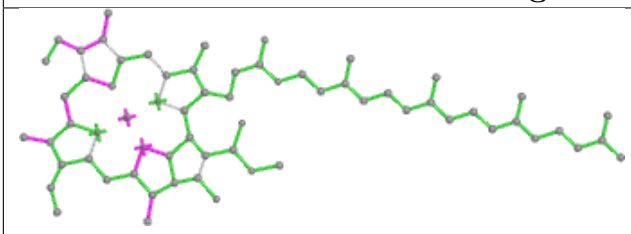


Rings

Ligand CLA c 512



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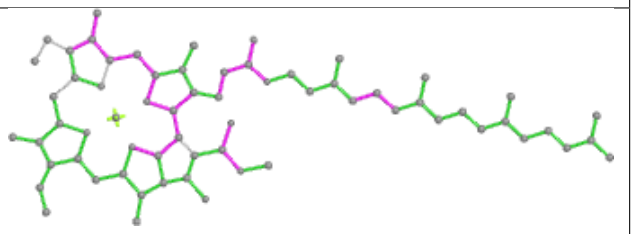

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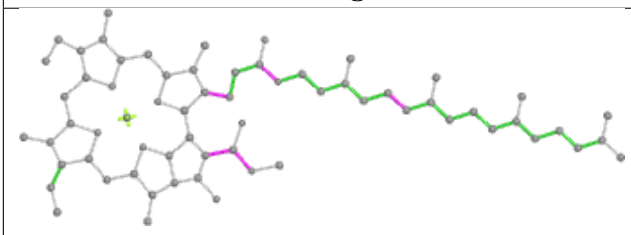

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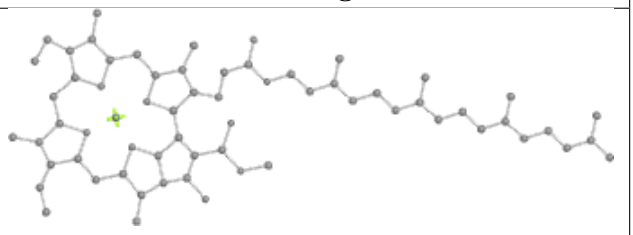
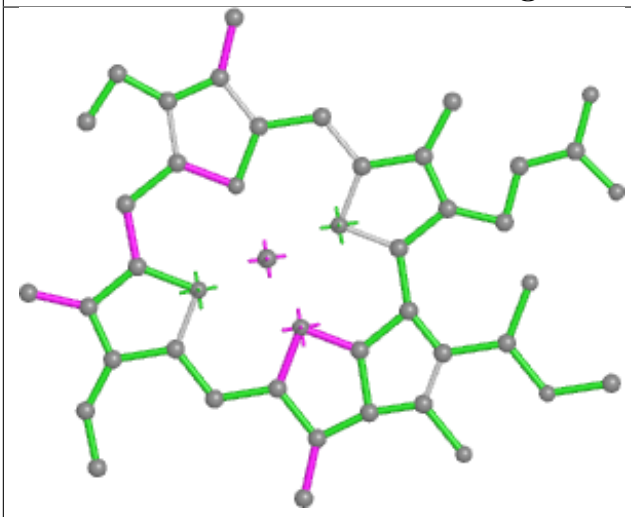


Rings

Ligand CLA 14 305



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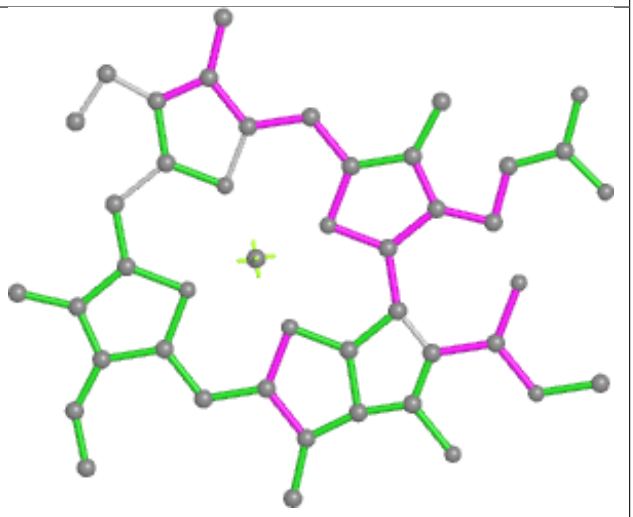

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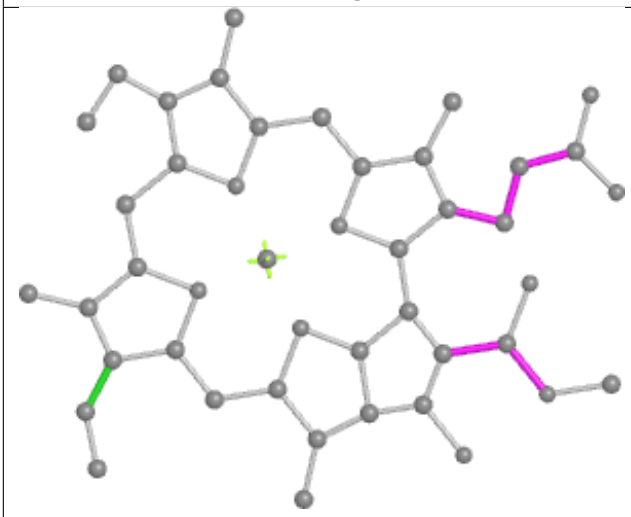

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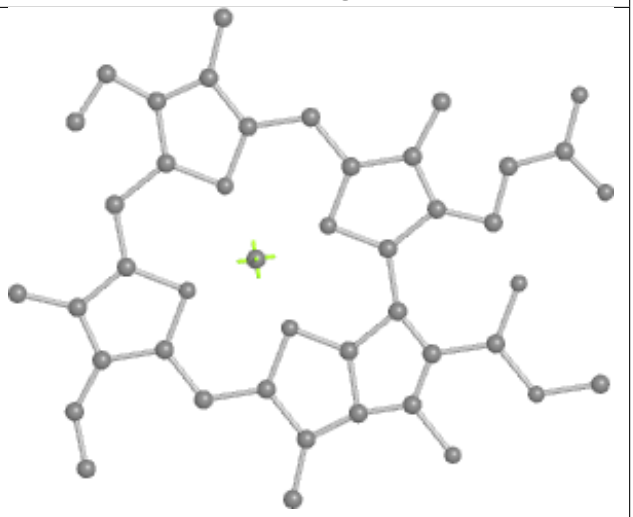
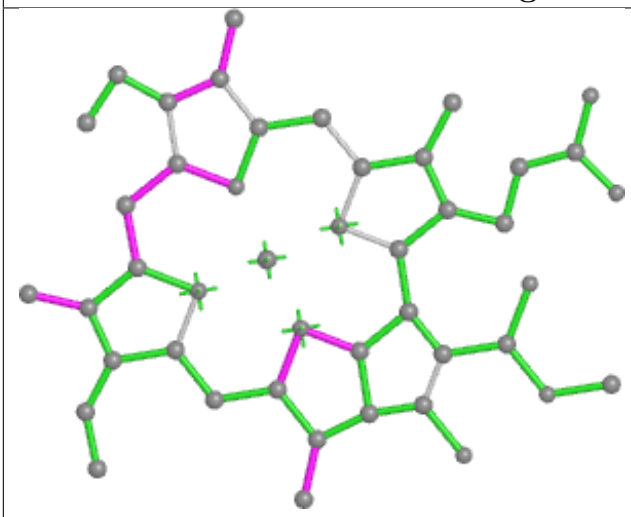


Rings

Ligand CLA 36 306



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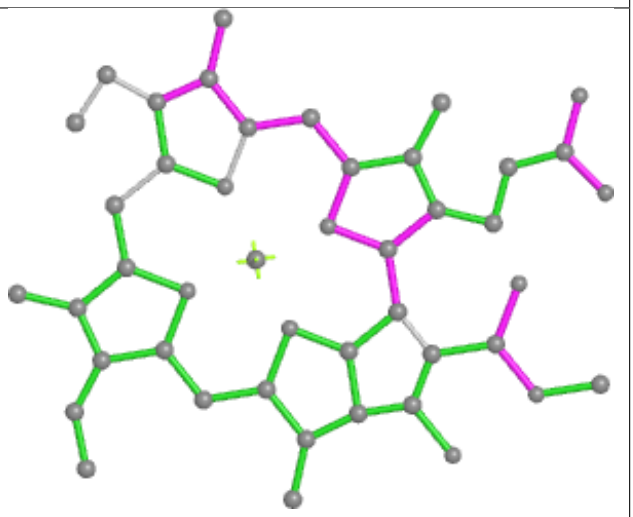

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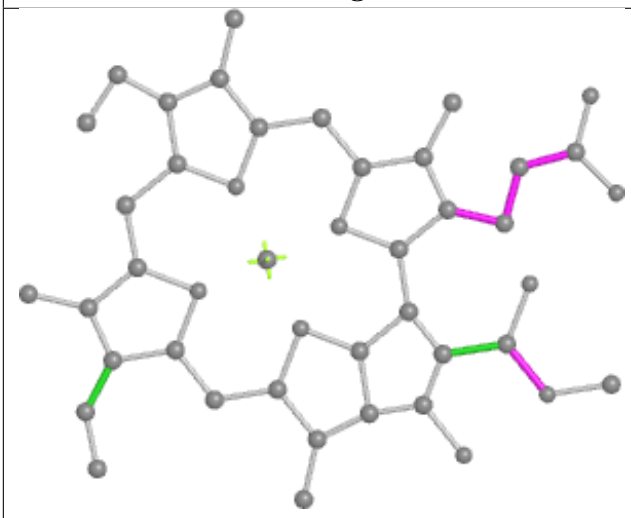

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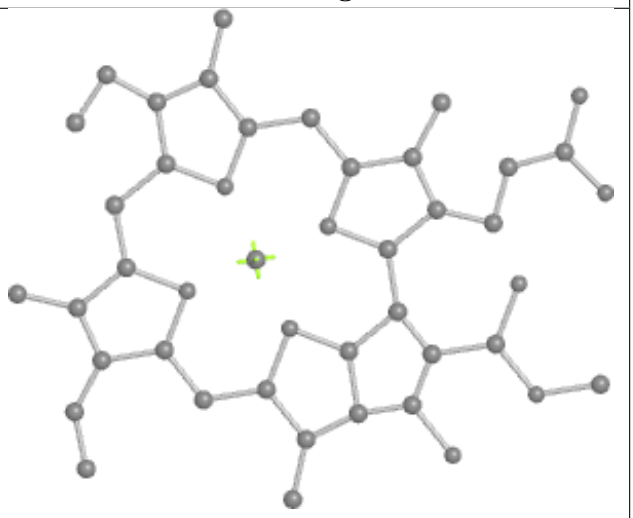
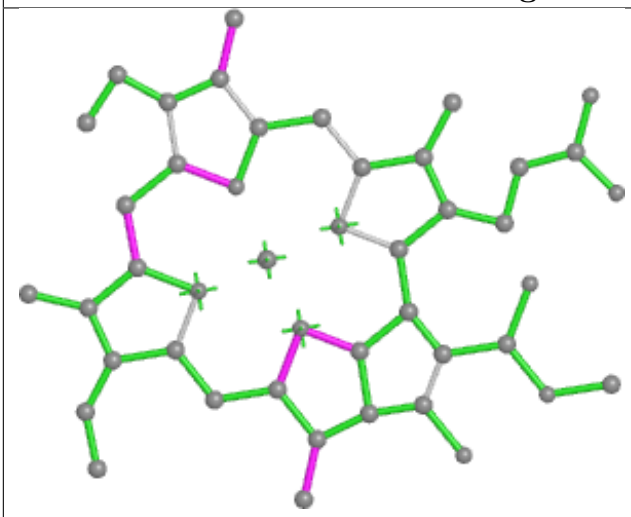


Rings

Ligand CLA 21 308



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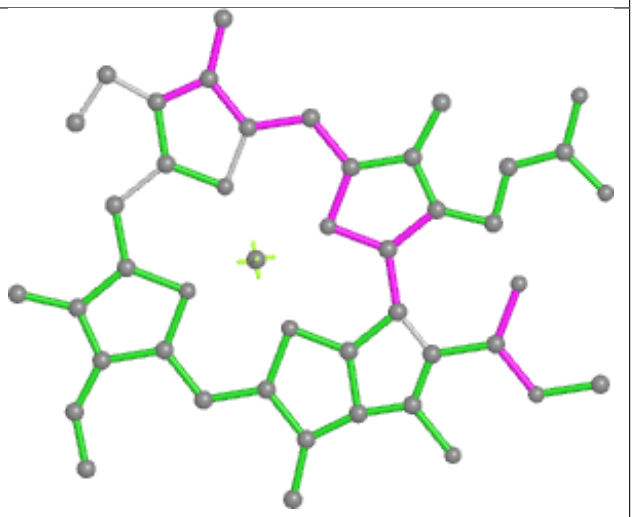

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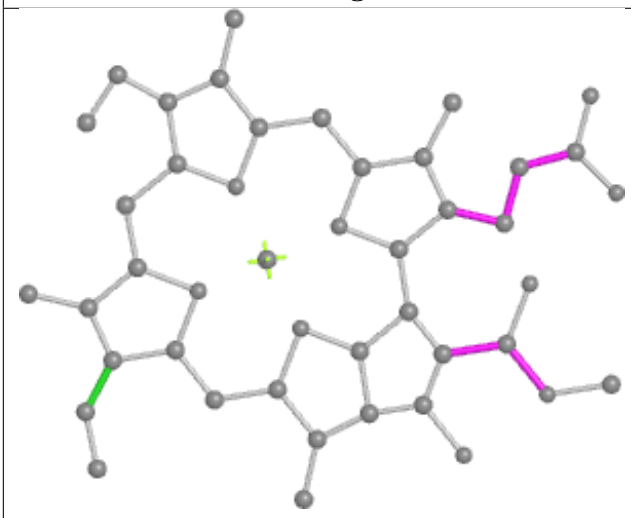

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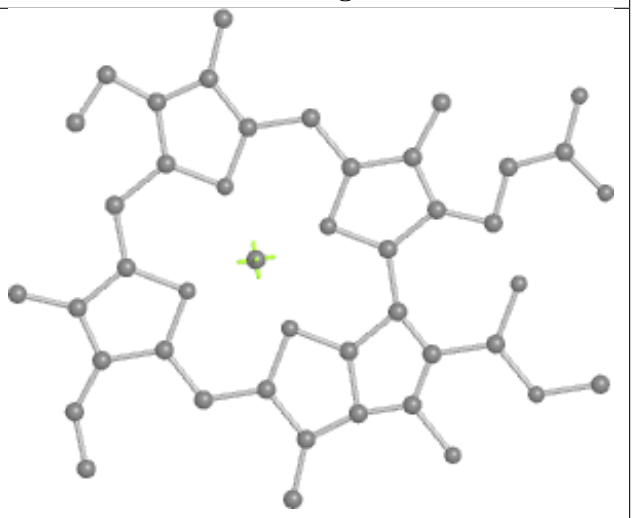
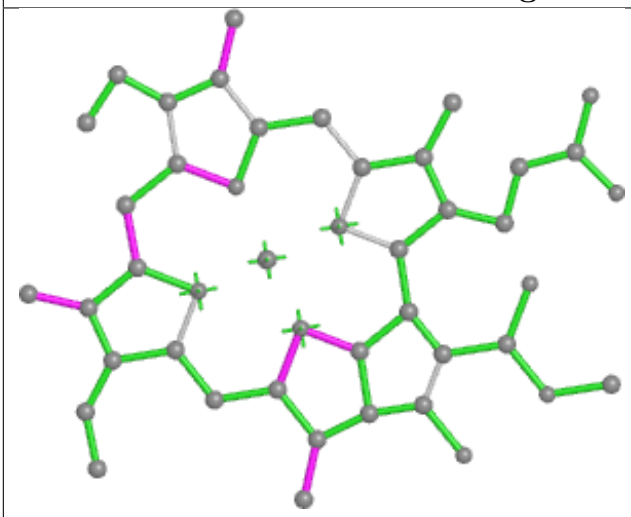


Rings

Ligand CLA 21 302



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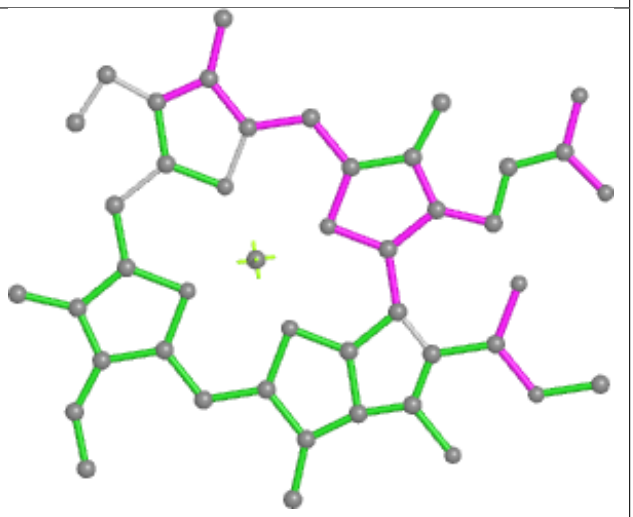

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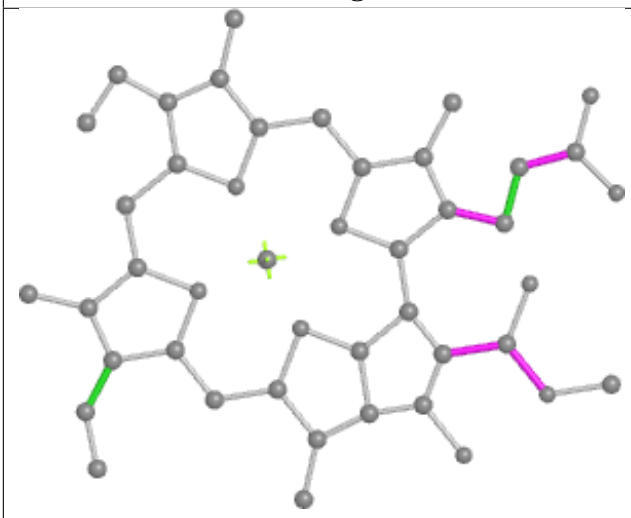

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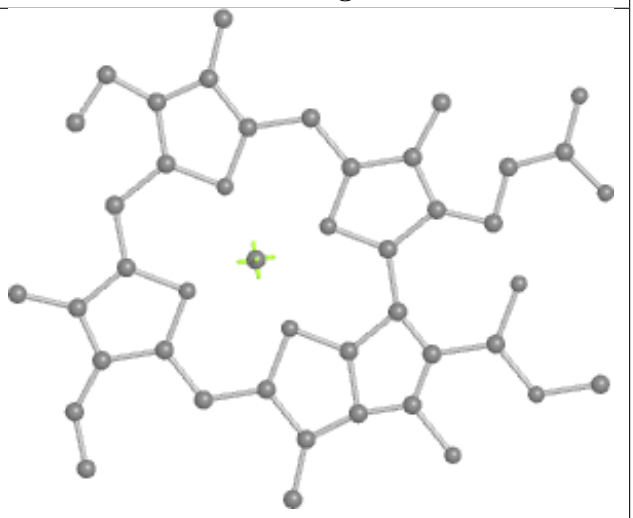
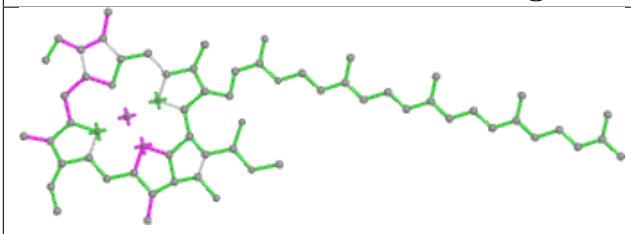


Rings

Ligand CLA d 402



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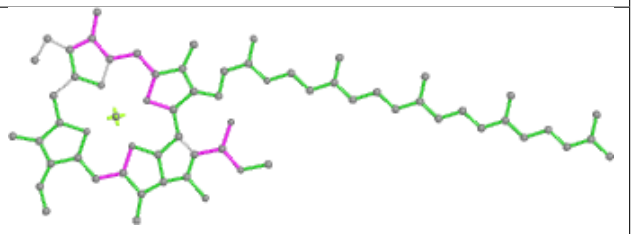

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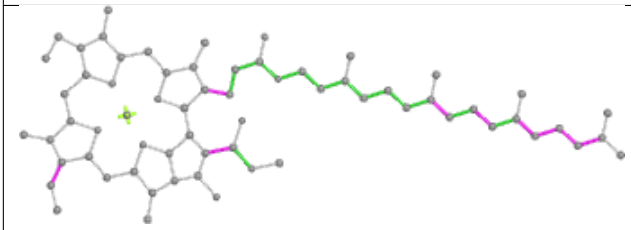

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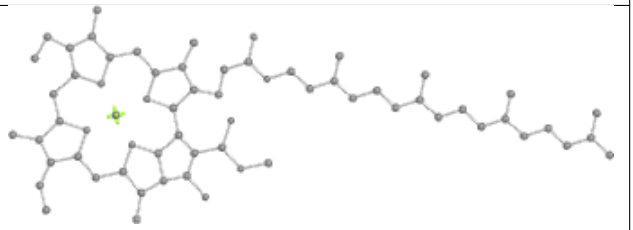
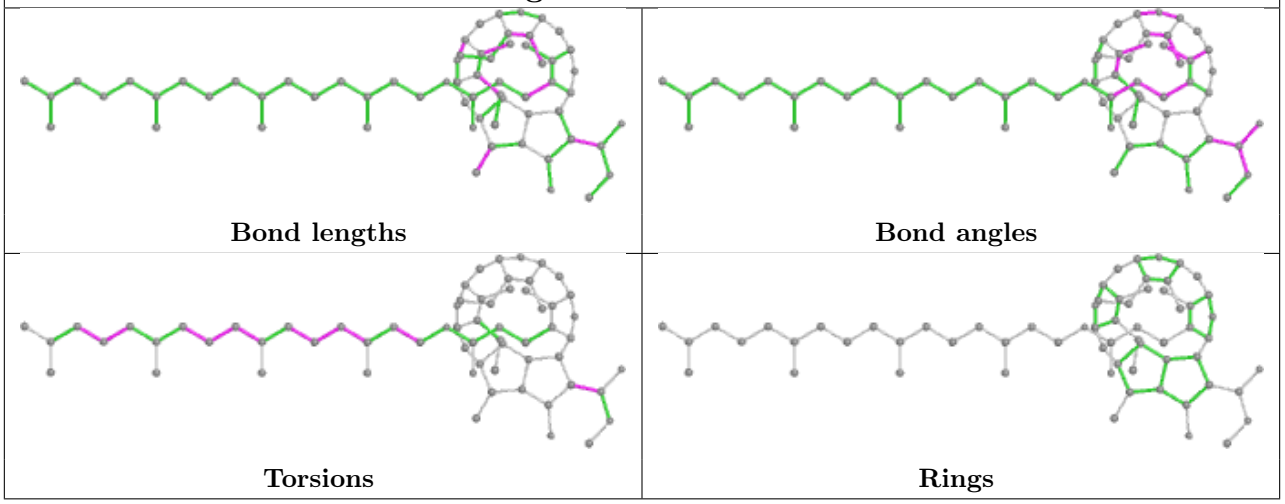
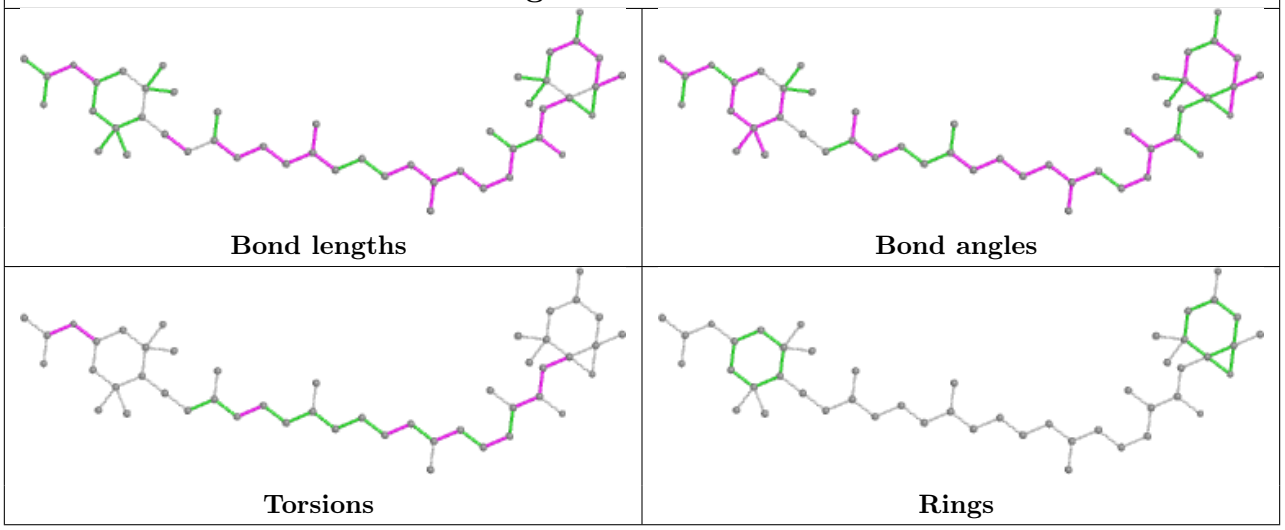


Rings

Ligand PHO d 403



Ligand A86 18 302



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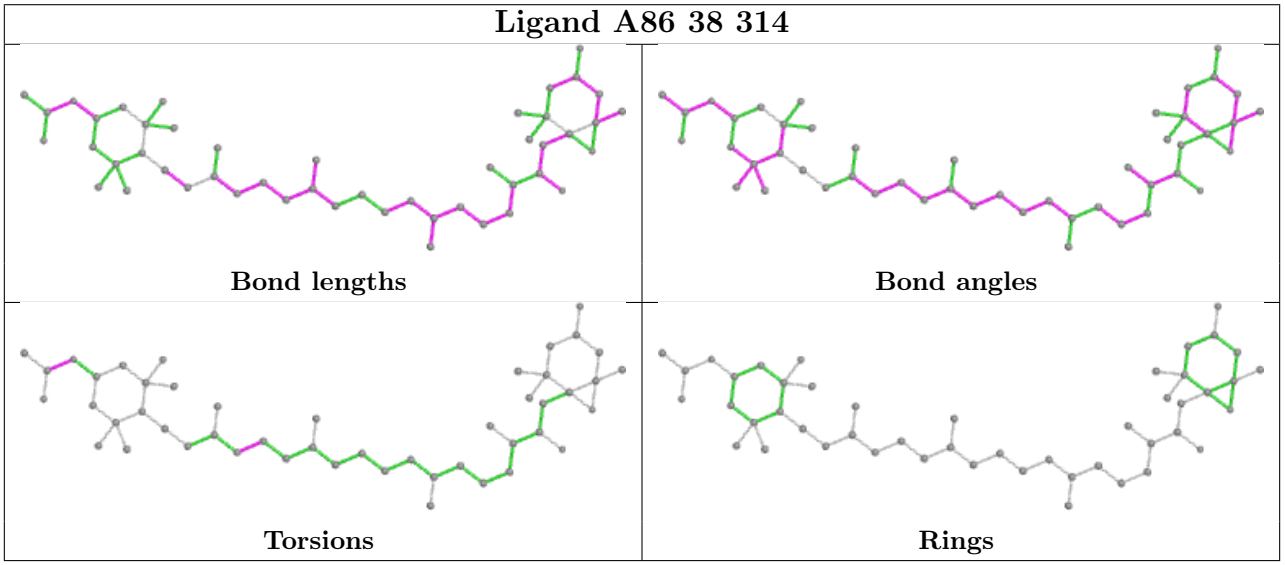
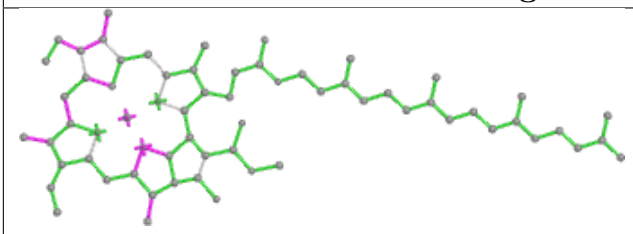
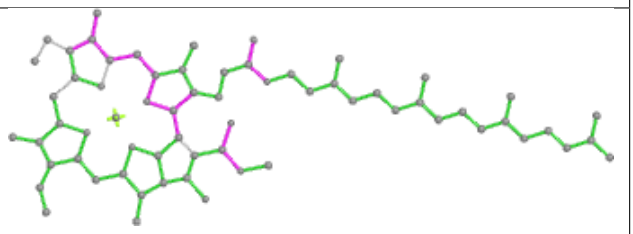


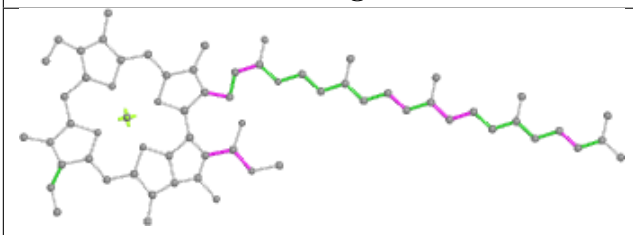
Ligand CLA 40 209



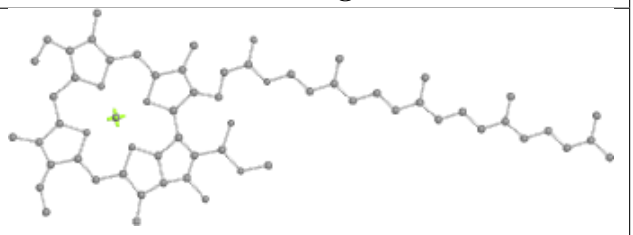
Bond lengths



Bond angles

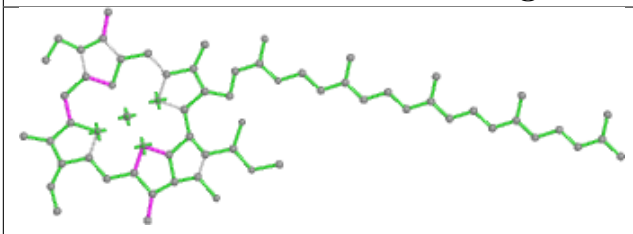


Torsions



Rings

Ligand CLA 21 307



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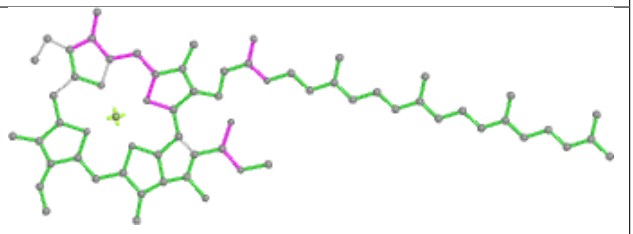
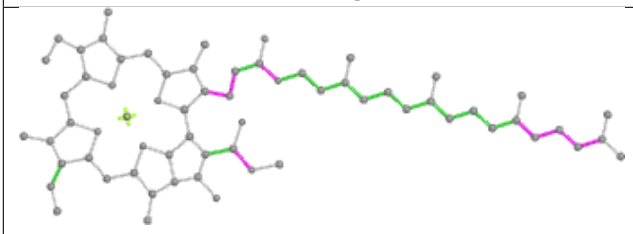


Bond angles



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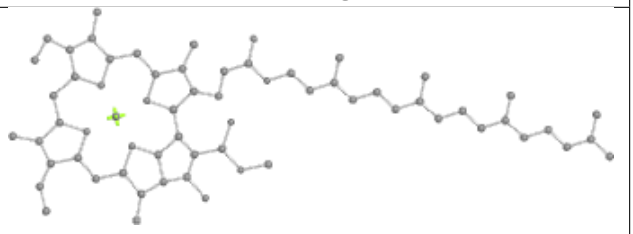
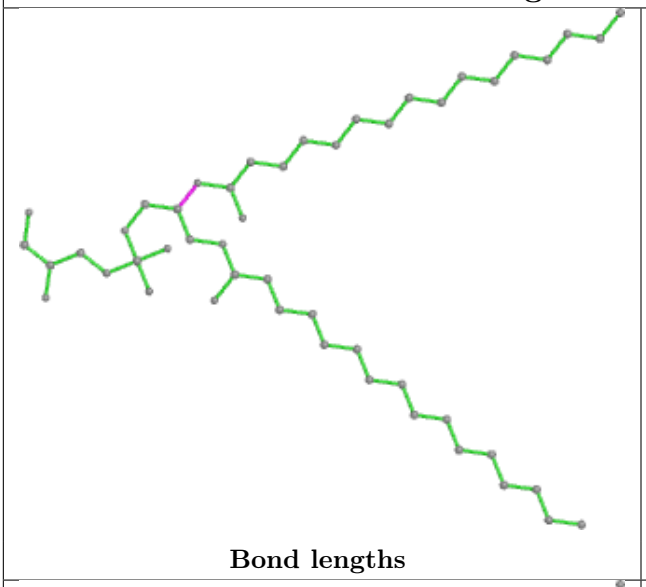


Rings

Ligand LHG L 101



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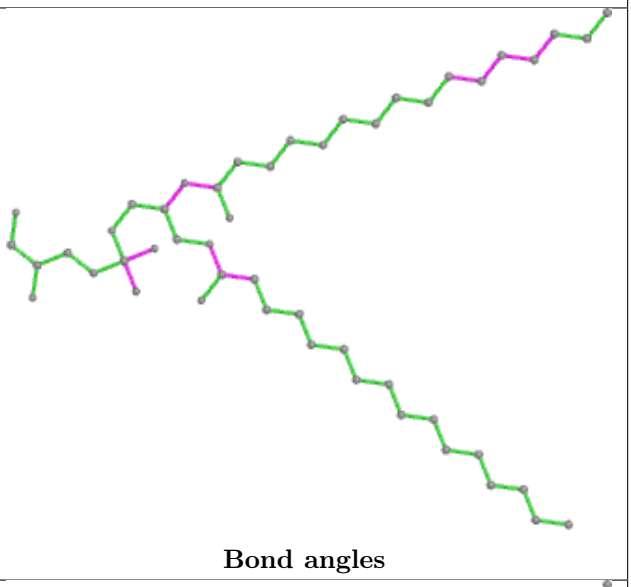
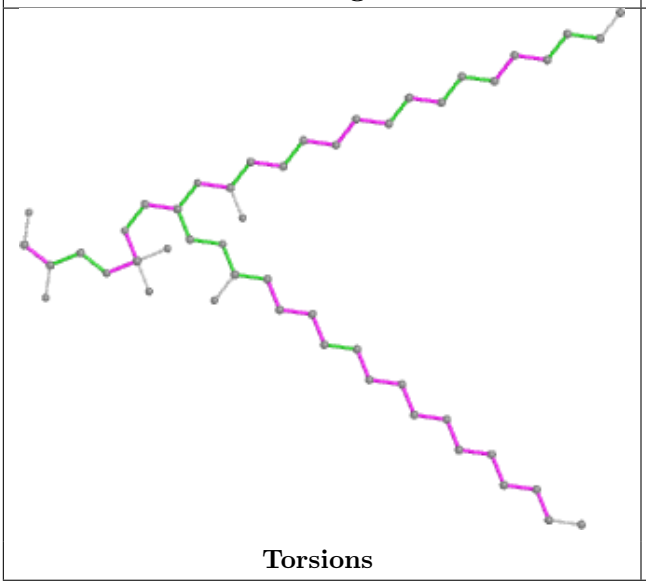
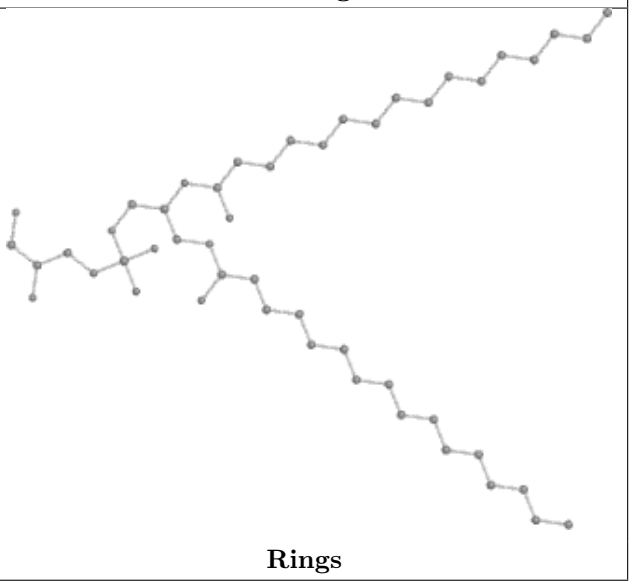


Bond angles

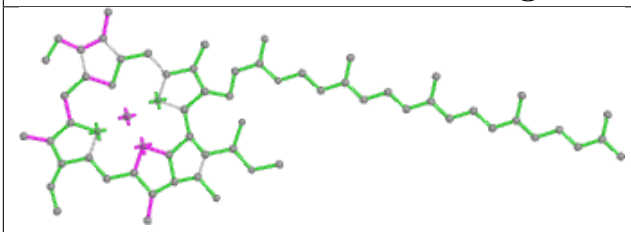


Torsions



Rings

Ligand CLA 33 303



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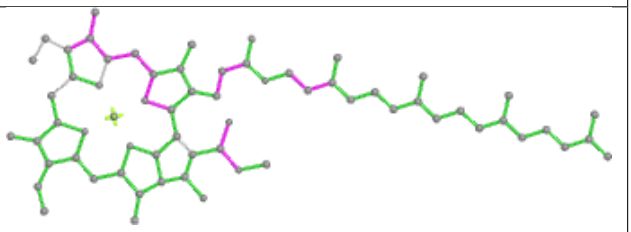
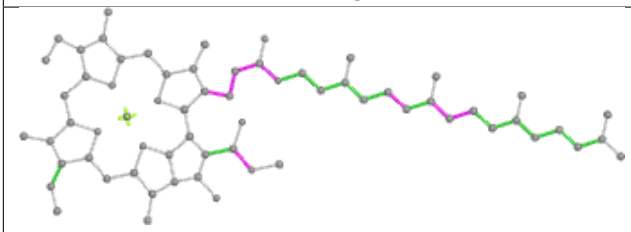


Bond angles



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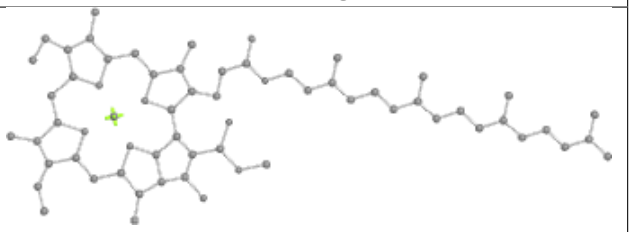
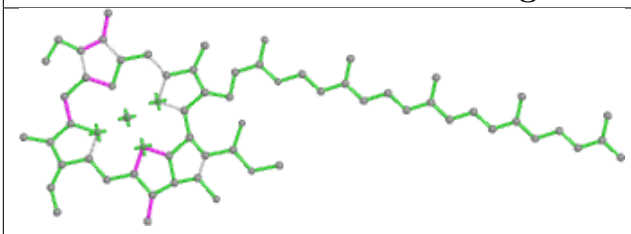


Rings

Ligand CLA 41 306



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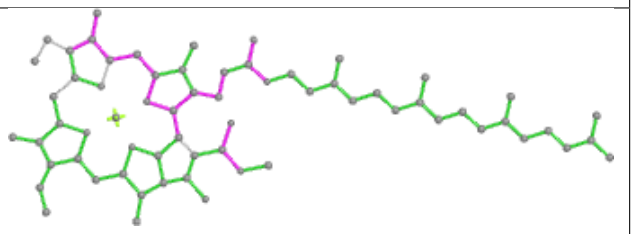

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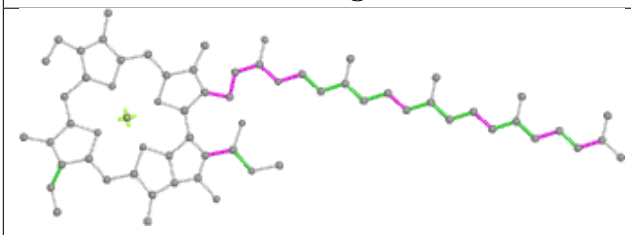

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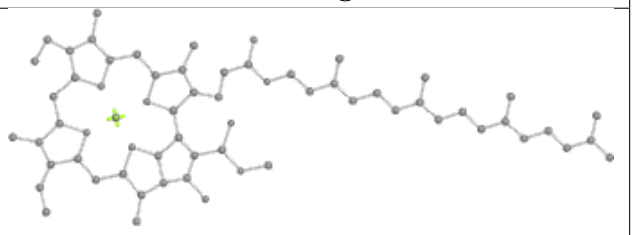
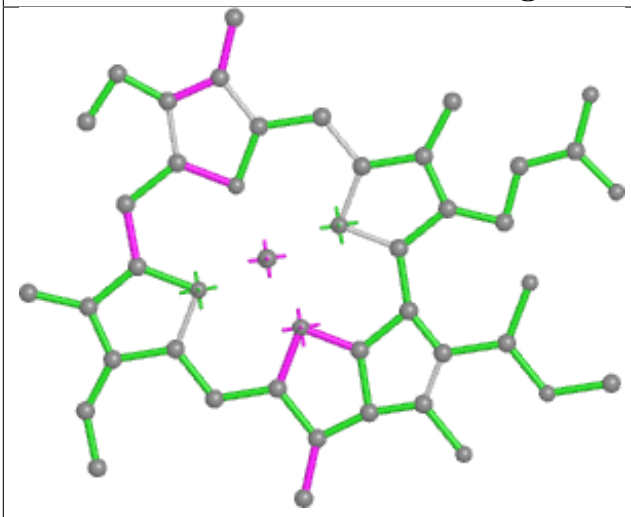


Rings

Ligand CLA 39 304



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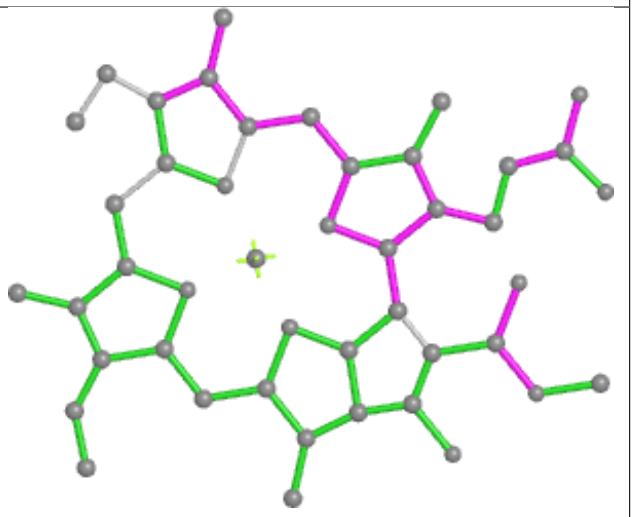

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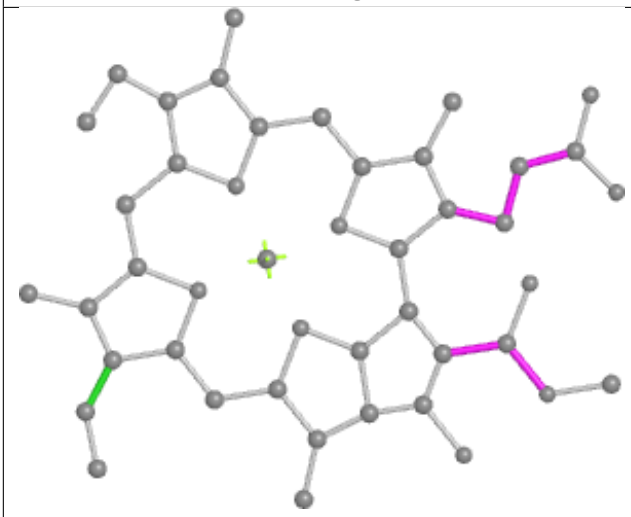

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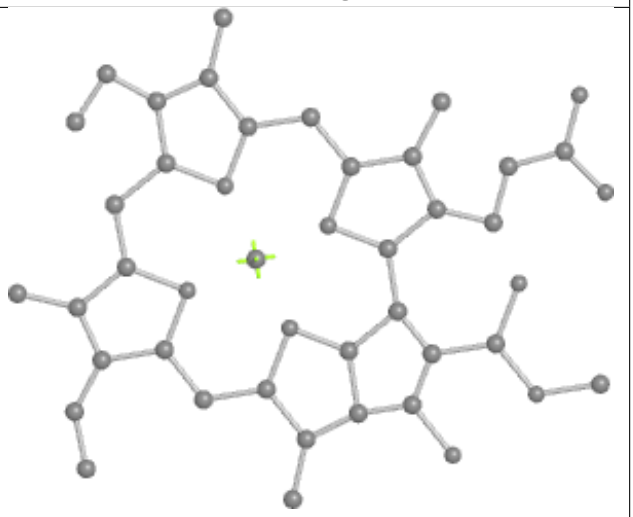
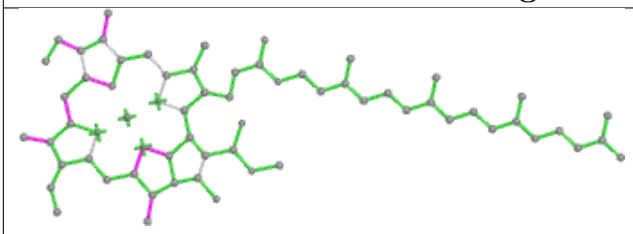


Rings

Ligand CLA 14 302



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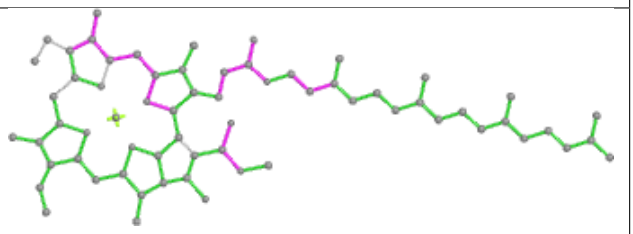
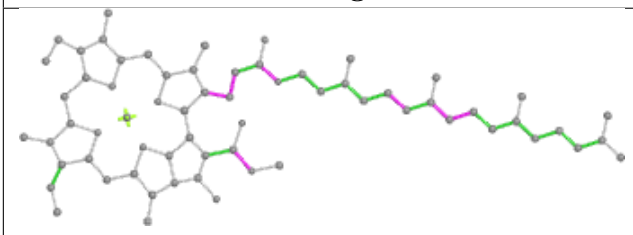


Bond angles



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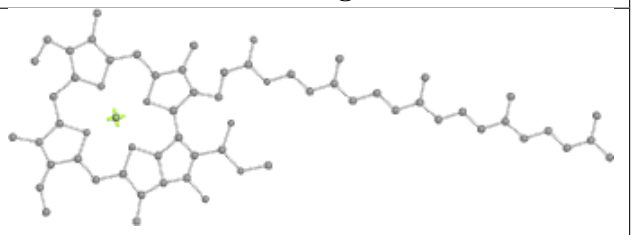
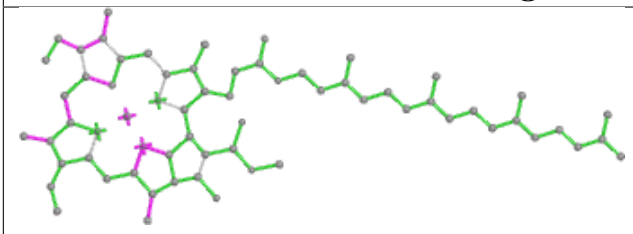


Rings

Ligand CLA 36 304



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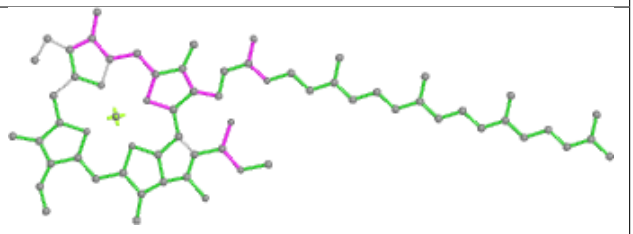

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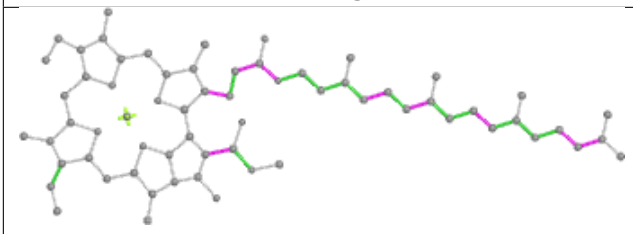

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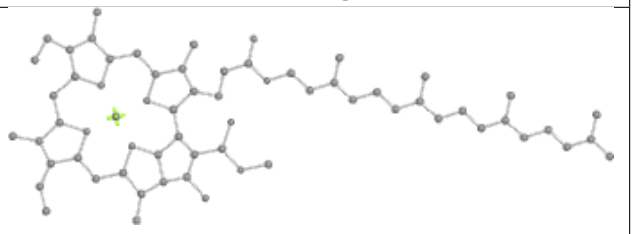
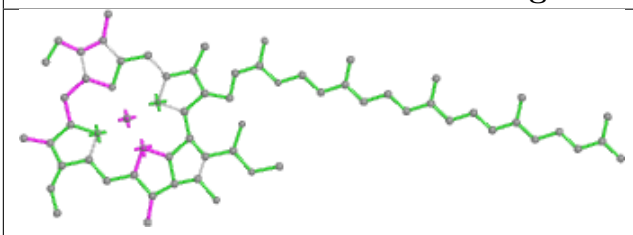


Rings

Ligand CLA c 504



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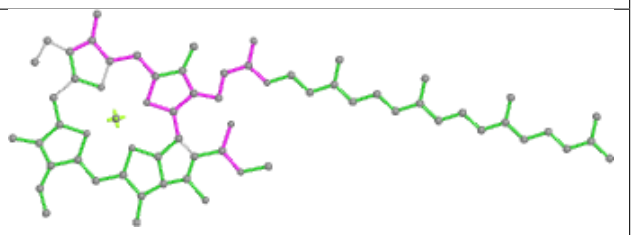

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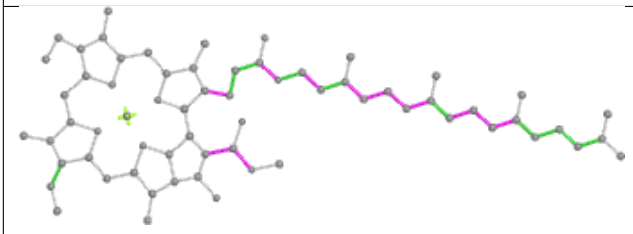

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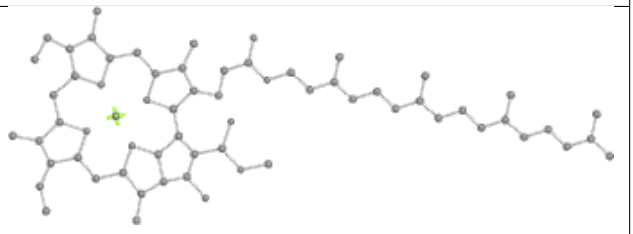
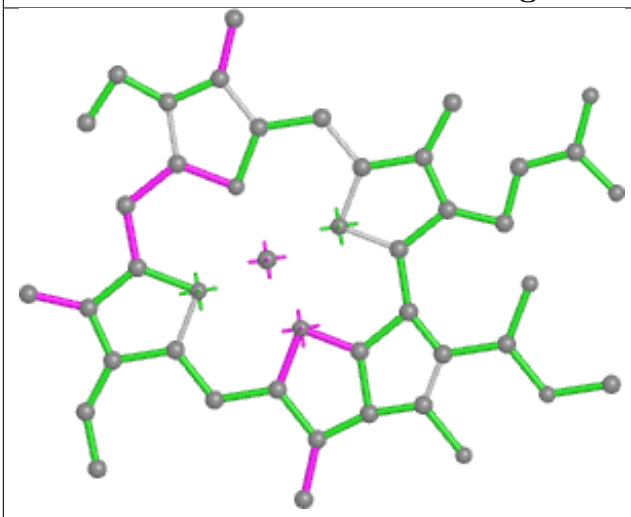


Rings

Ligand CLA 36 305



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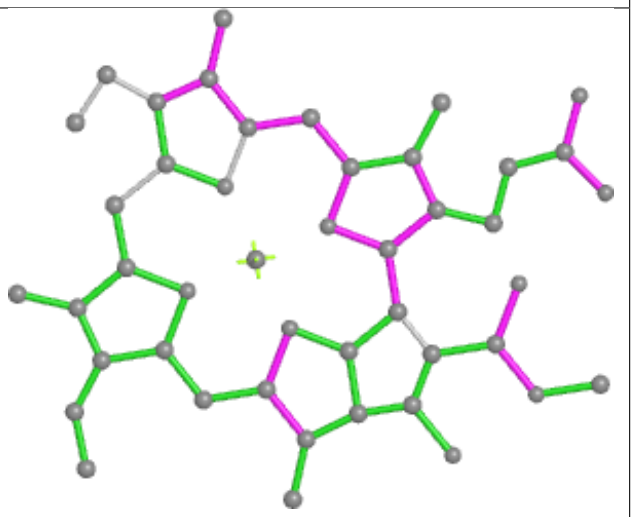
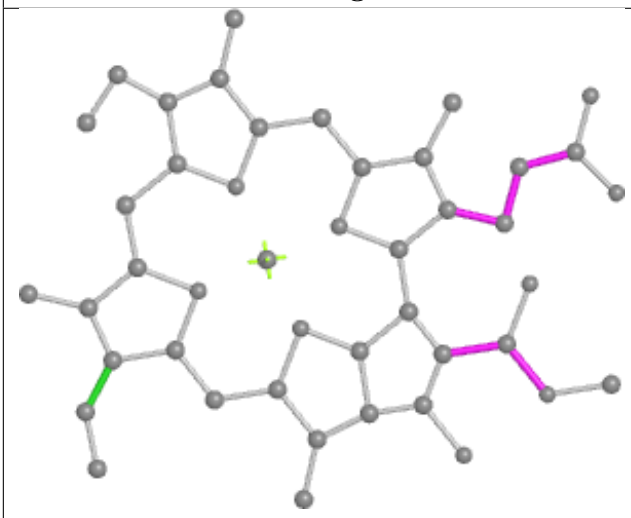


Bond angles



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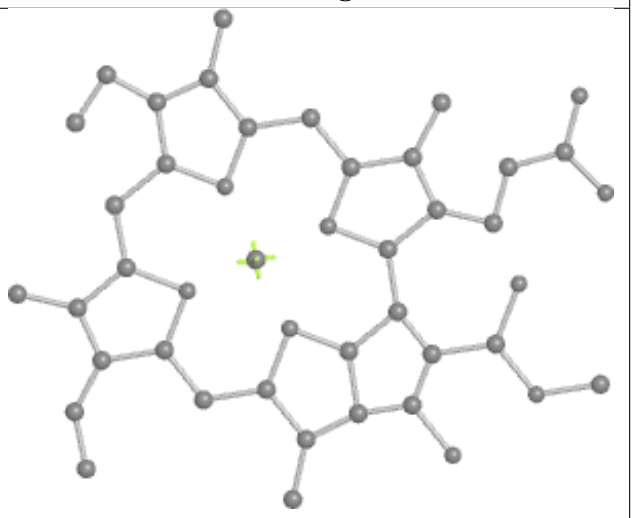
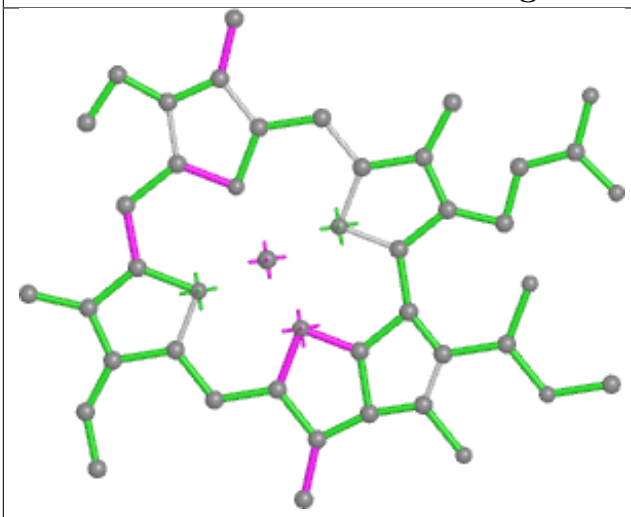


Rings

Ligand CLA 38 308



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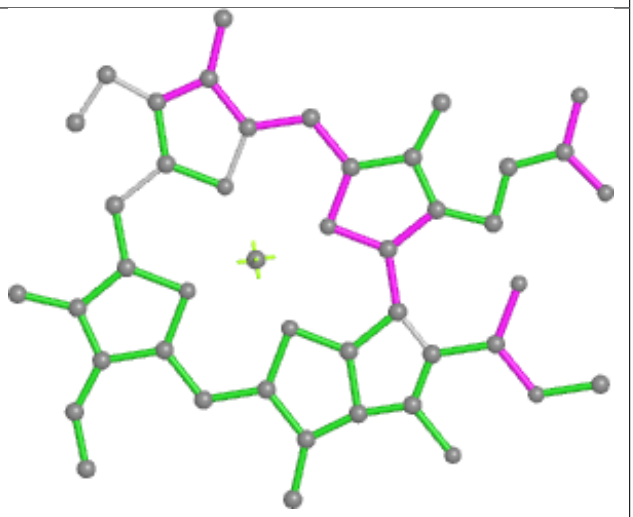

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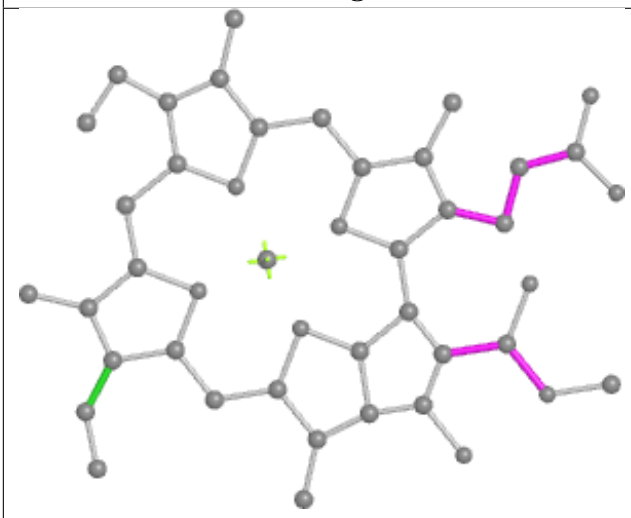

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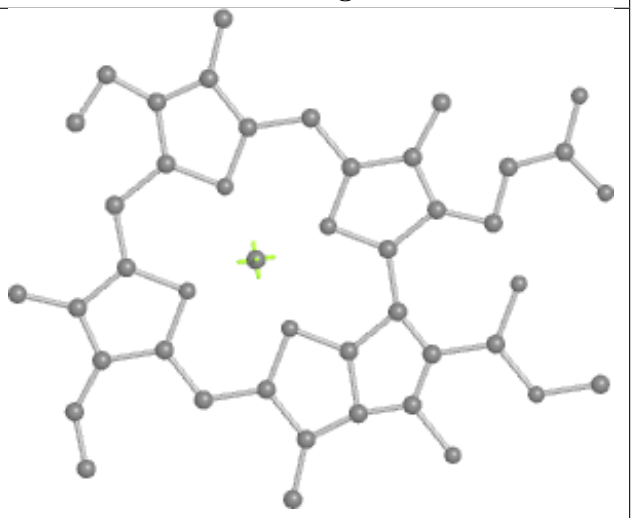
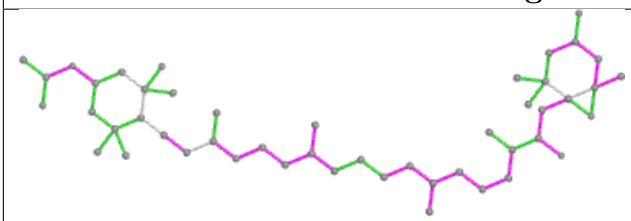


Rings

Ligand A86 31 310



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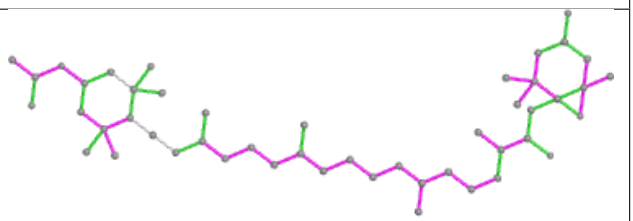

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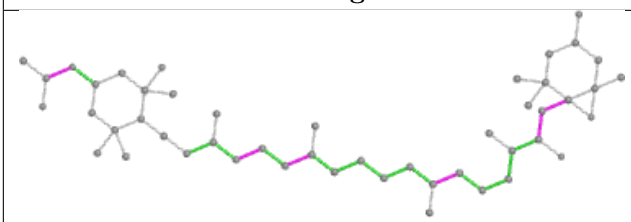

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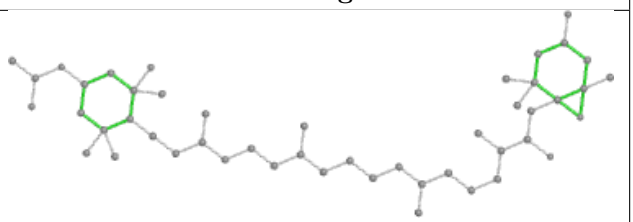
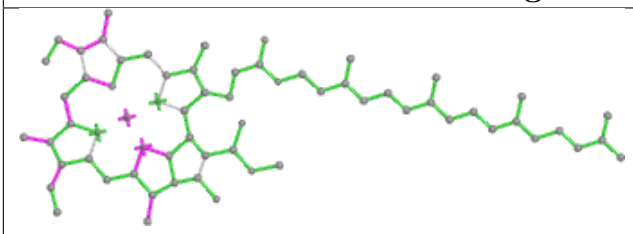


Rings

Ligand CLA B 610



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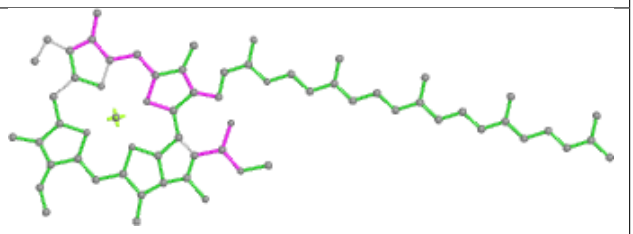
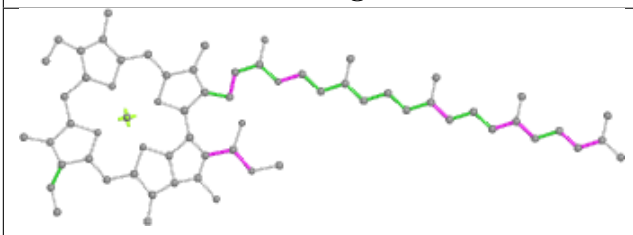


Bond angles



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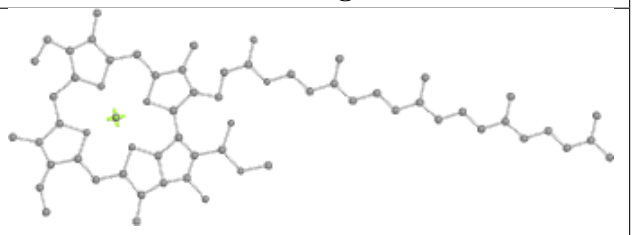
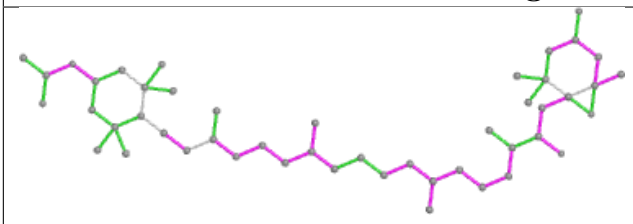


Rings

Ligand A86 37 316



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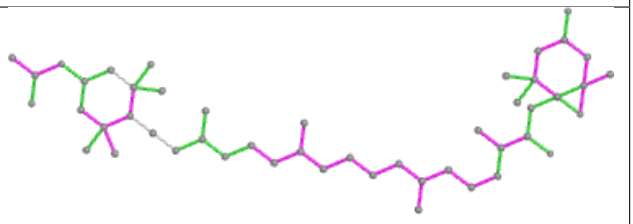
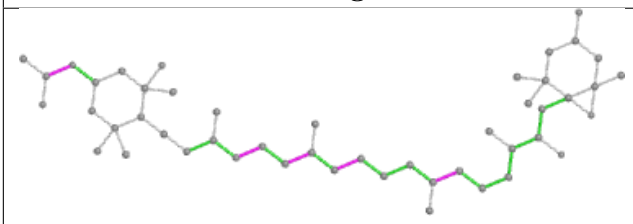
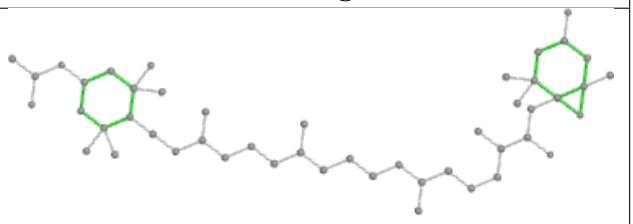


Bond angles

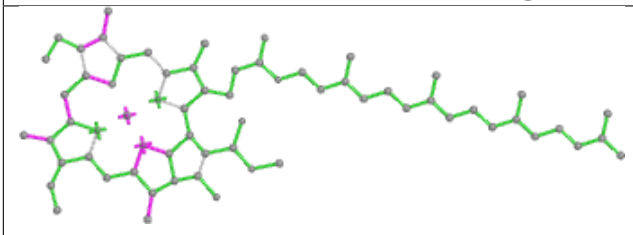


Torsions



Rings

Ligand CLA 34 301



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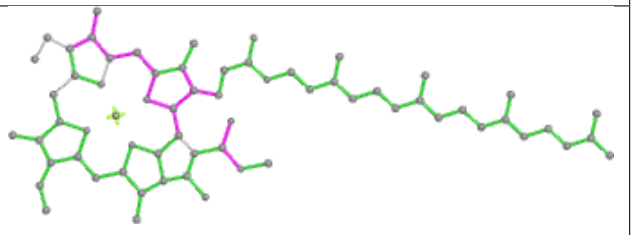
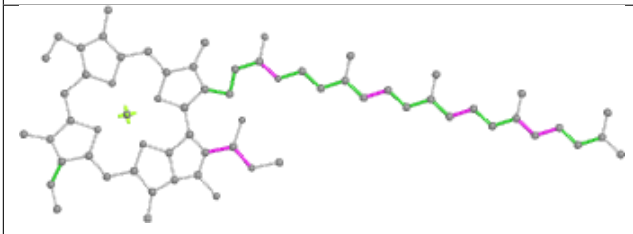


Bond angles



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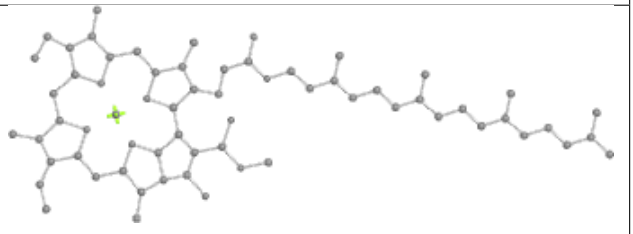
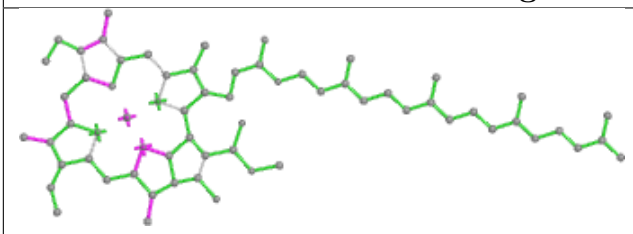


Rings

Ligand CLA 11 315



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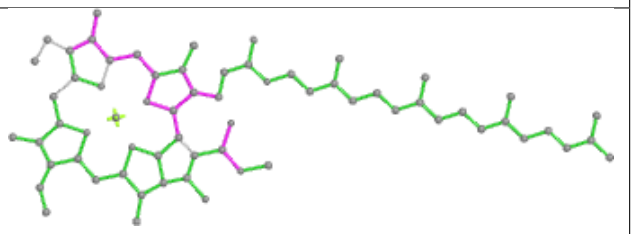
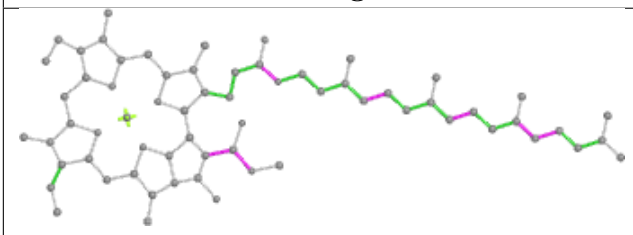


Bond angles



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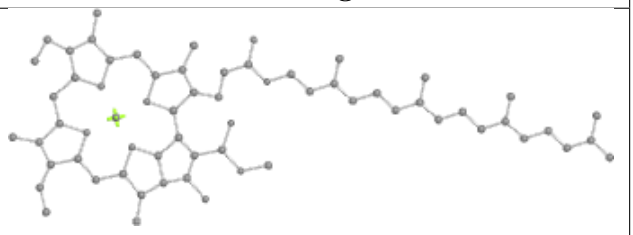
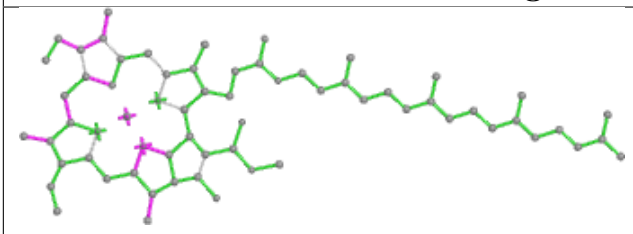


Rings

Ligand CLA B 609



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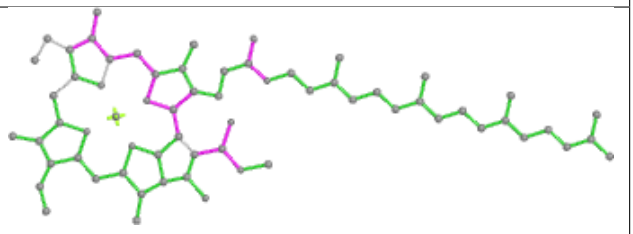
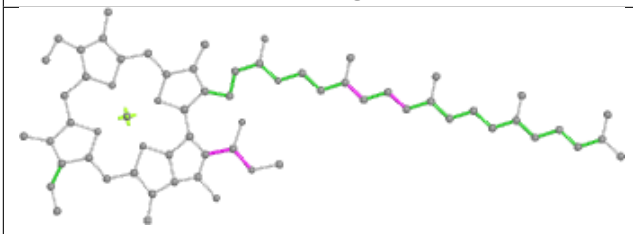
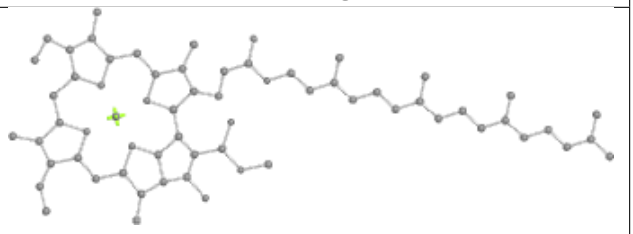


Bond angles

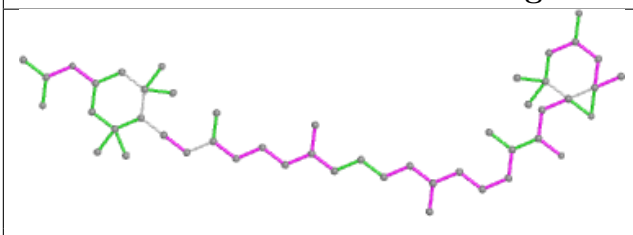


Torsions



Rings

Ligand A86 16 311



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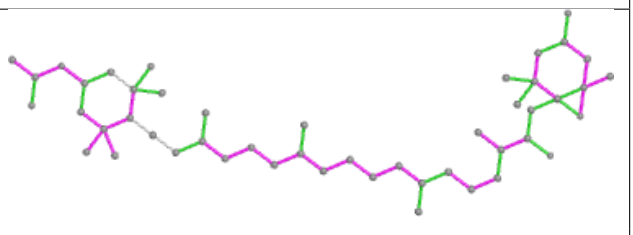

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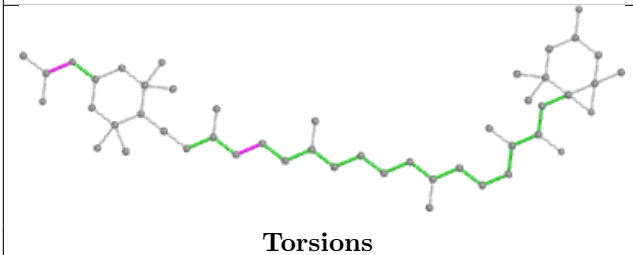

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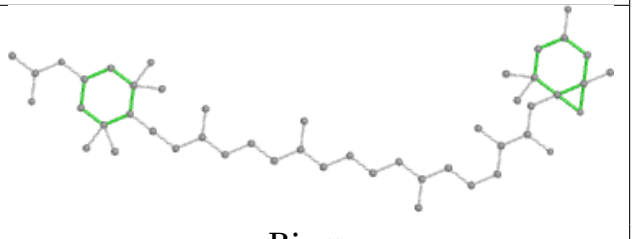
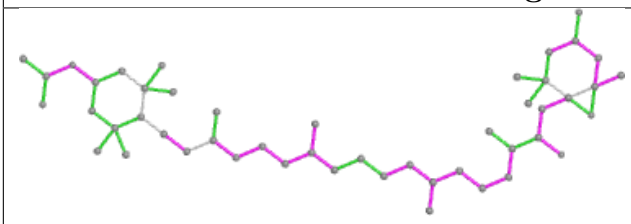


Rings

Ligand A86 34 312



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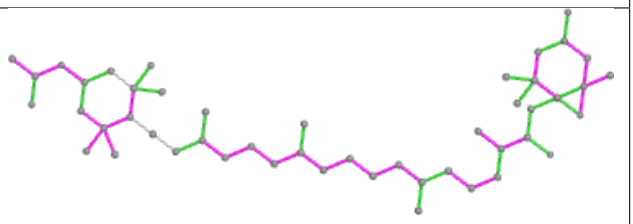

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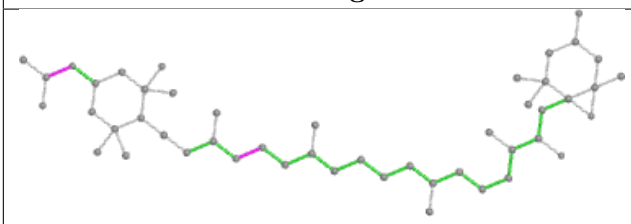

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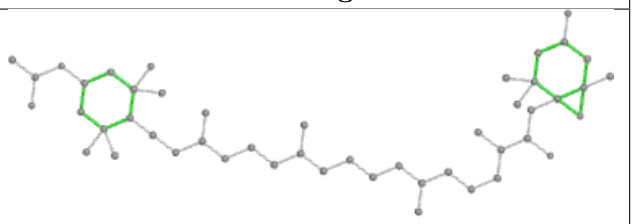
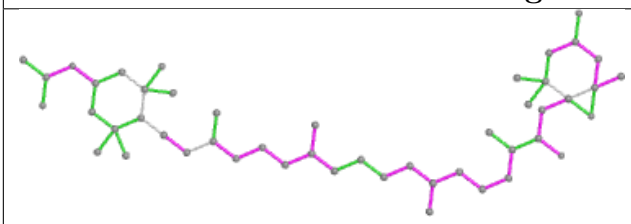


Rings

Ligand A86 11 310



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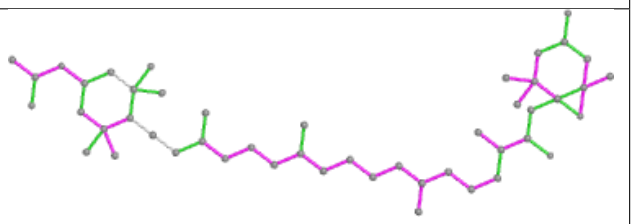

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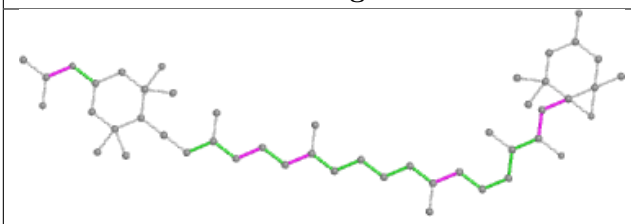

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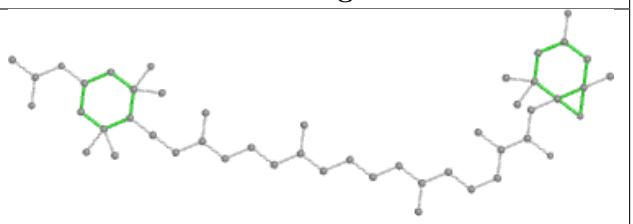
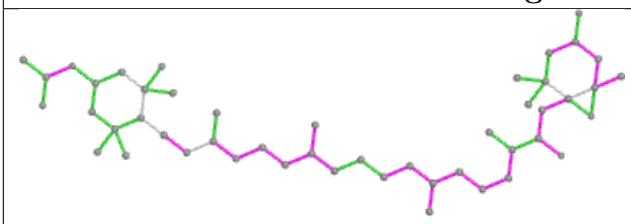


Rings

Ligand A86 34 313



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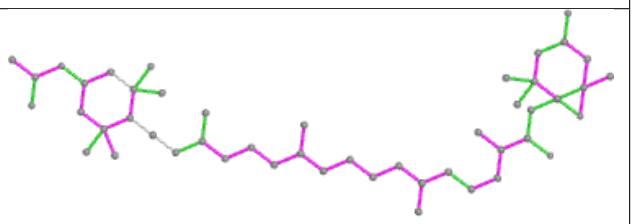

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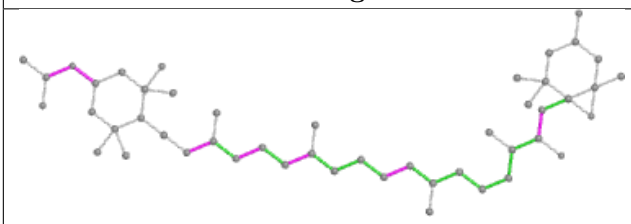

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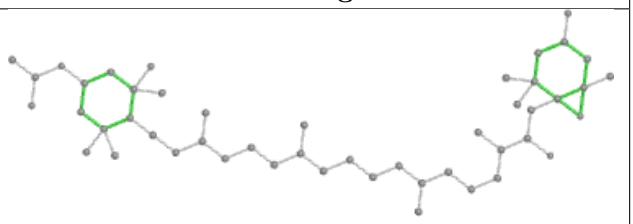
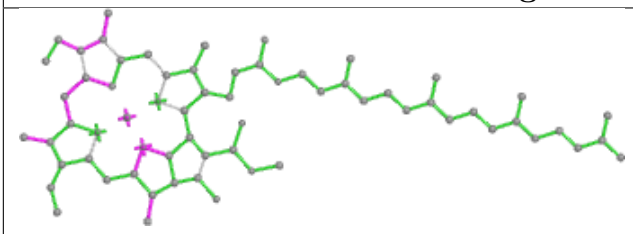


Rings

Ligand CLA 18 301



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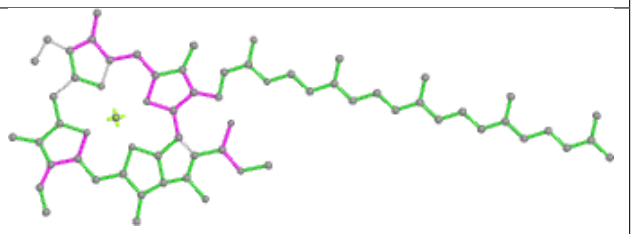

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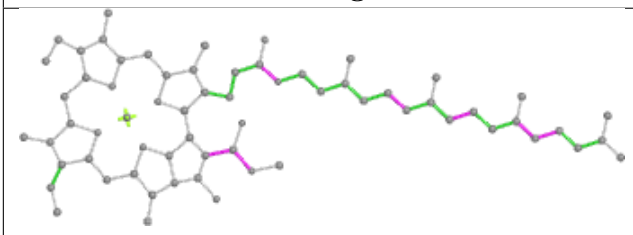

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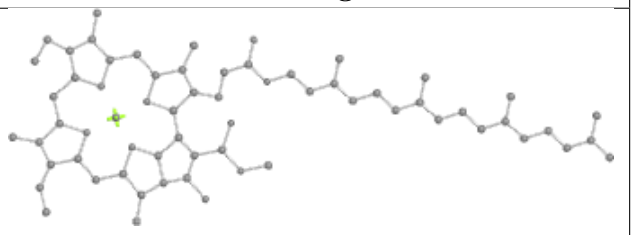

Rings

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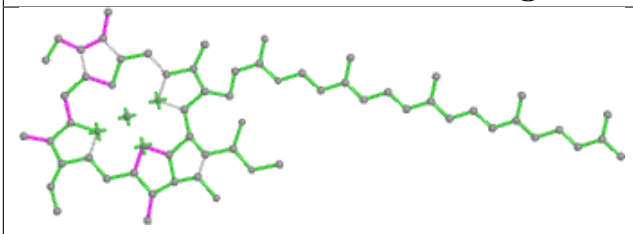

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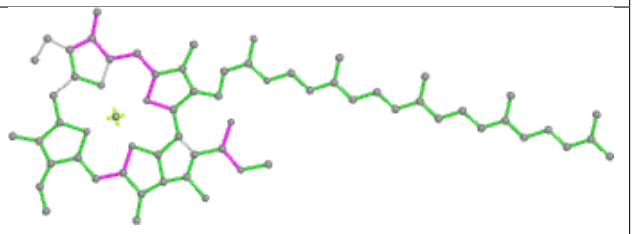

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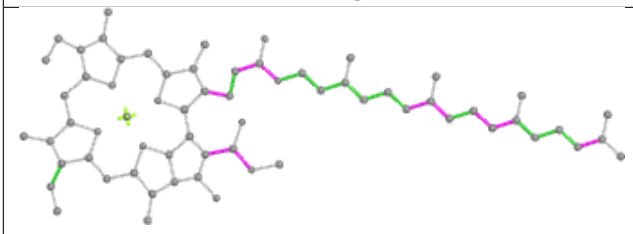

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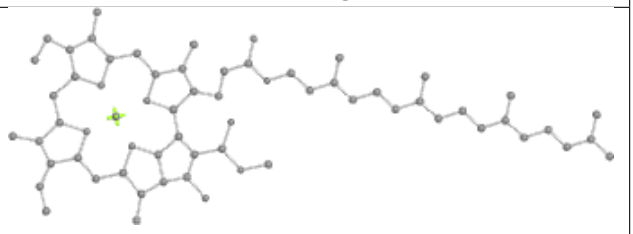
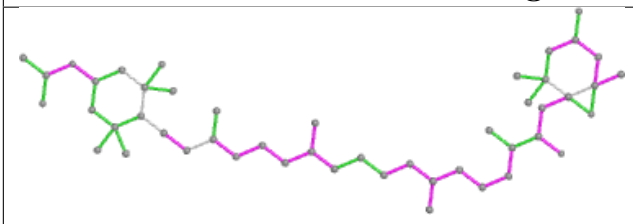


Rings

Ligand A86 15 314



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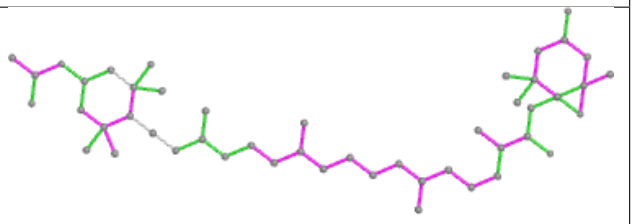

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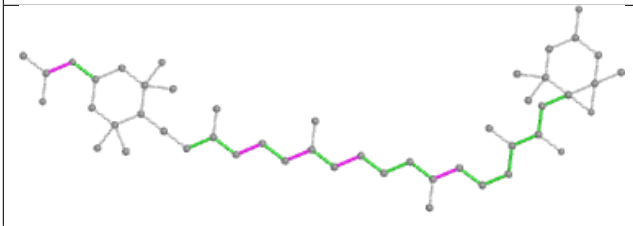

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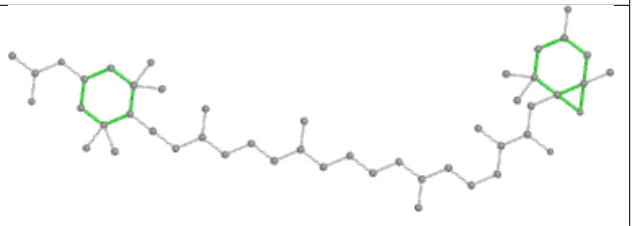
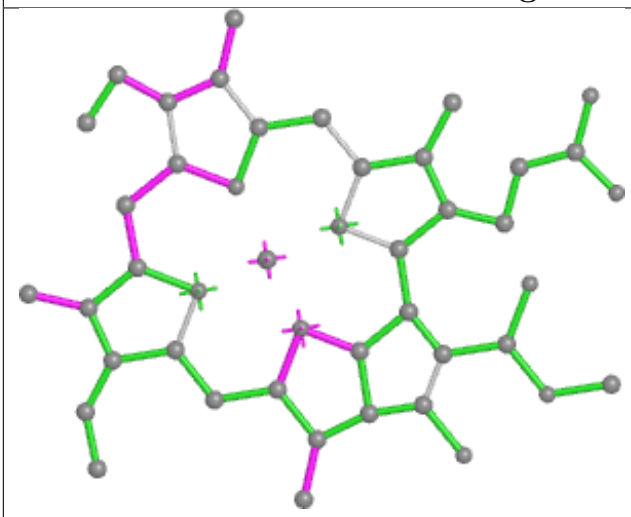


Rings

Ligand CLA 33 310



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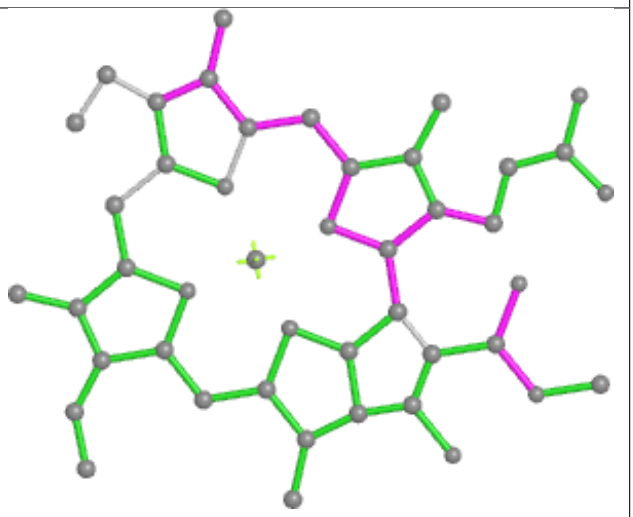

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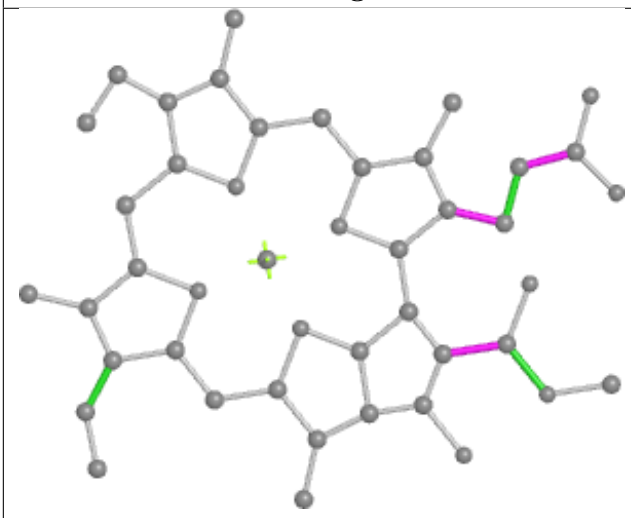

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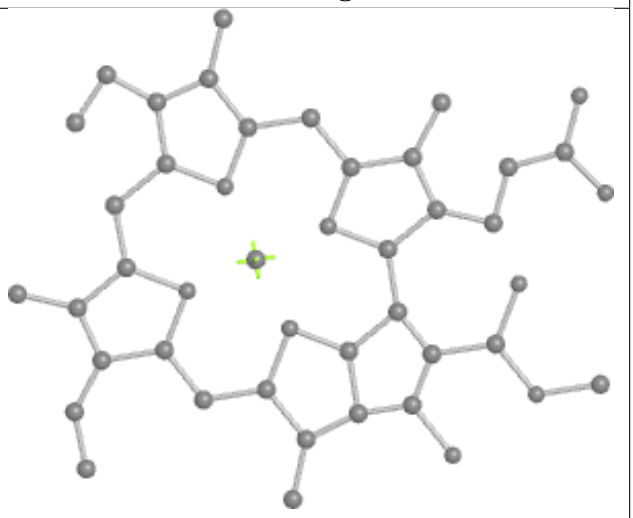
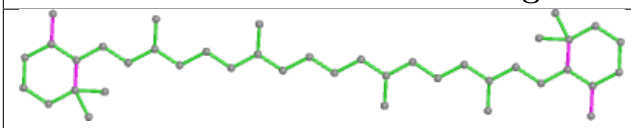


Rings

Ligand BCR C 515



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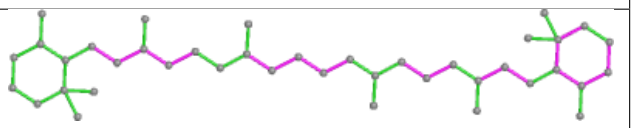

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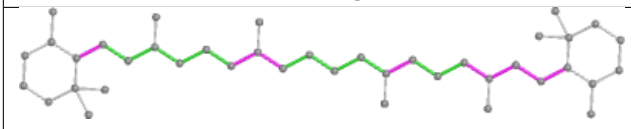
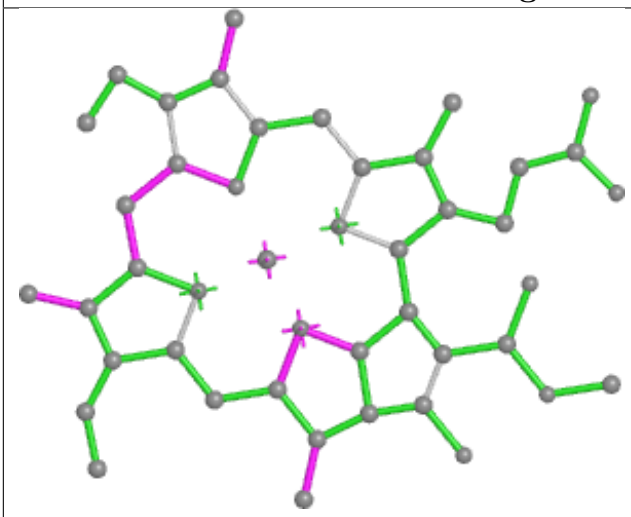


Torsions

Rings

Ligand CLA 39 307



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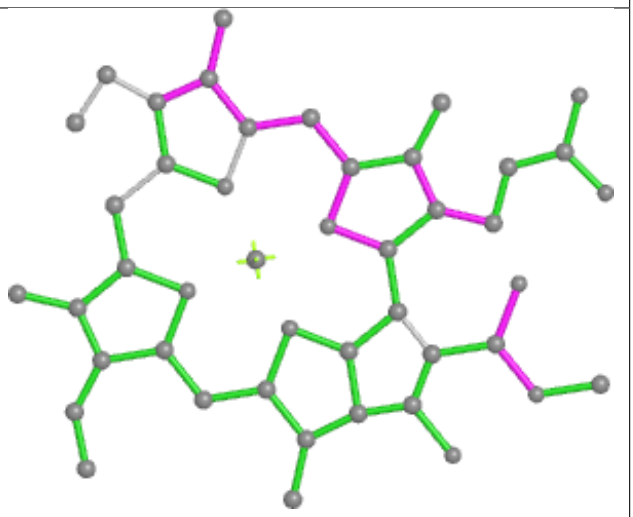

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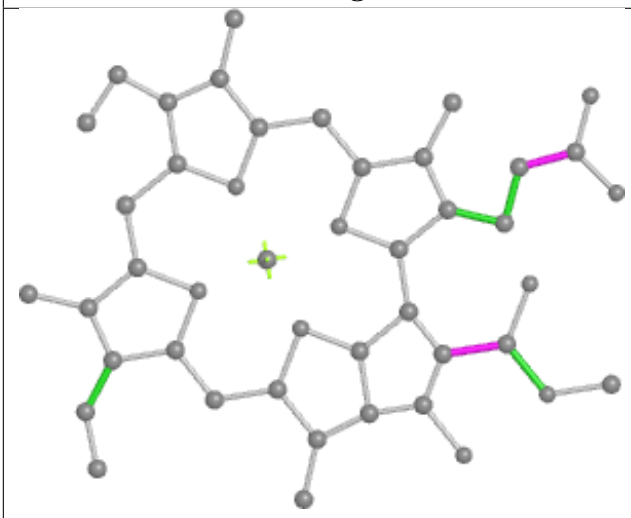

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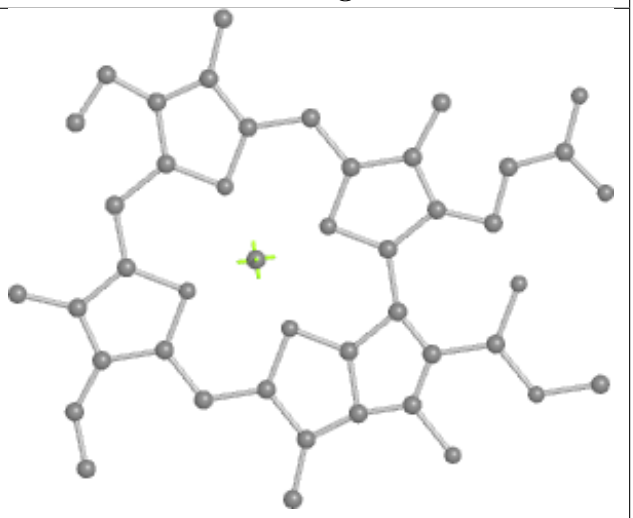
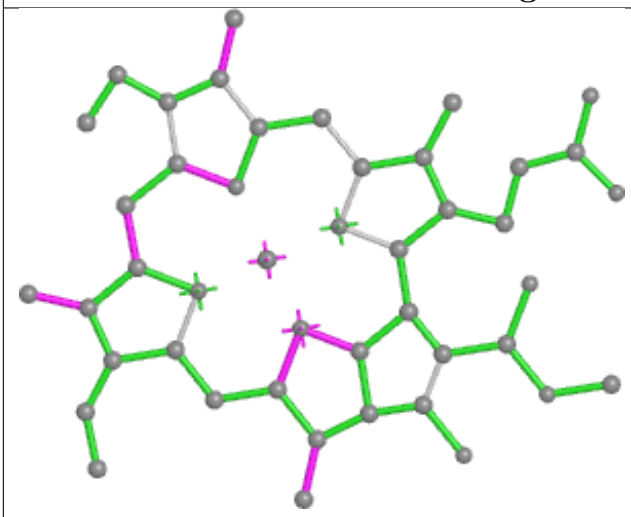


Rings

Ligand CLA 36 303



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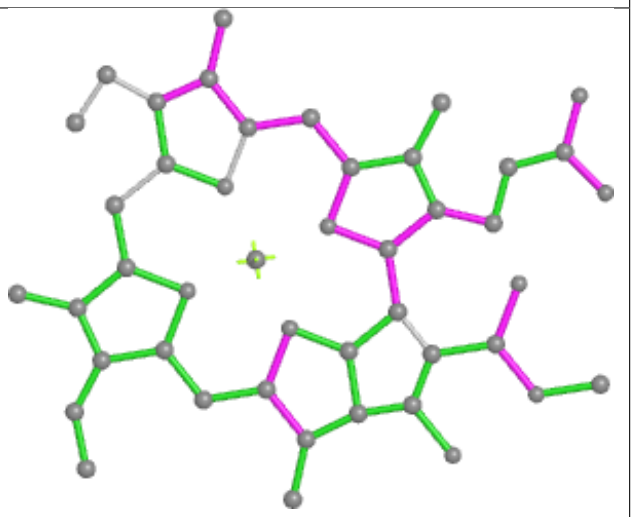

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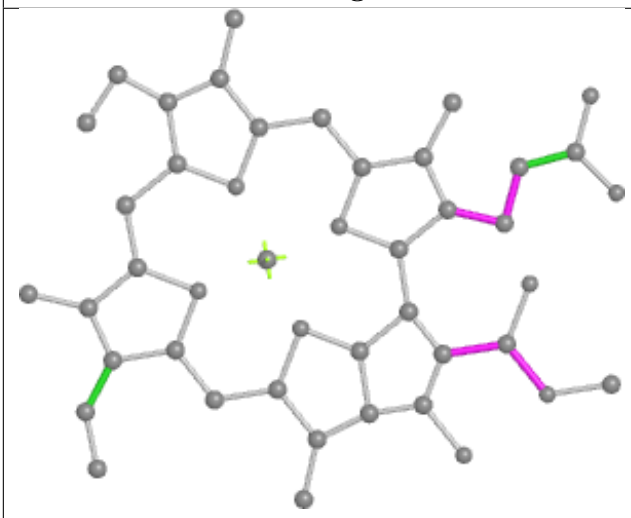

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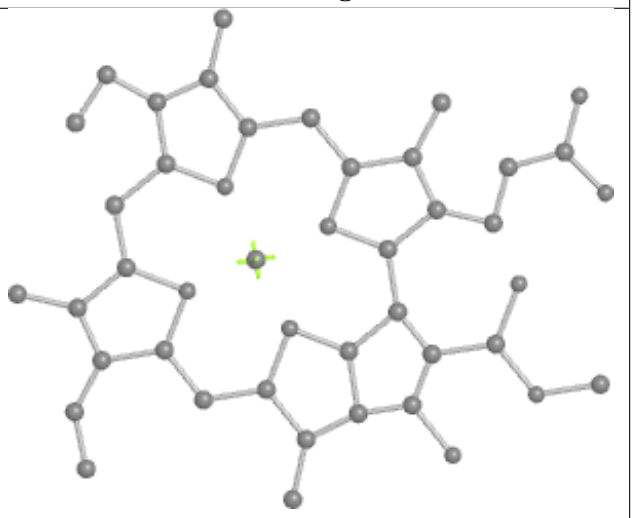
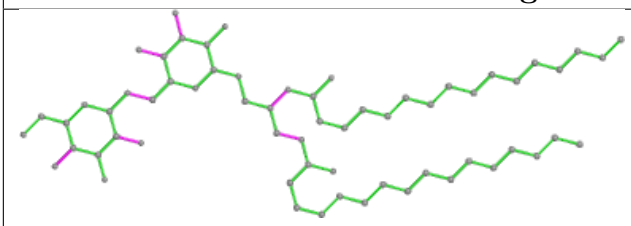


Rings

Ligand DGD C 516



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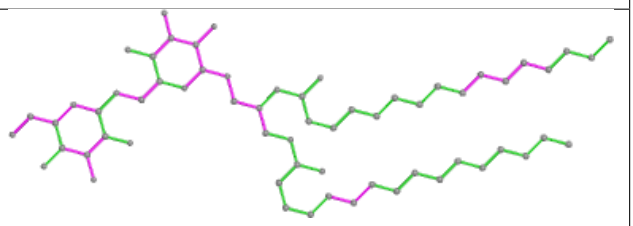

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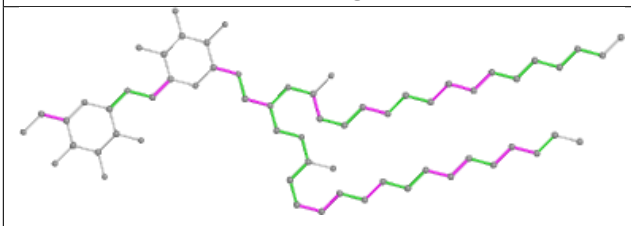

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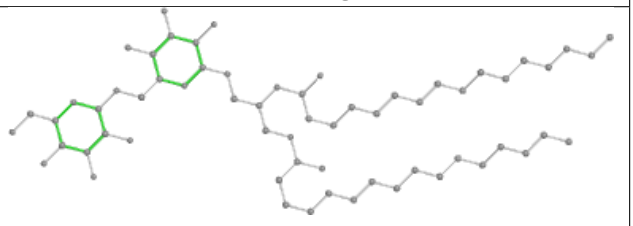
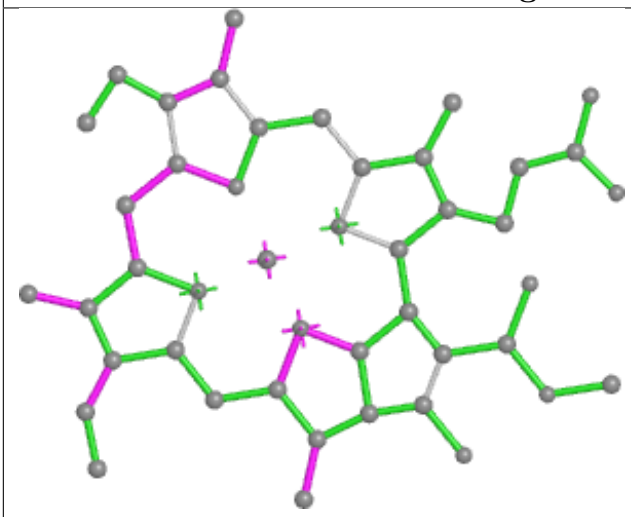


Rings

Ligand CLA 17 304



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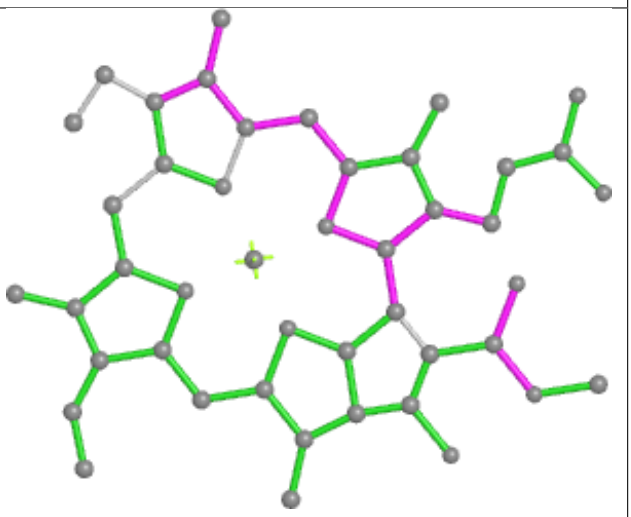

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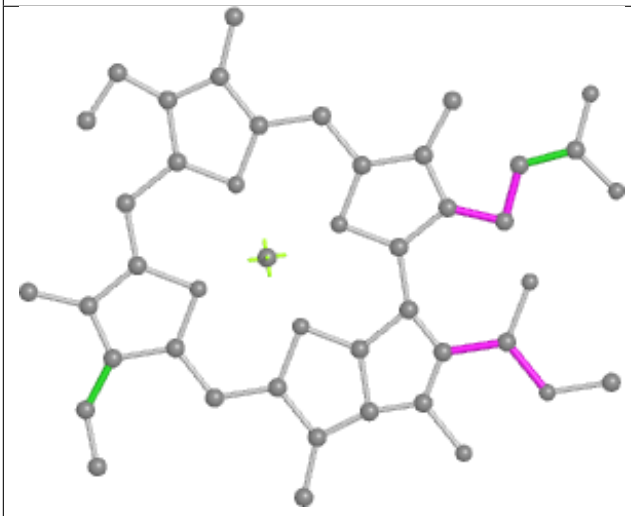

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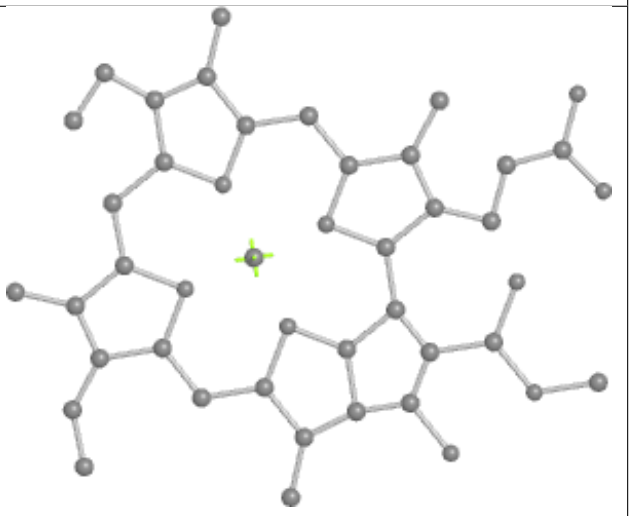
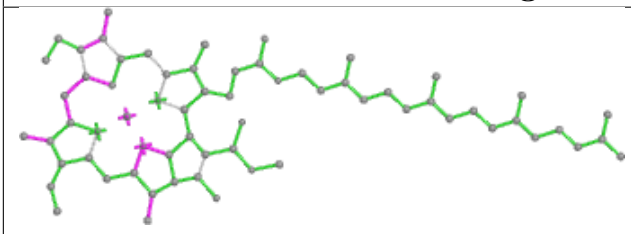


Rings

Ligand CLA 37 301



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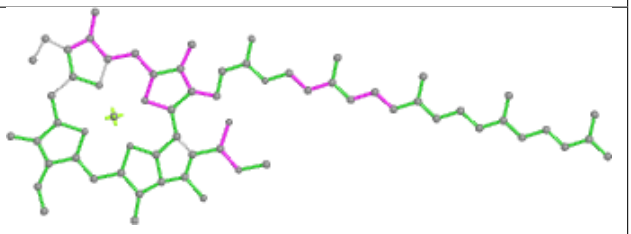

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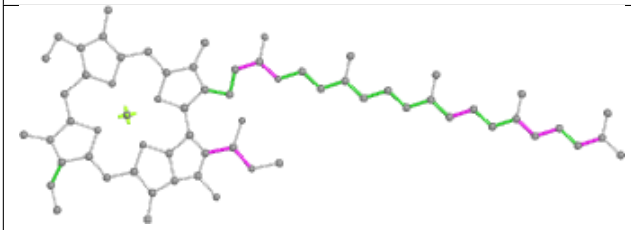
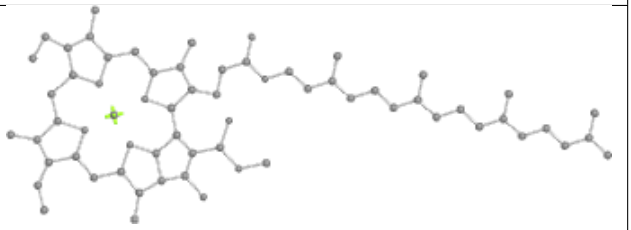
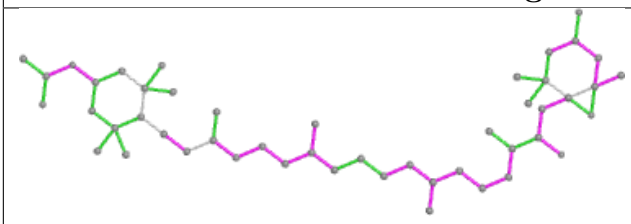


Torsions



Rings

Ligand A86 33 316



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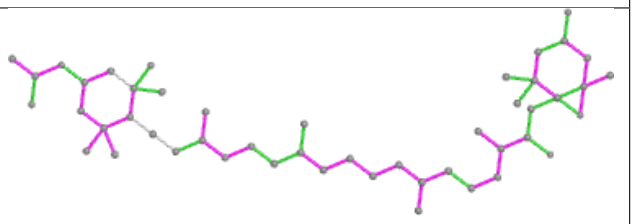

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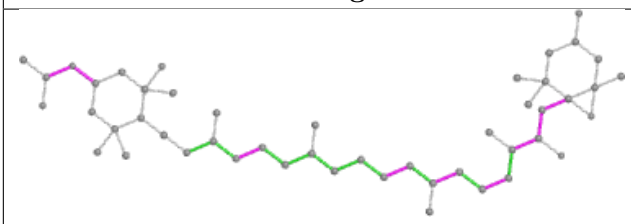

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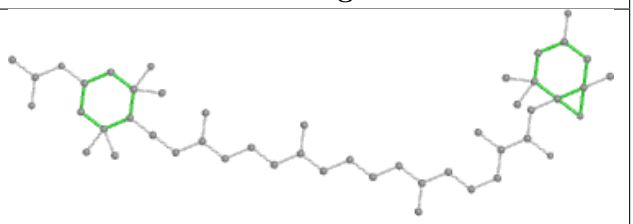

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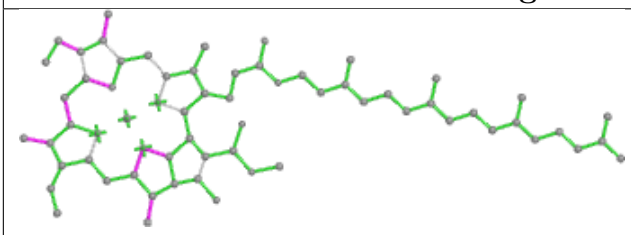

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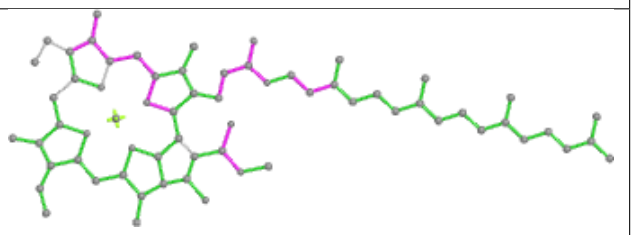

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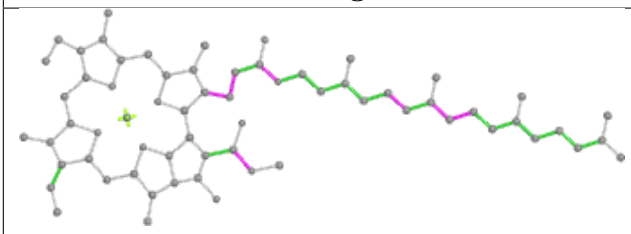

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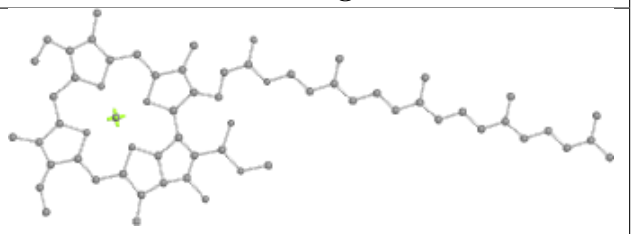

Rings

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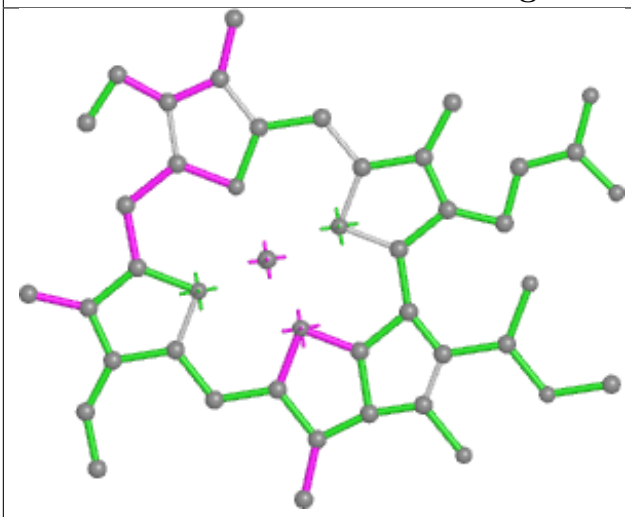

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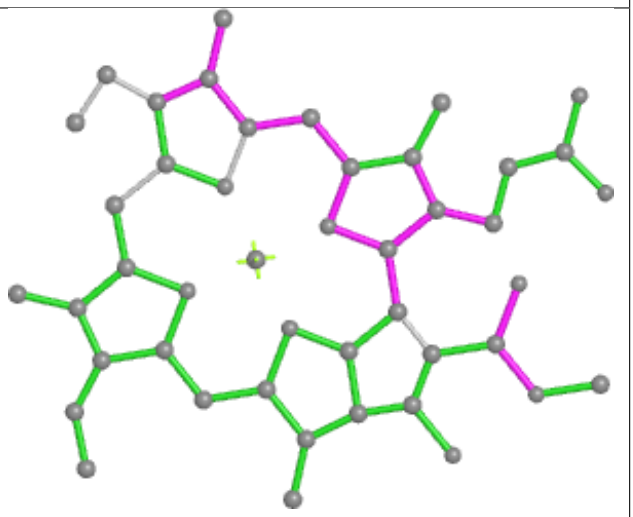

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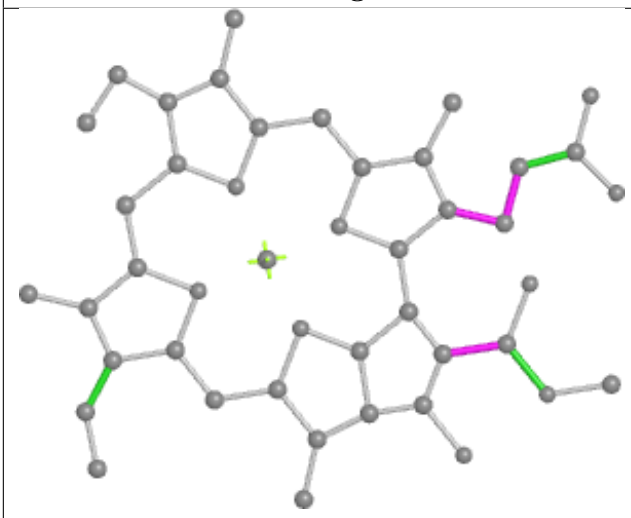

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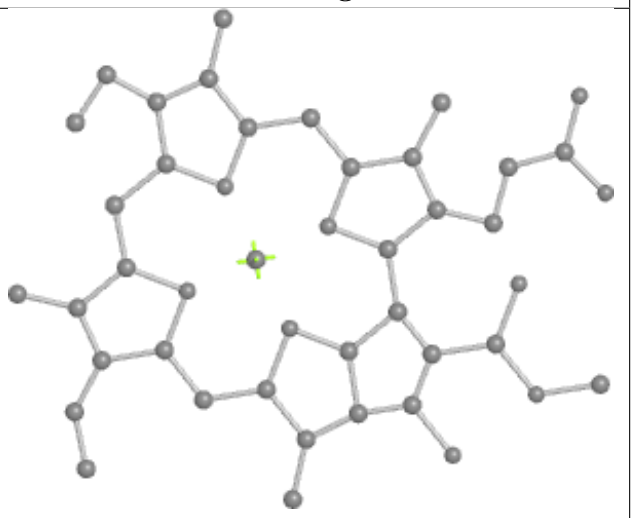

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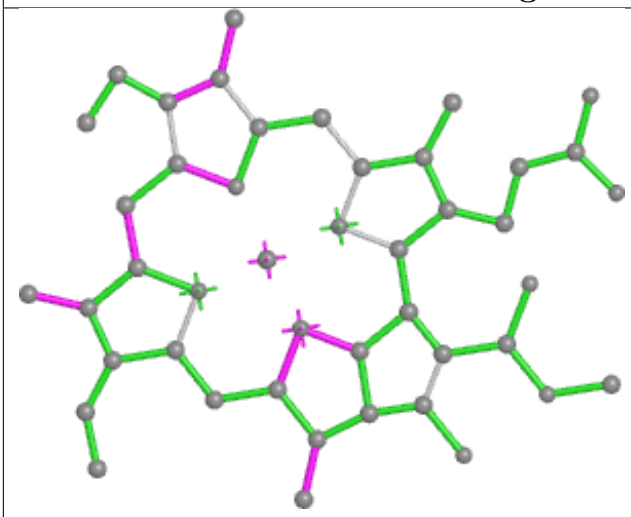

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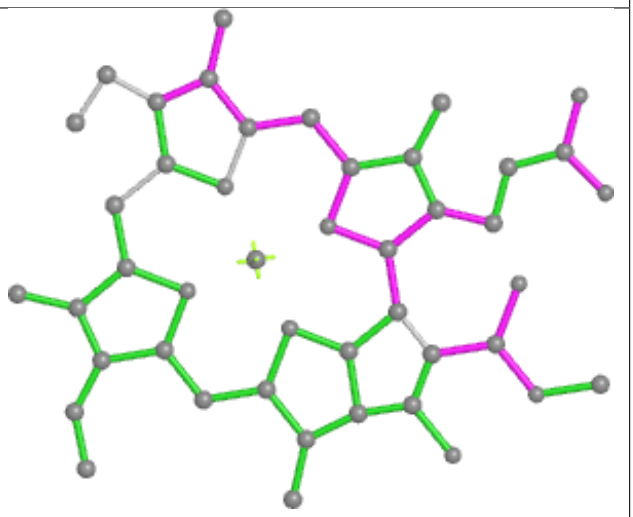

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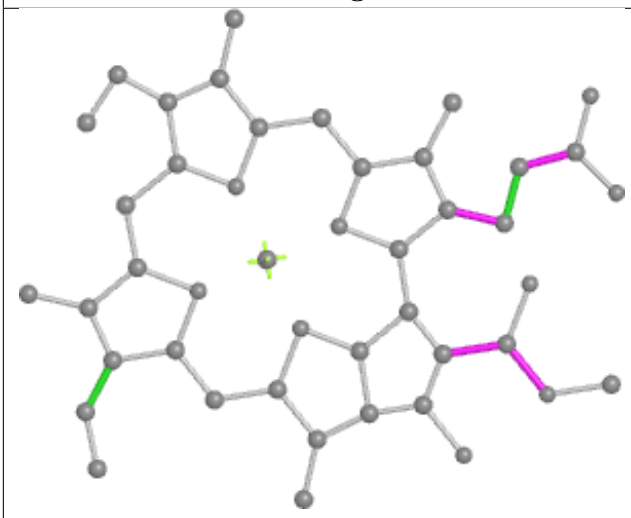

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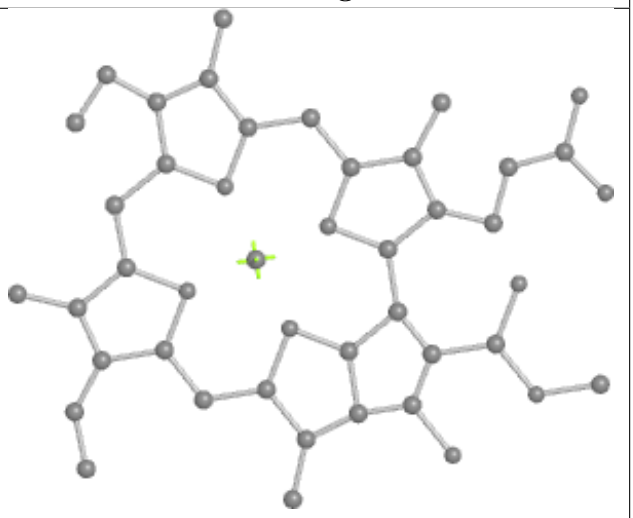
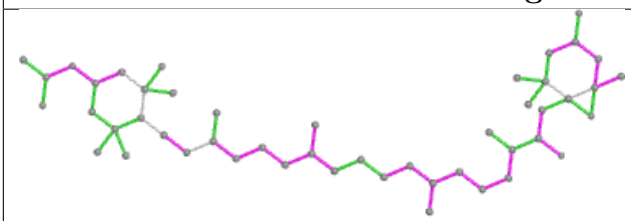


Rings

Ligand A86 37 302



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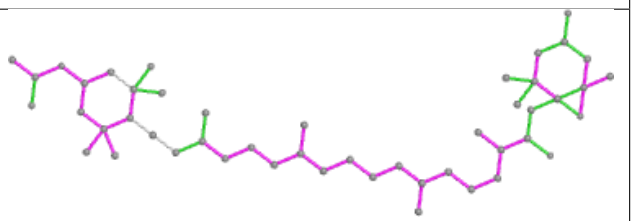

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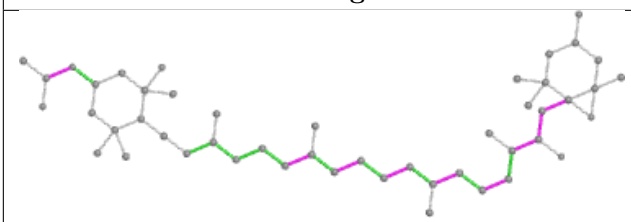

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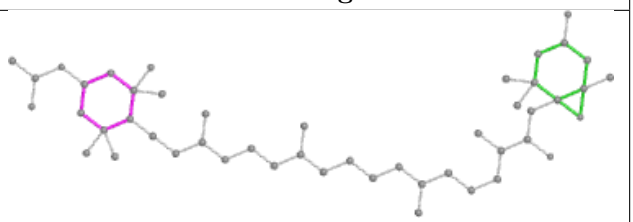

Rings

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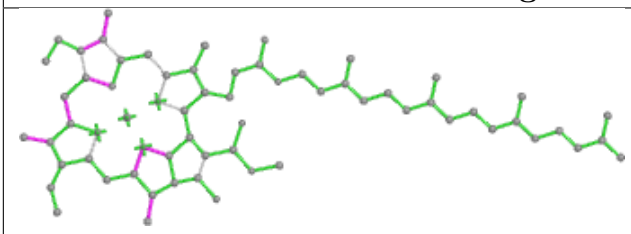

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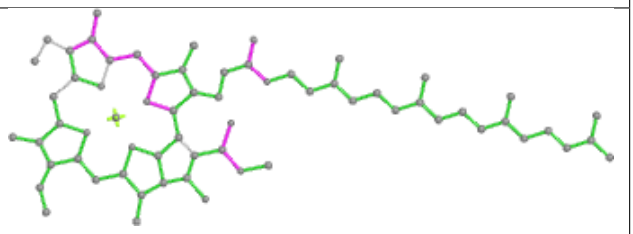

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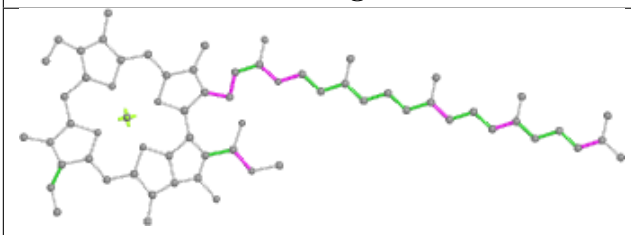

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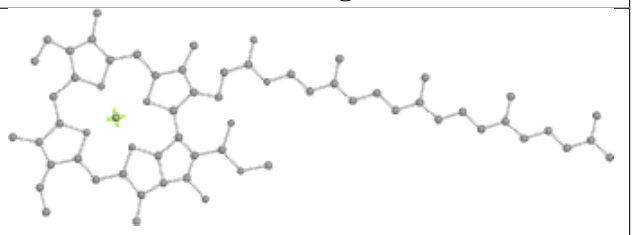

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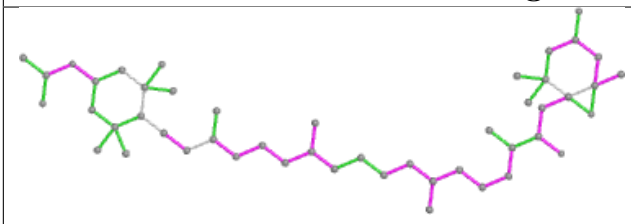

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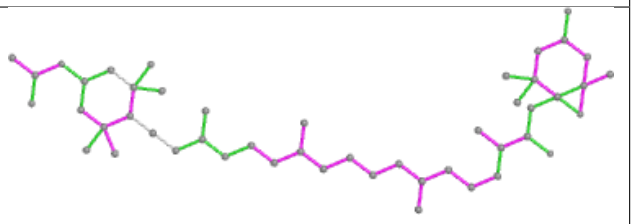

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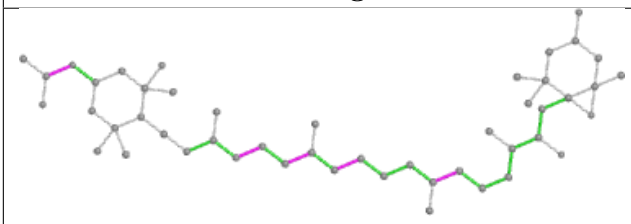

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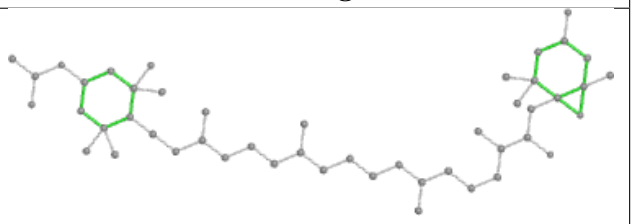

Rings

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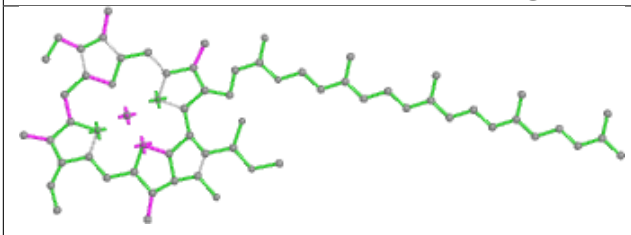

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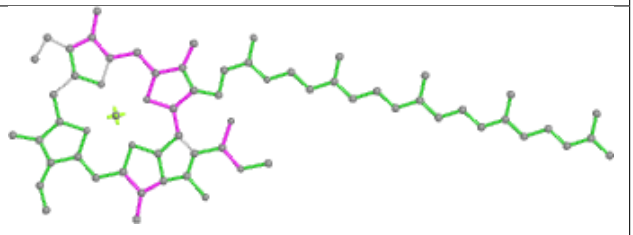

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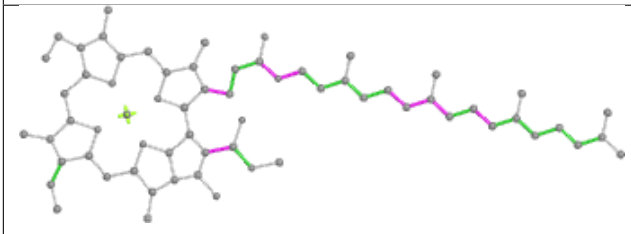

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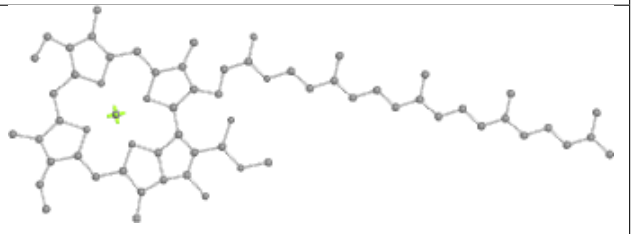

Rings

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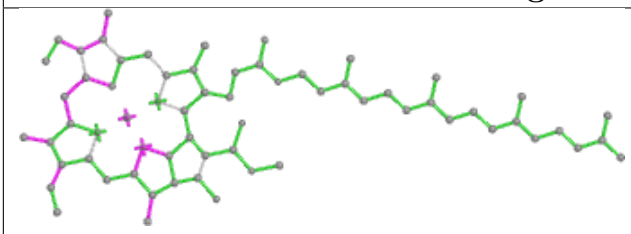

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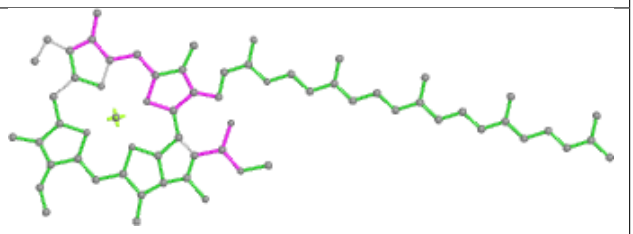

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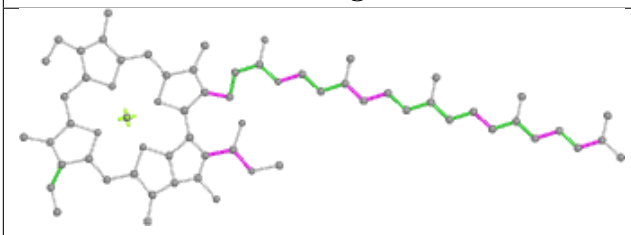

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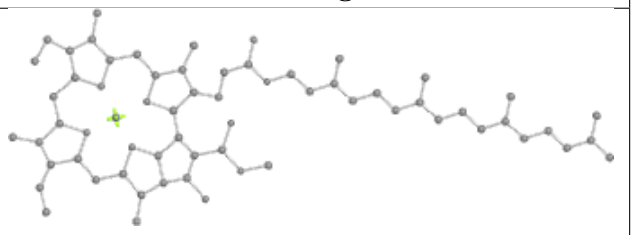

Rings

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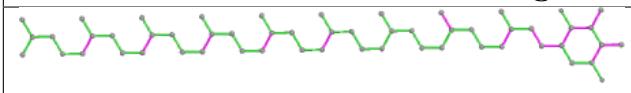

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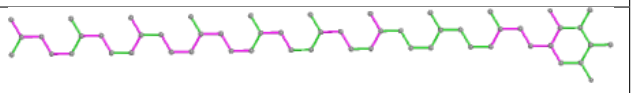

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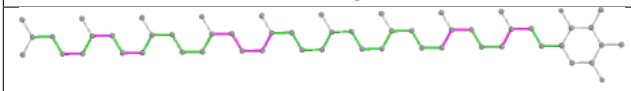

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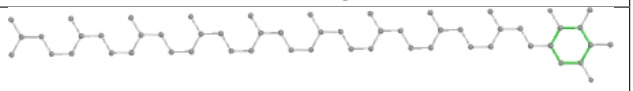

Rings

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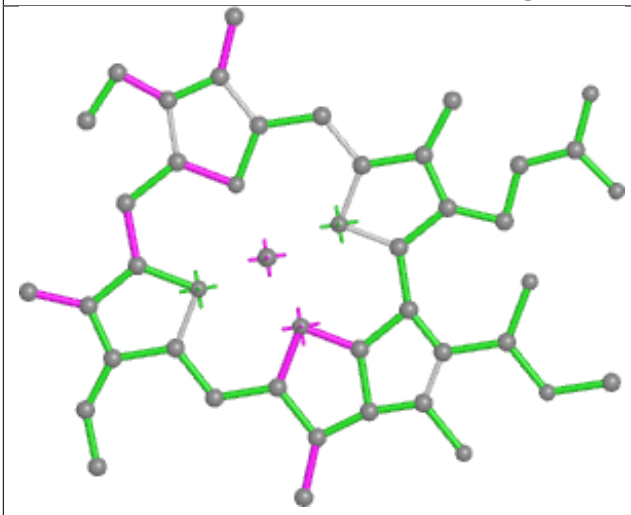

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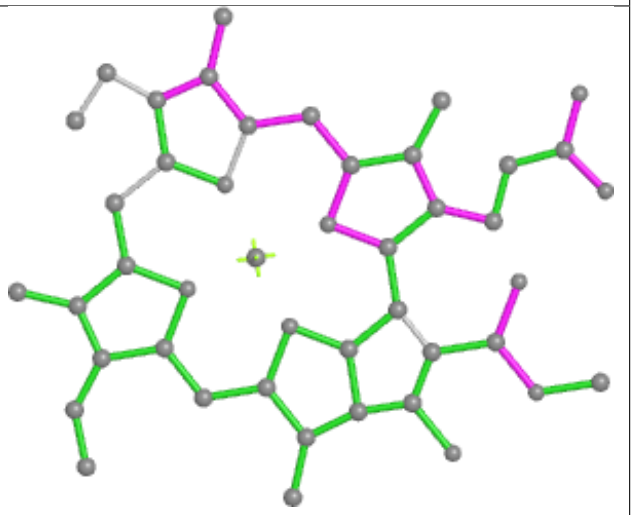

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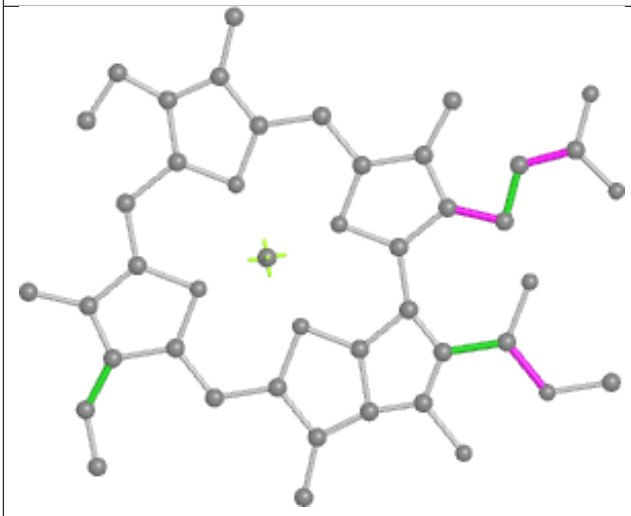

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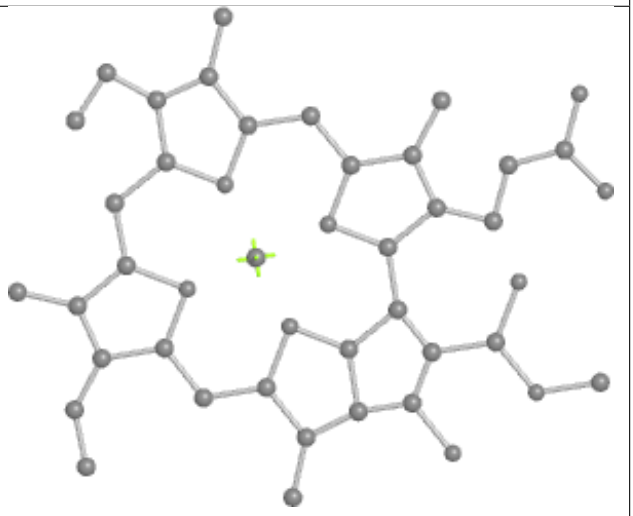

Rings

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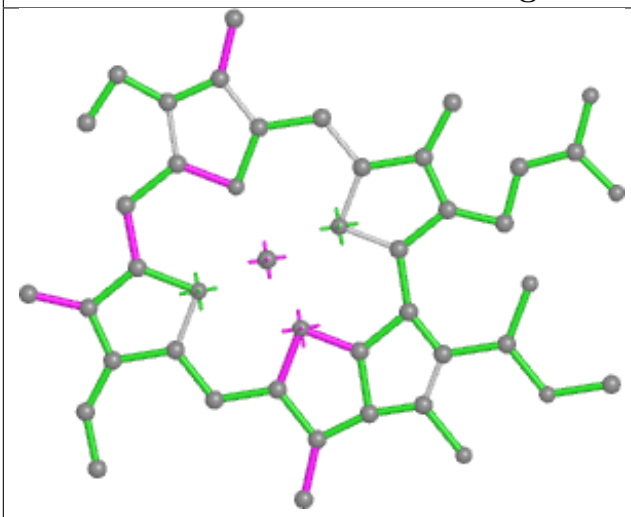

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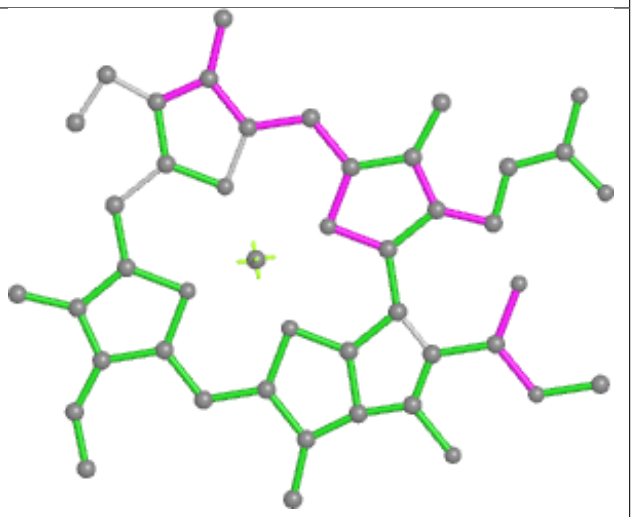

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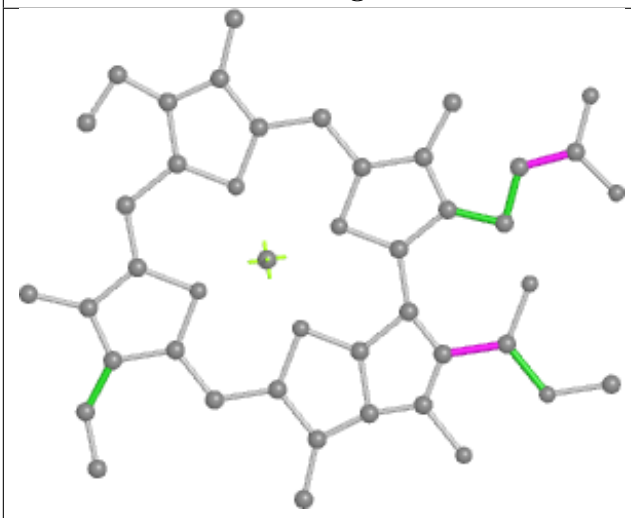

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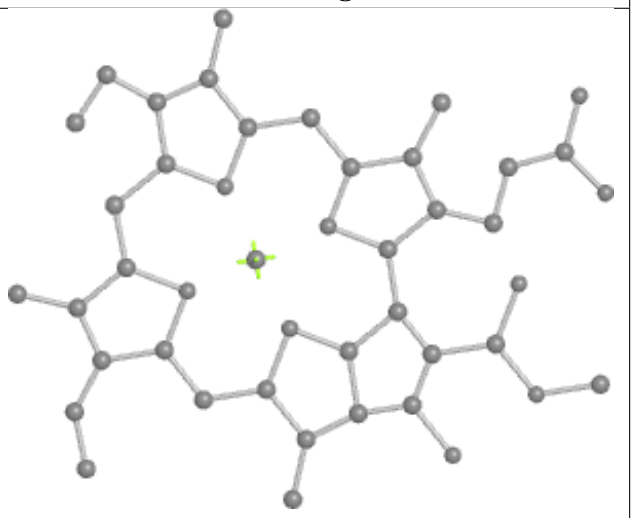
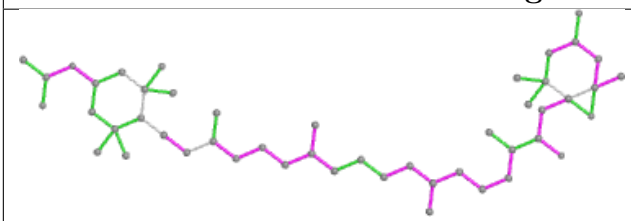


Rings

Ligand A86 35 313



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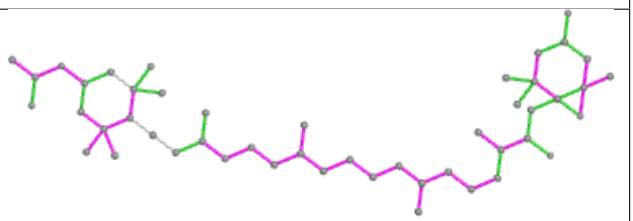

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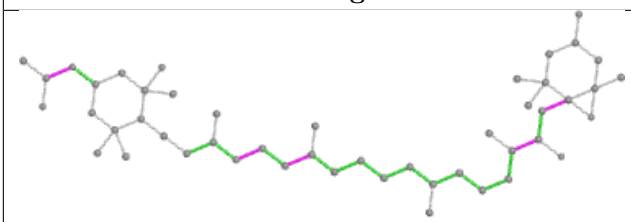

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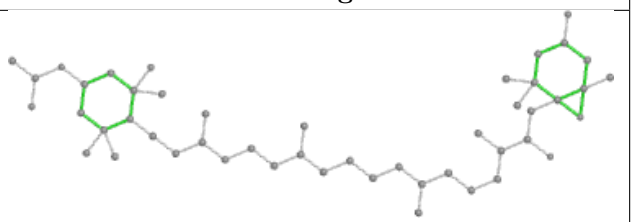

Rings

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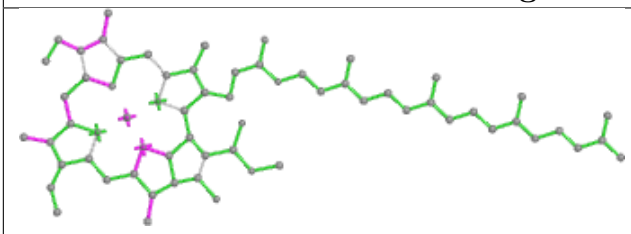

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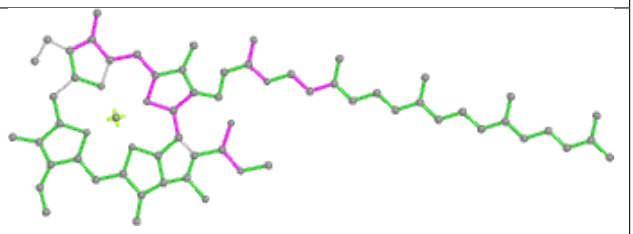

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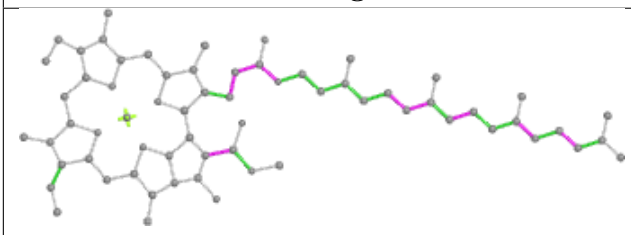
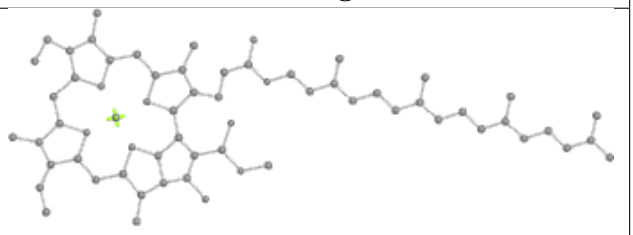
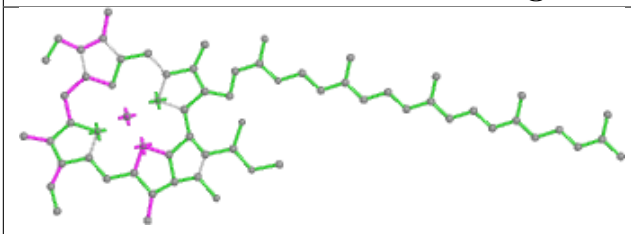


Torsions

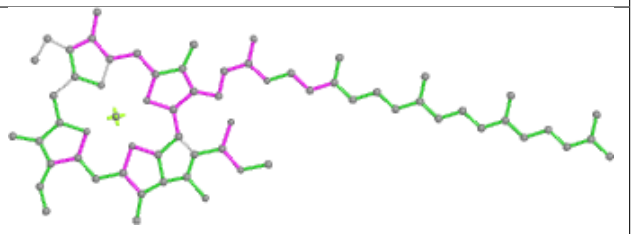


Rings

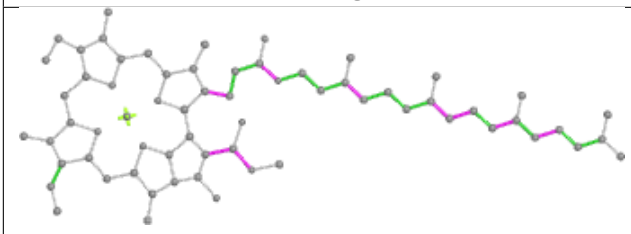
Ligand CLA b 604



Bond lengths



Bond angles



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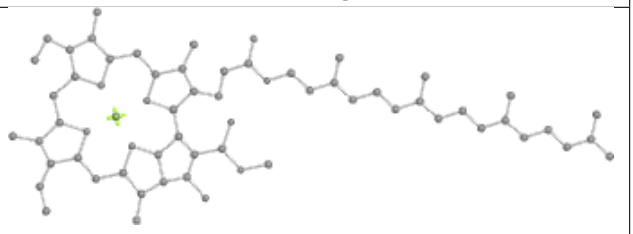
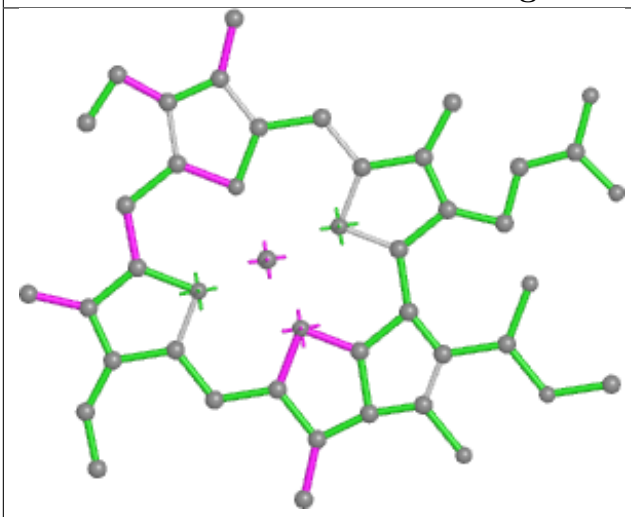


Rings

Ligand CLA 34 306



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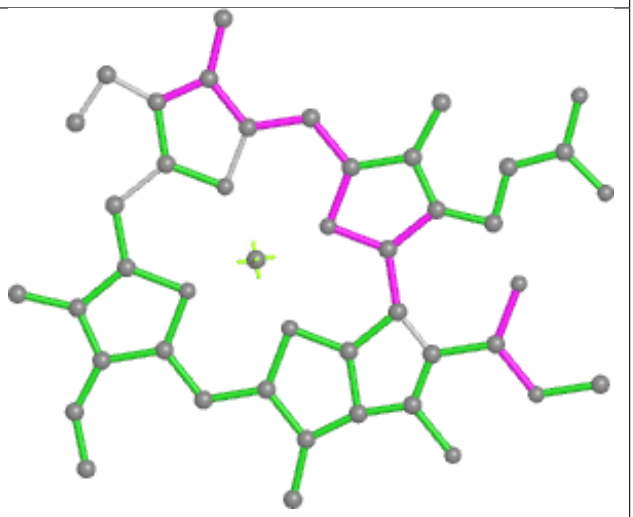

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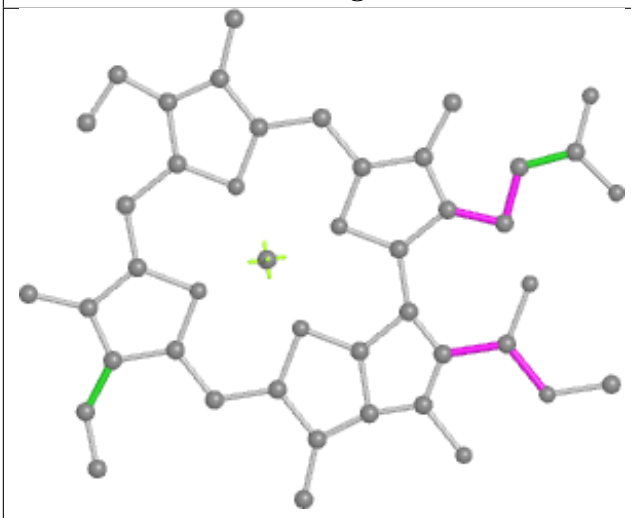

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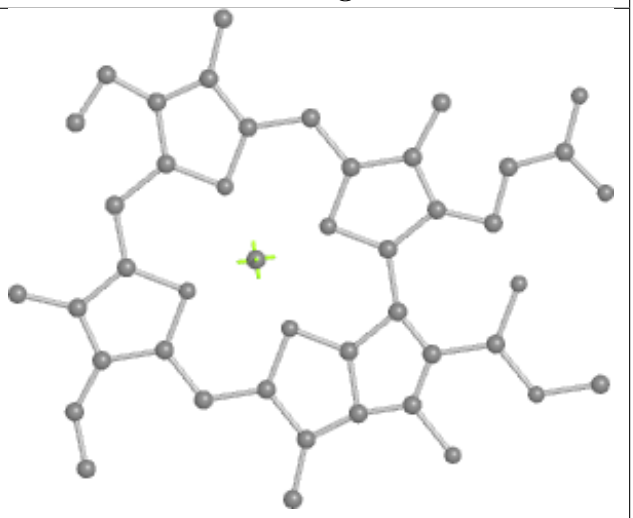
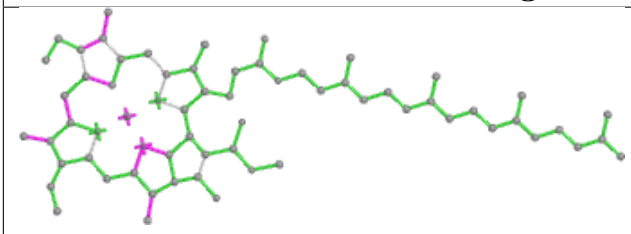


Rings

Ligand CLA 31 315



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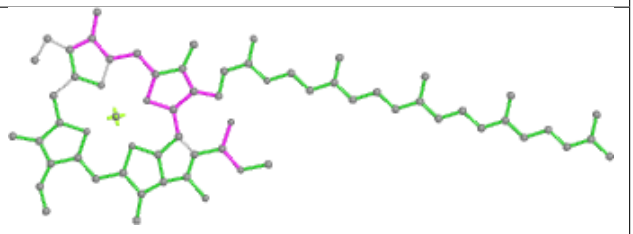

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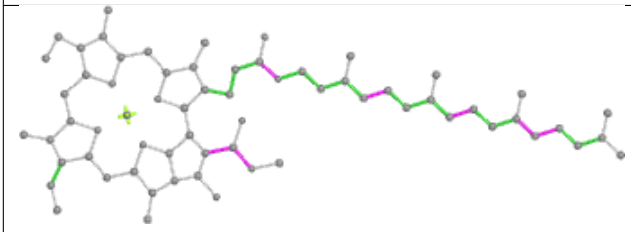

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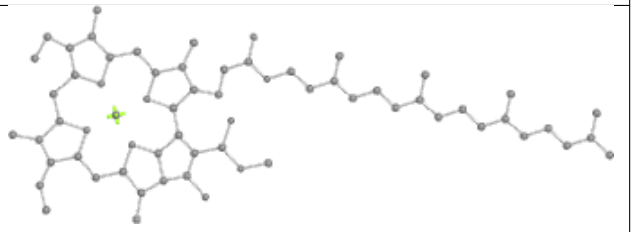
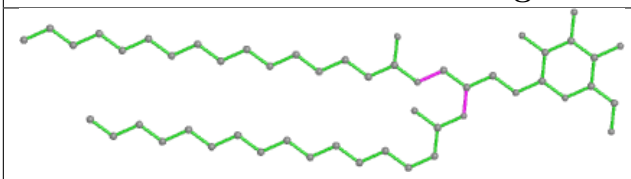


Rings

Ligand LMG W 101



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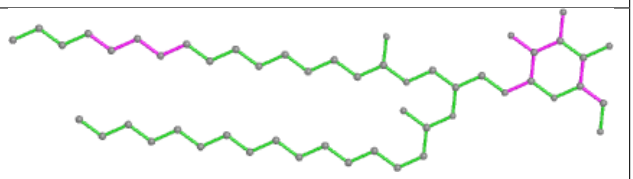
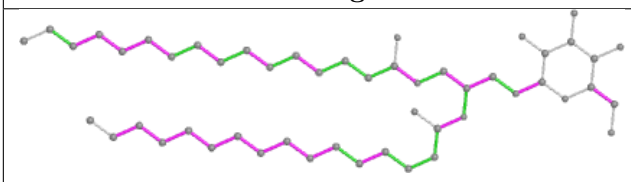


Bond angles



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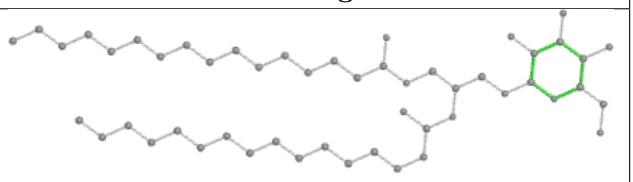
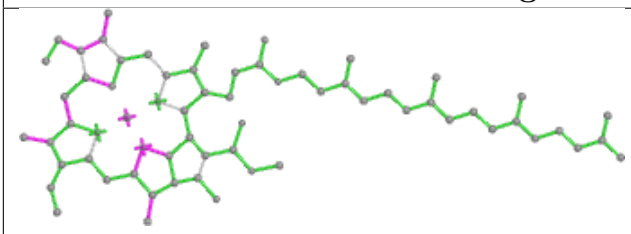


Rings

Ligand CLA 39 303



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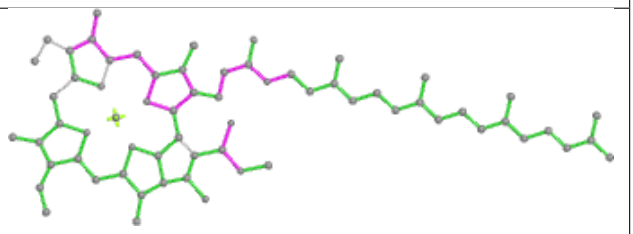

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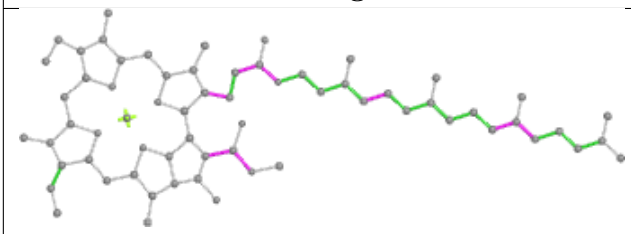

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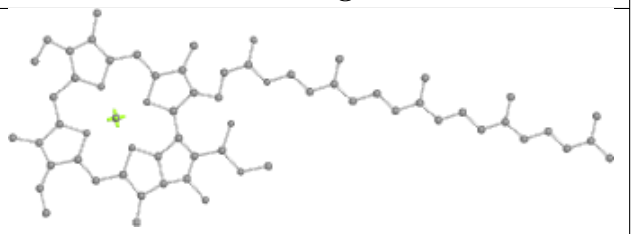
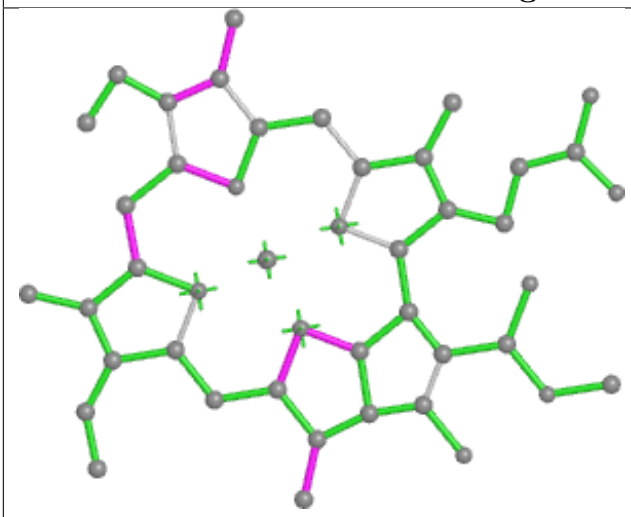


Rings

Ligand CLA 13 307



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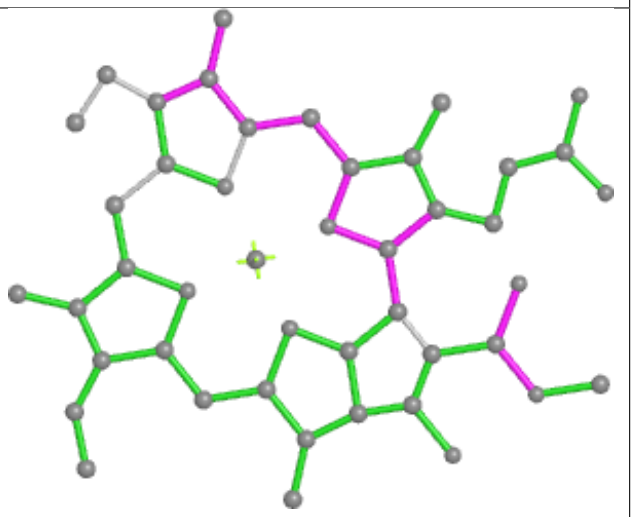

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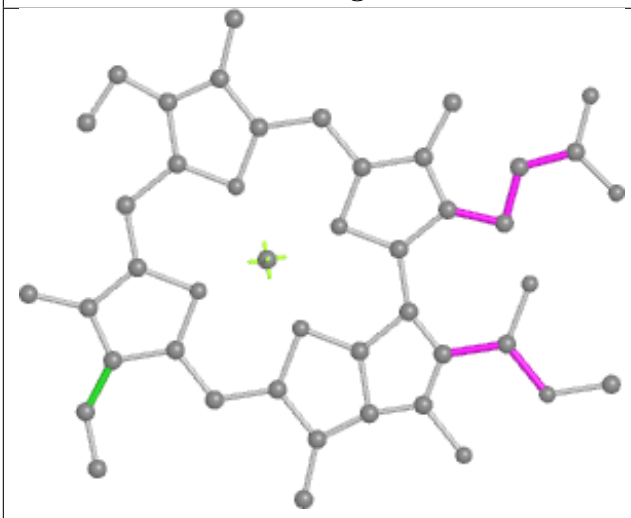

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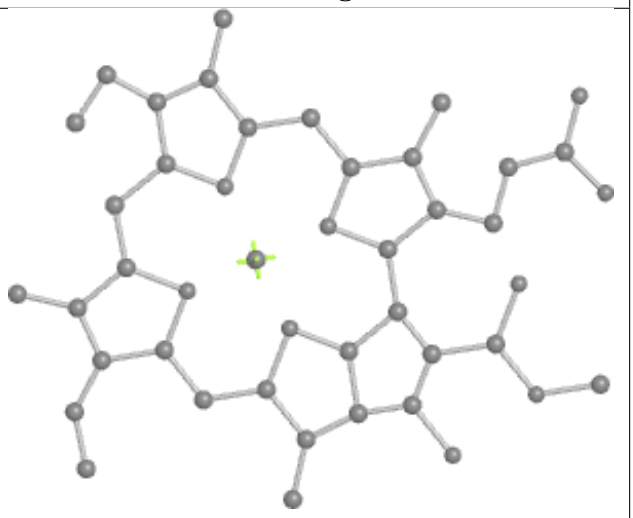
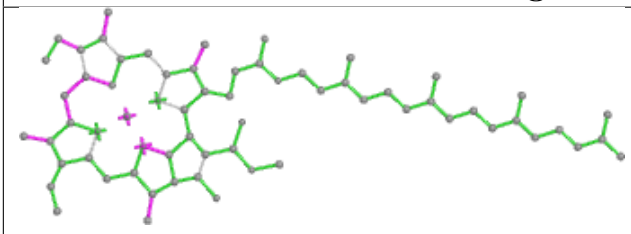


Rings

Ligand CLA b 612



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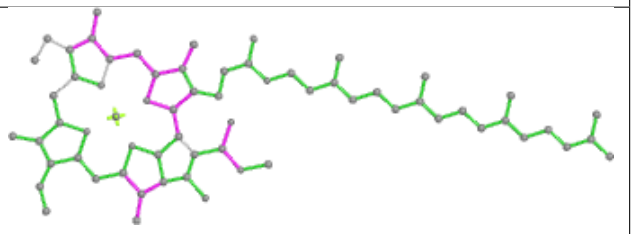

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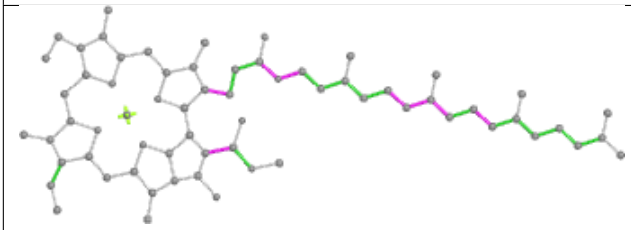

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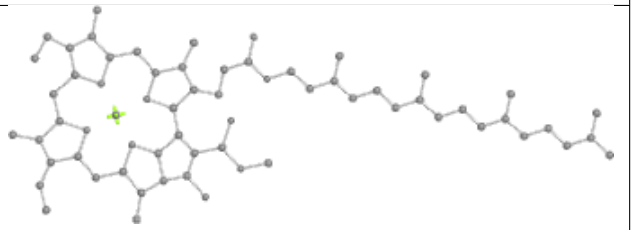
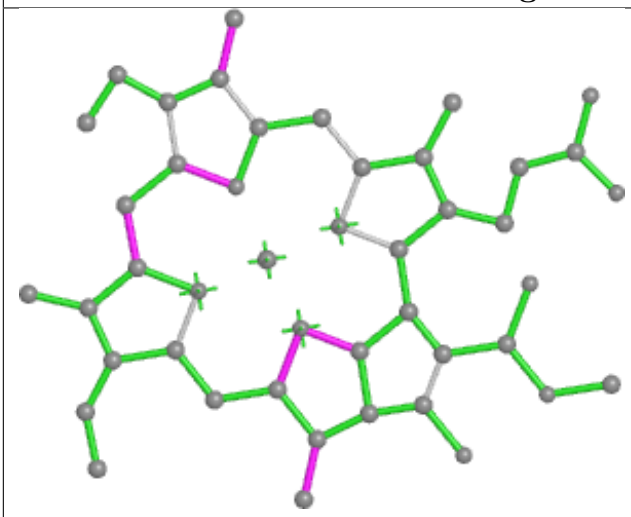


Rings

Ligand CLA 21 305



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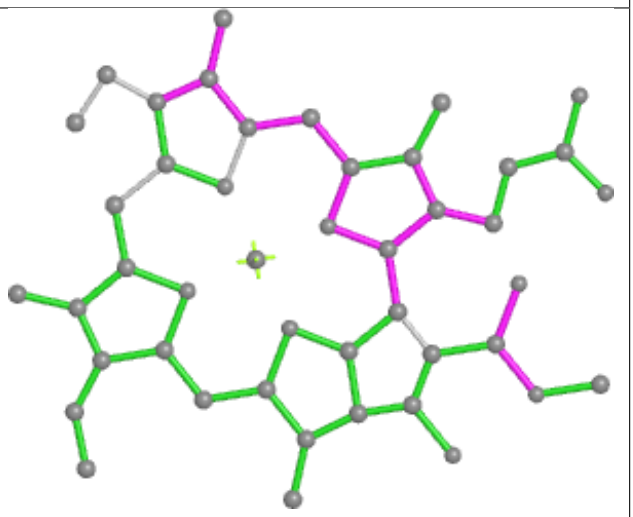

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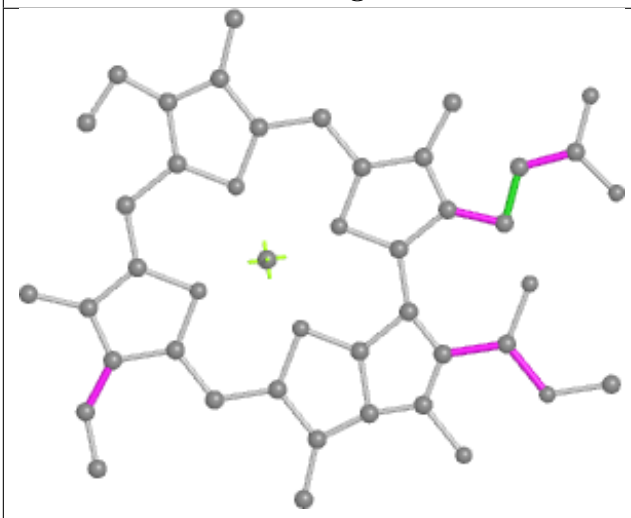

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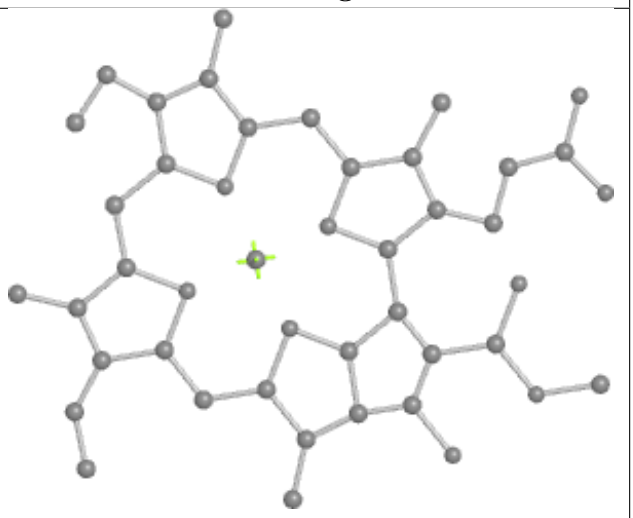
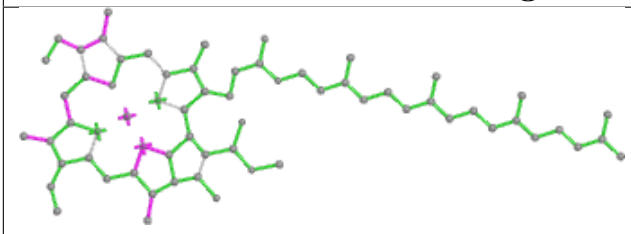


Rings

Ligand CLA 33 309



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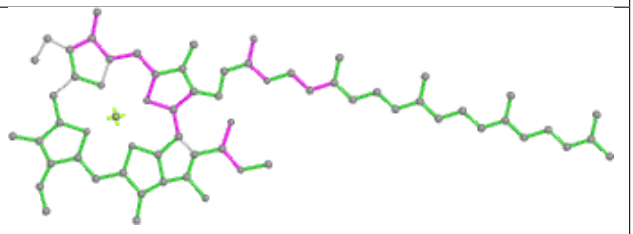

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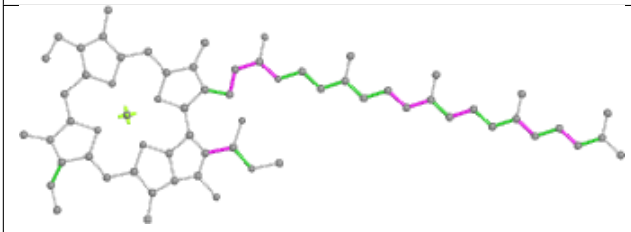

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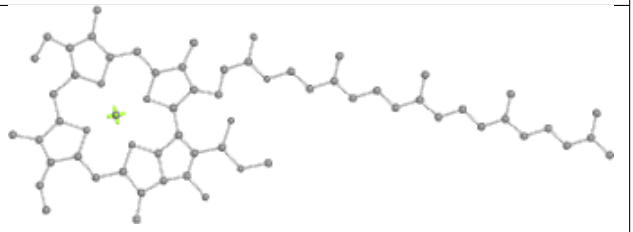
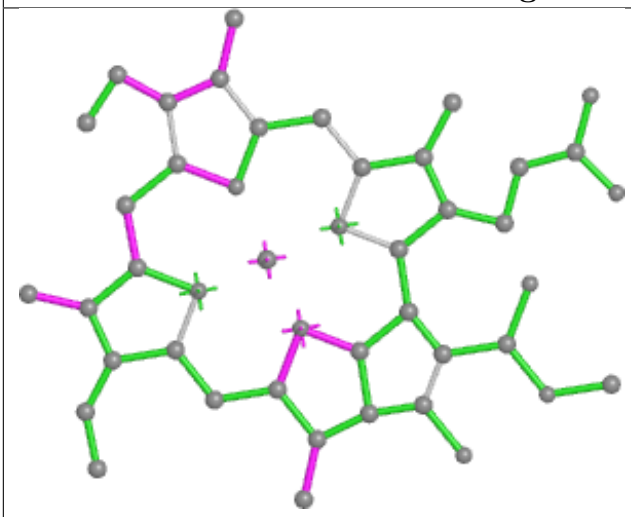


Rings

Ligand CLA 35 308



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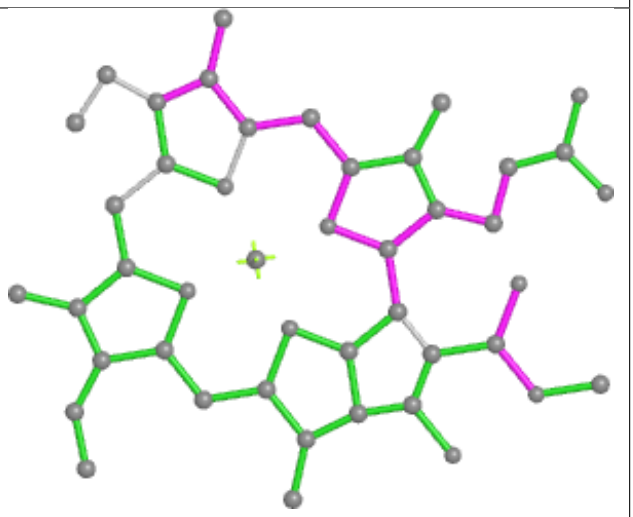

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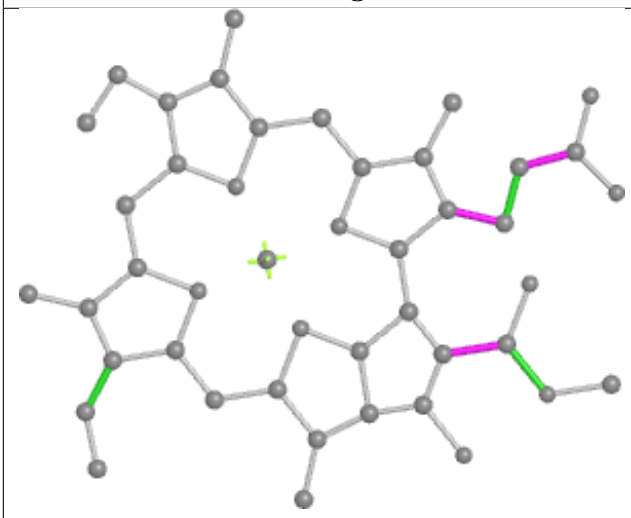

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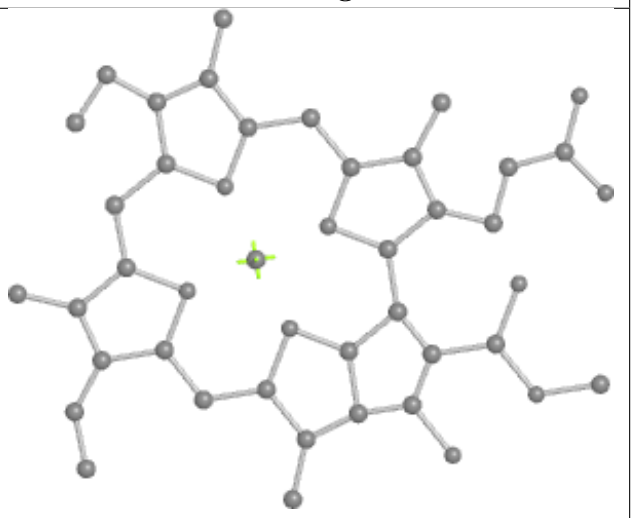
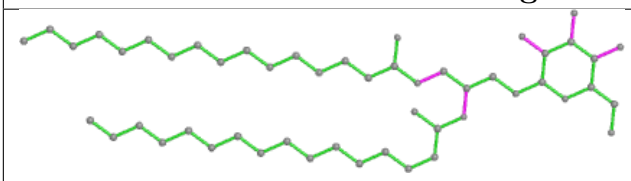


Rings

Ligand LMG B 620



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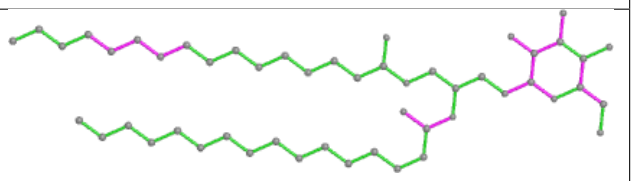
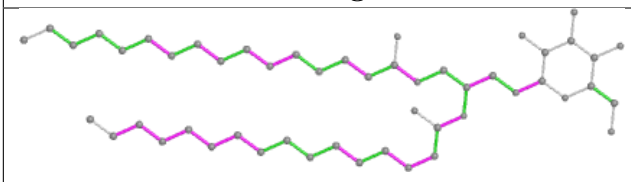


Bond angles



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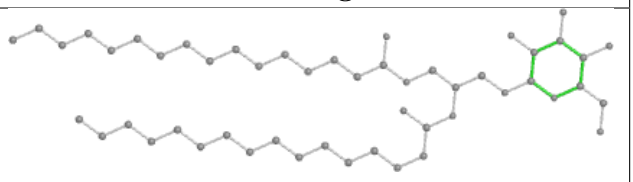
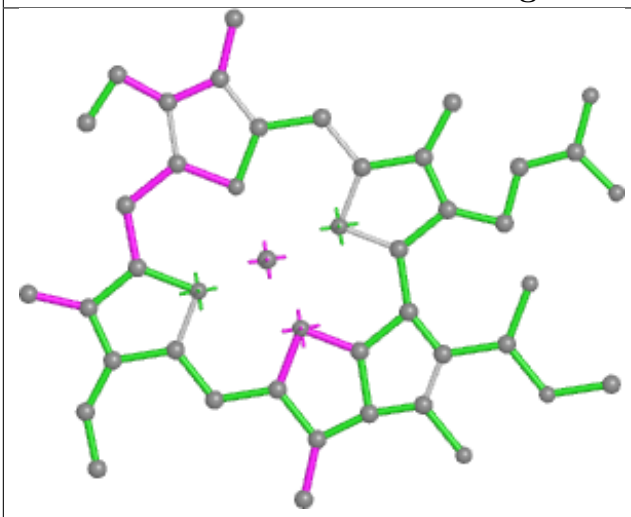


Rings

Ligand CLA 31 308



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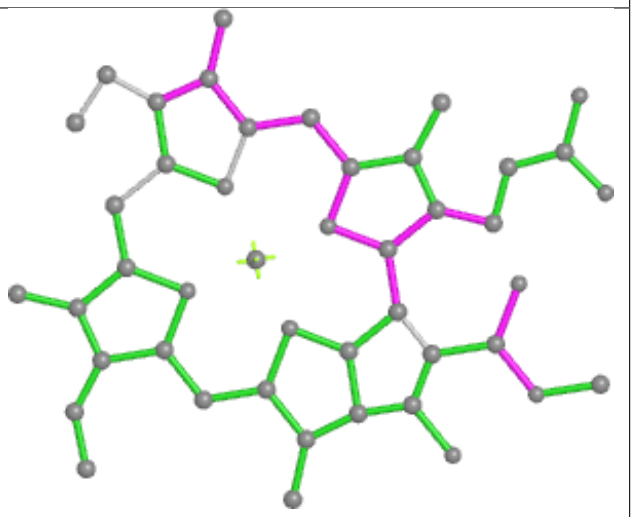
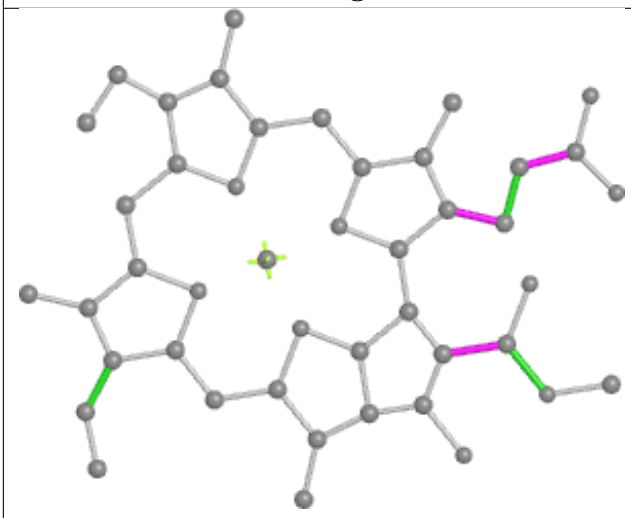


Bond angles



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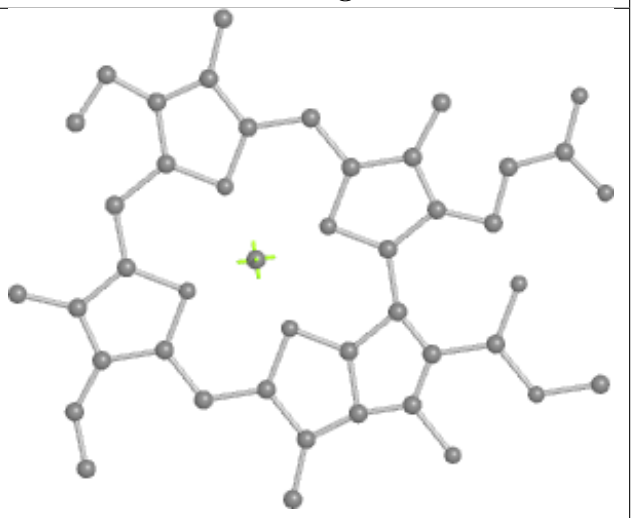
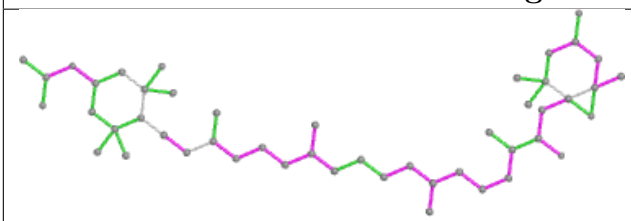


Rings

Ligand A86 31 316



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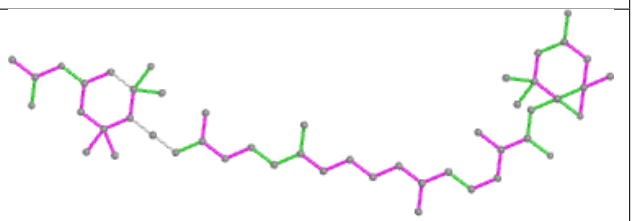
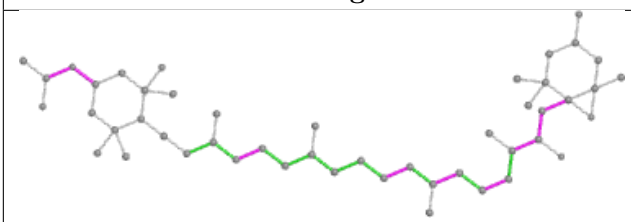
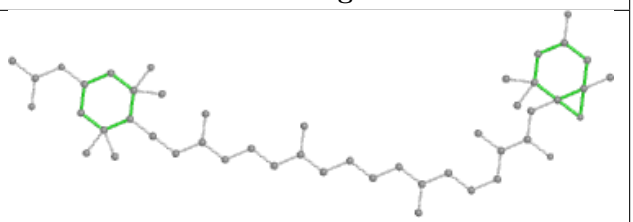


Bond angles

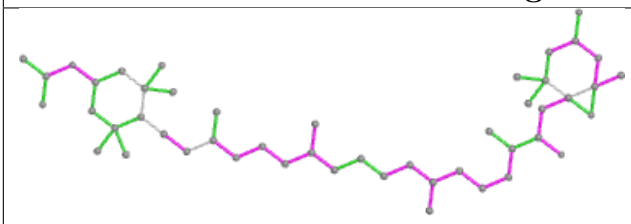


Torsions



Rings

Ligand A86 40 213



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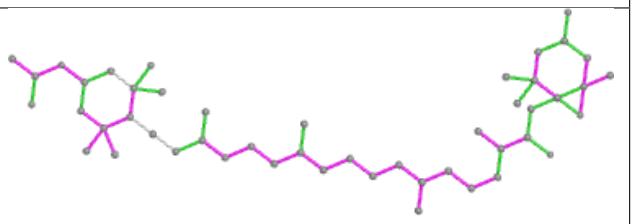
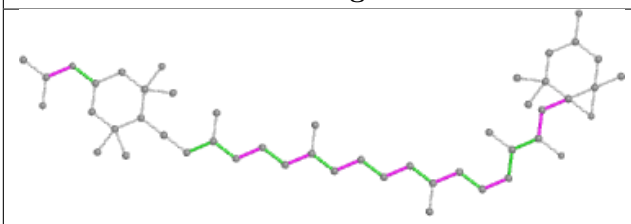
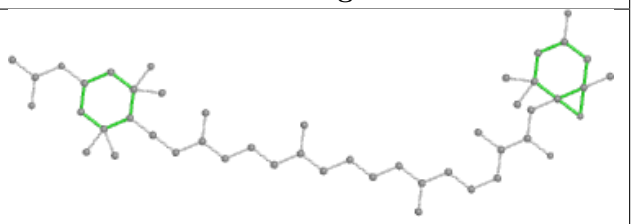


Bond angles

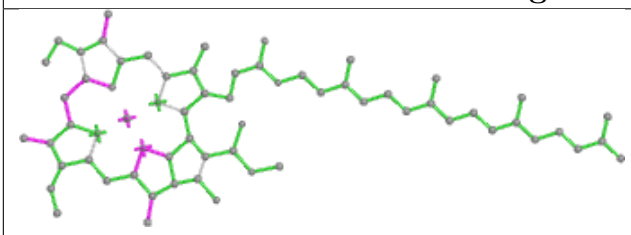


Torsions

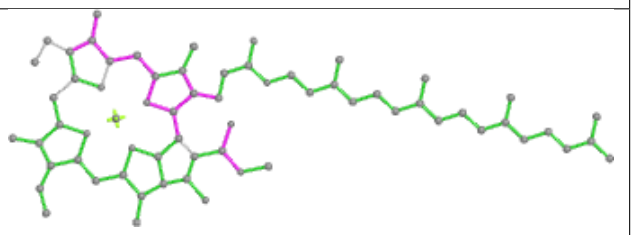


Rings

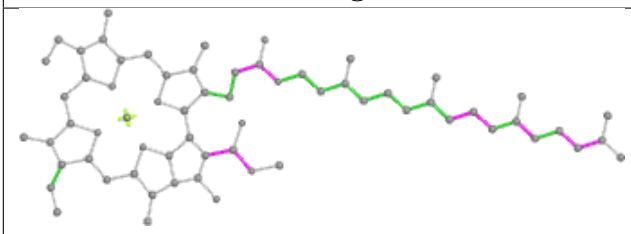
Ligand CLA c 514



Bond lengths



Bond angles



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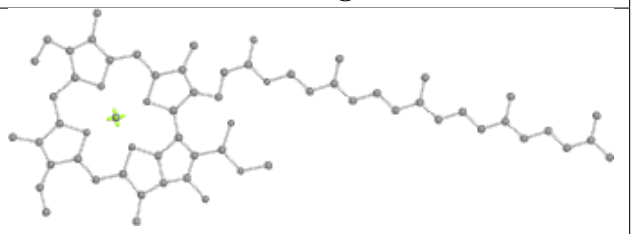
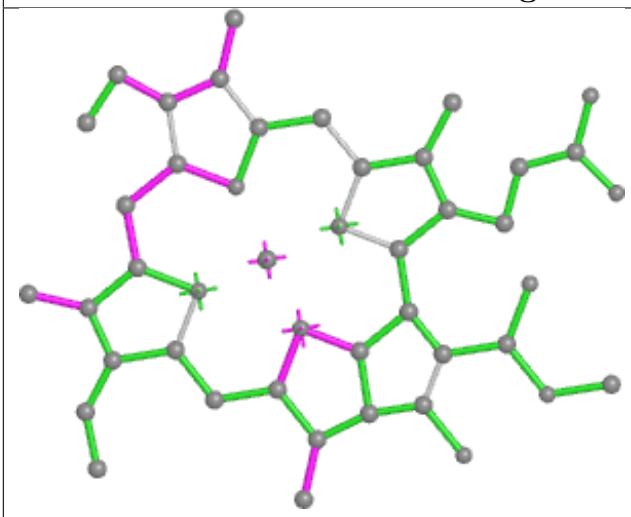


Rings

Ligand CLA 39 306



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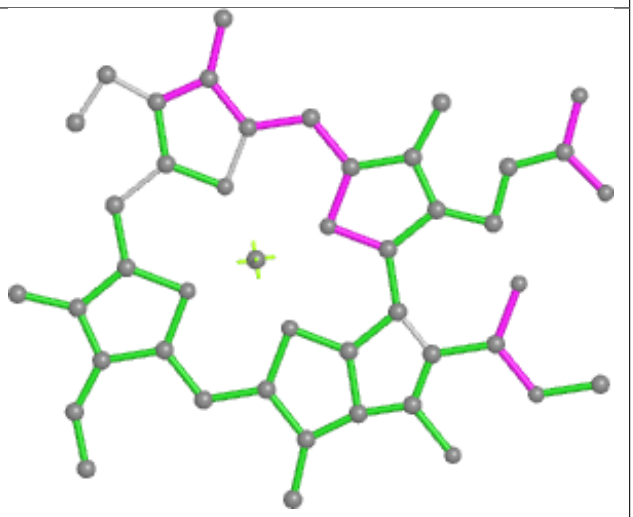

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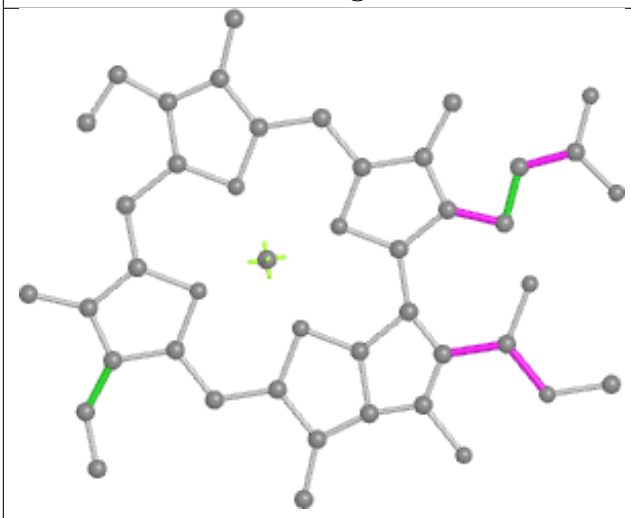

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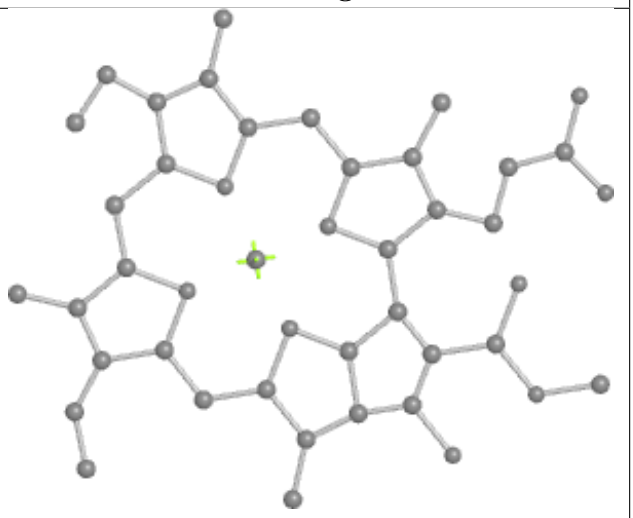
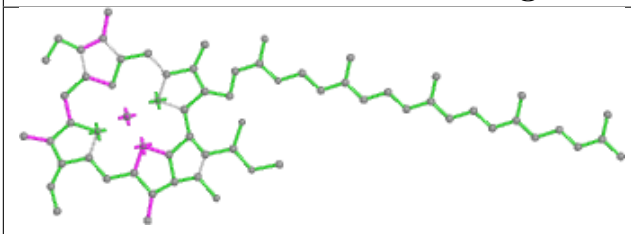


Rings

Ligand CLA 14 301



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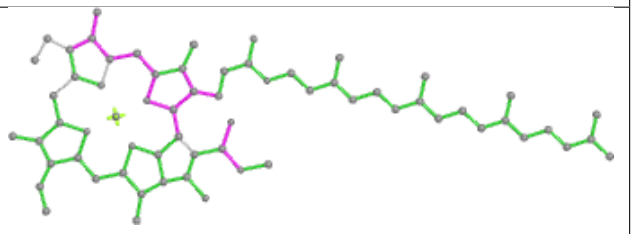

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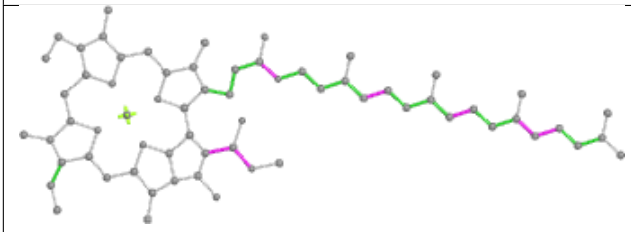

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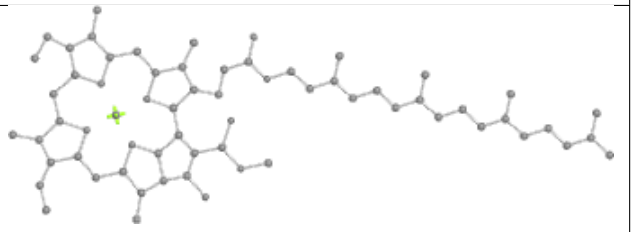
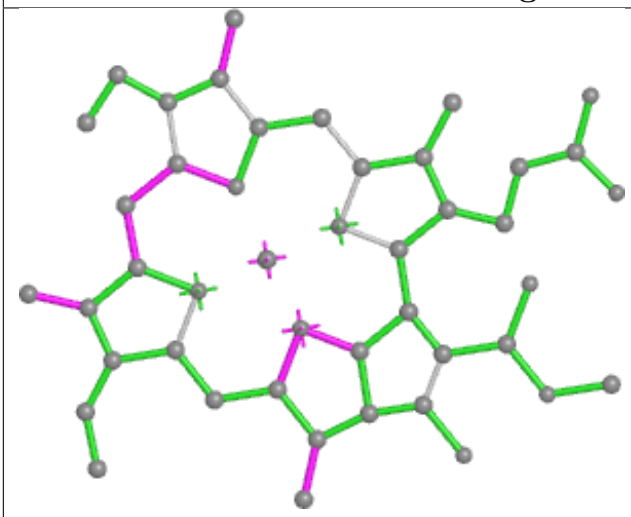


Rings

Ligand CLA 34 305



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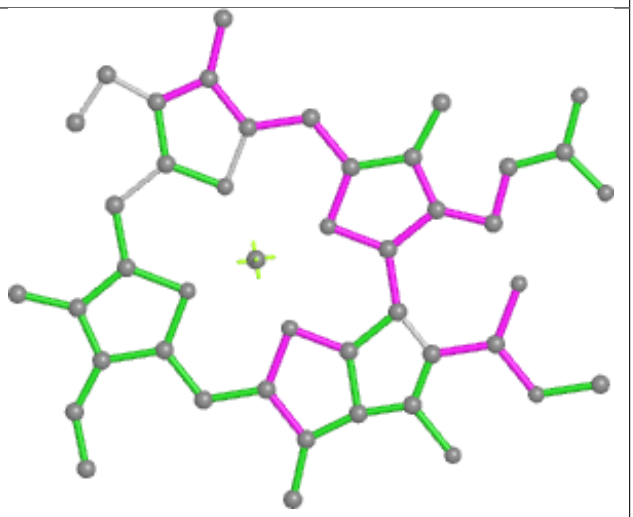

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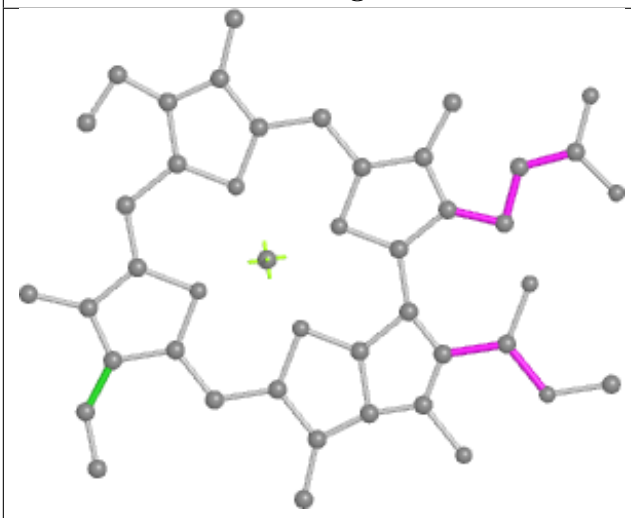

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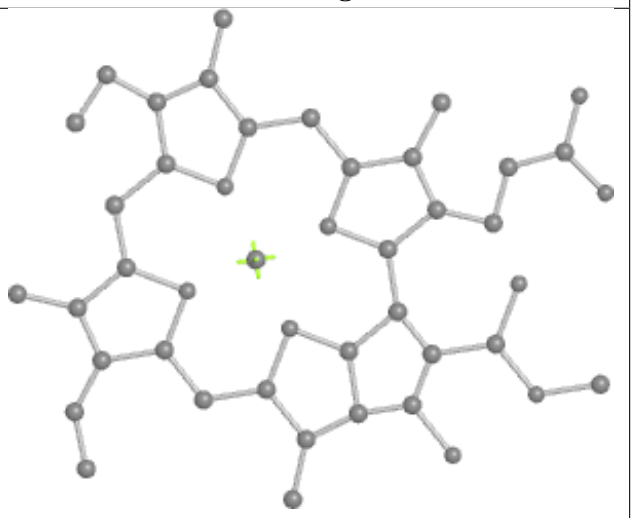
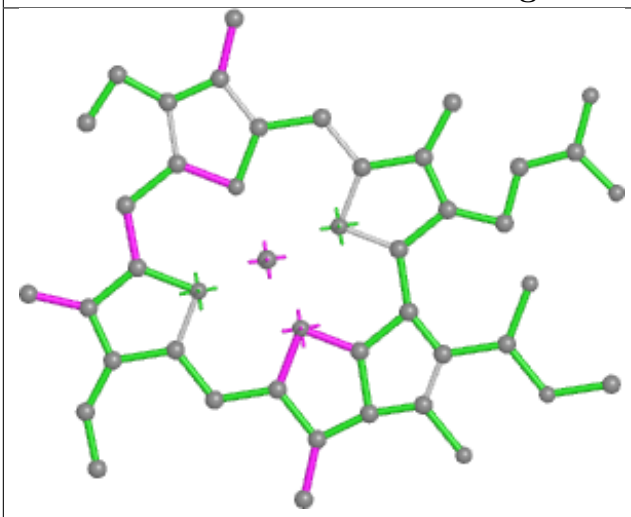


Rings

Ligand CLA 17 310



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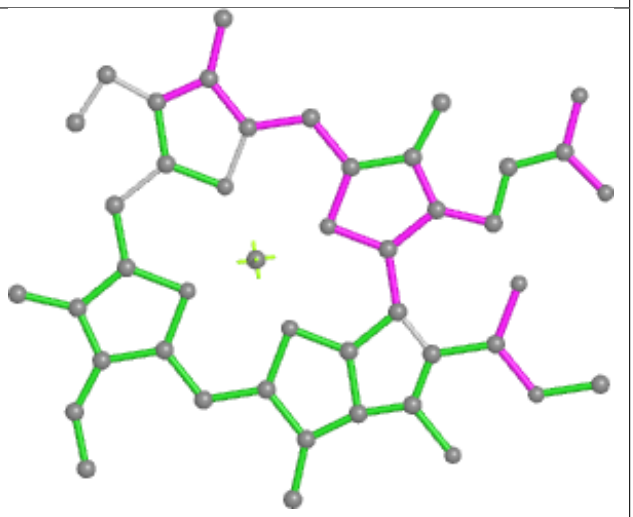

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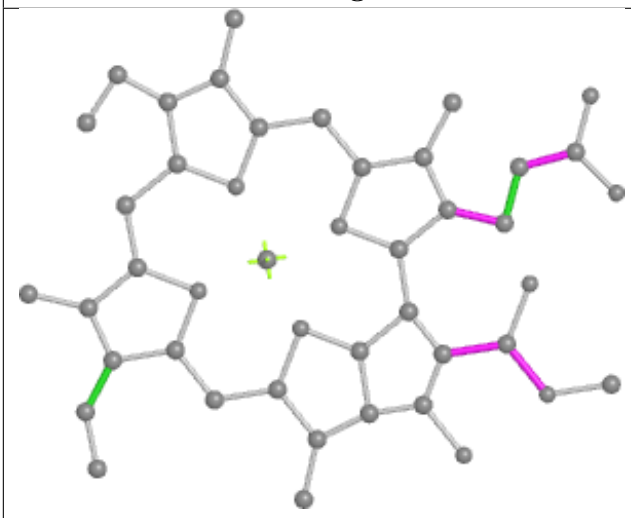

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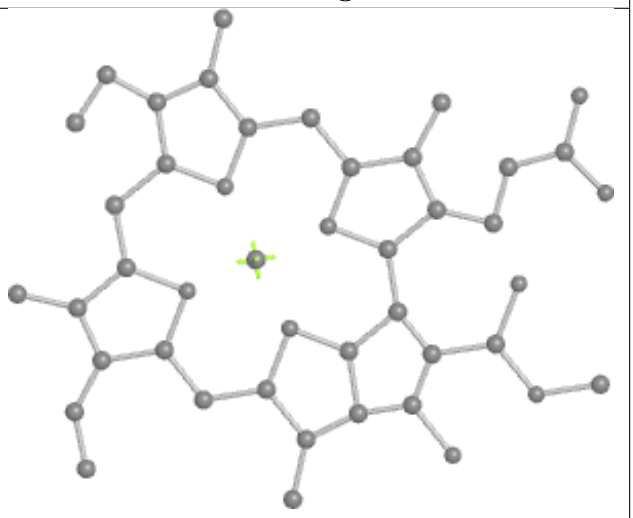
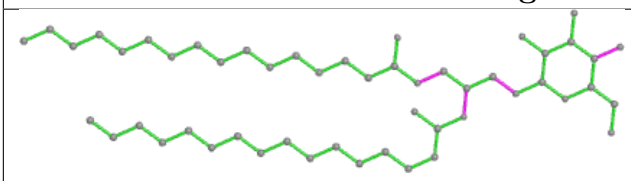


Rings

Ligand LMG Q 301



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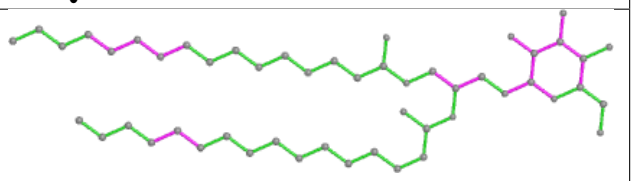

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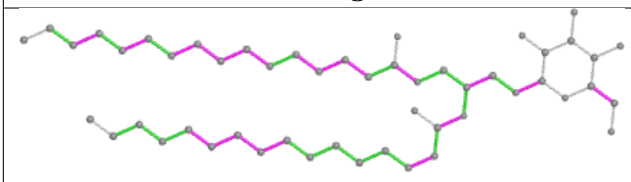

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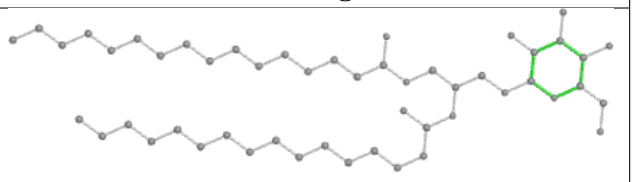
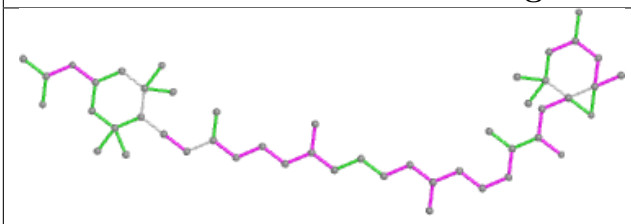


Rings

Ligand A86 33 315



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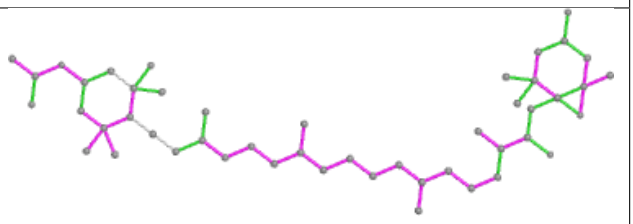

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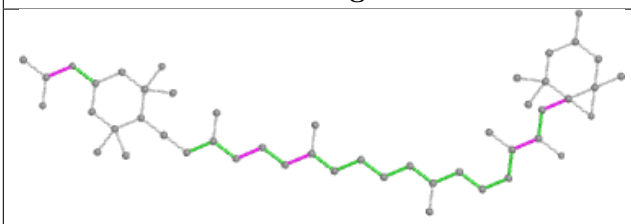

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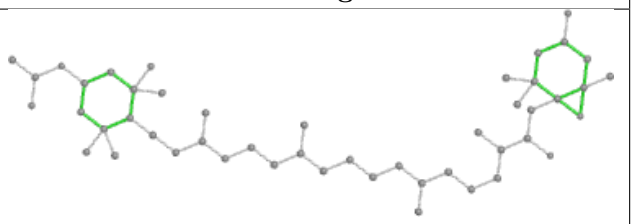
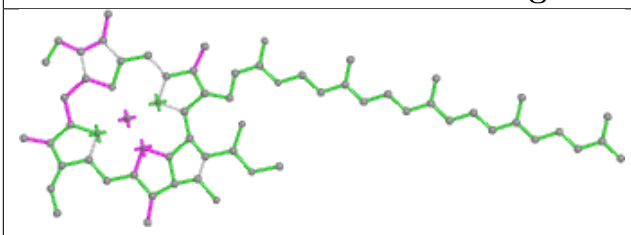


Rings

Ligand CLA c 510



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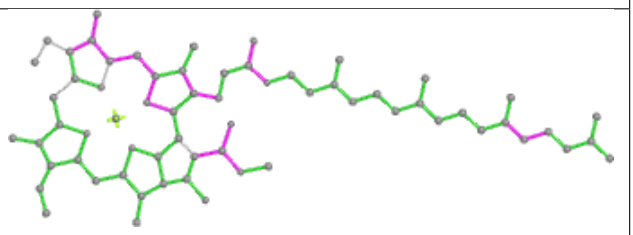

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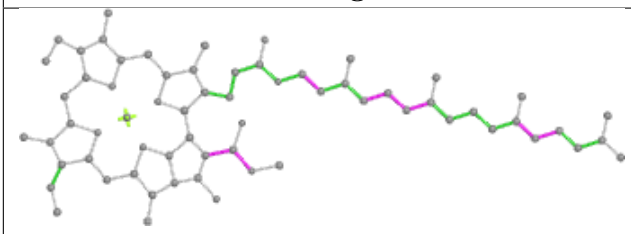

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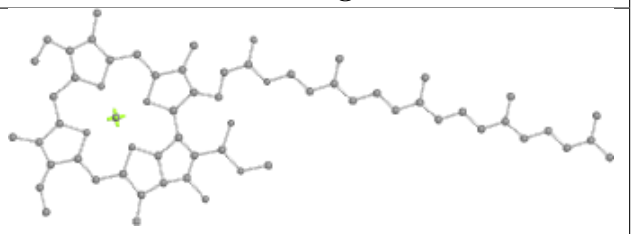
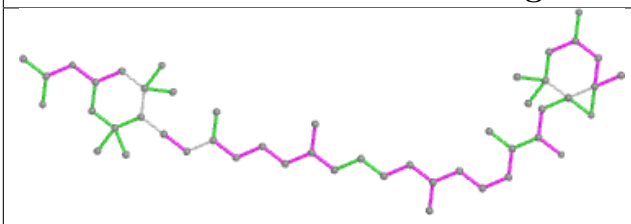


Rings

Ligand A86 17 302



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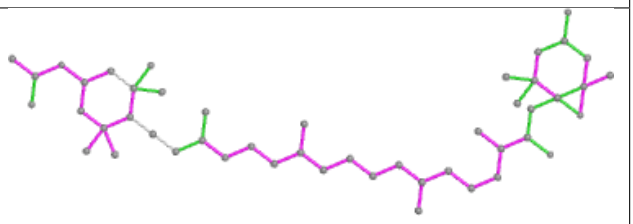

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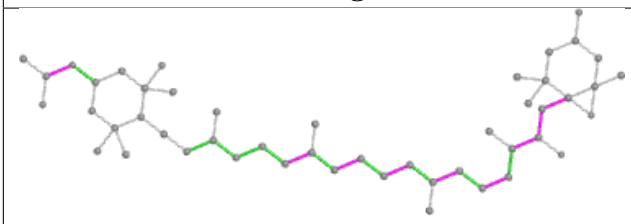

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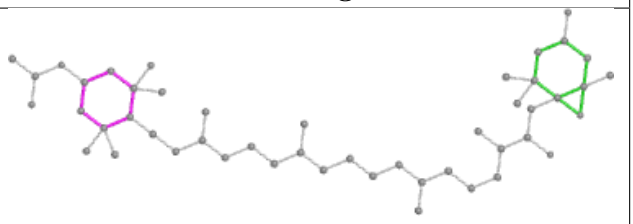
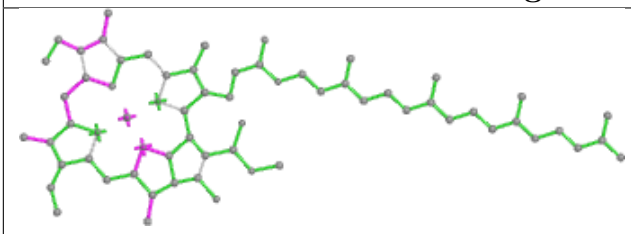


Rings

Ligand CLA B 603



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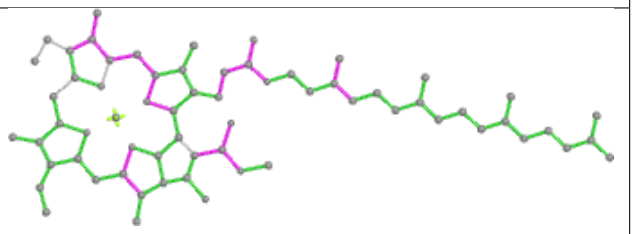

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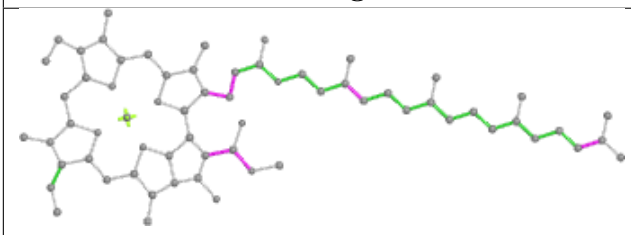

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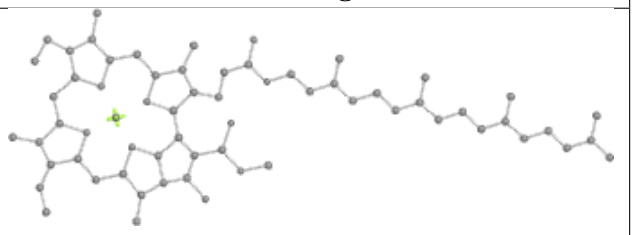
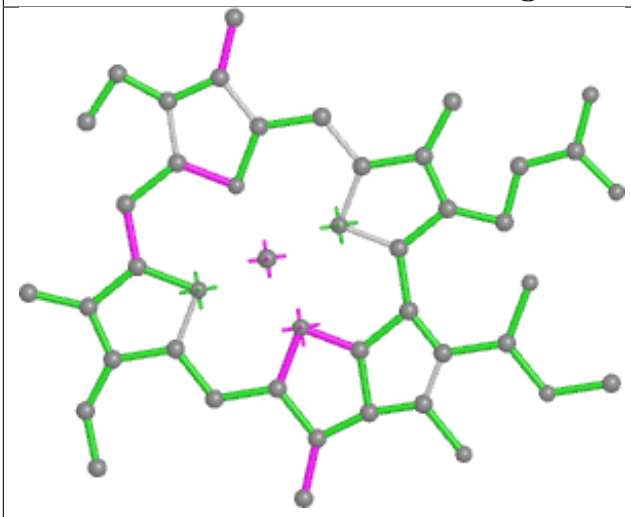


Rings

Ligand CLA 18 306



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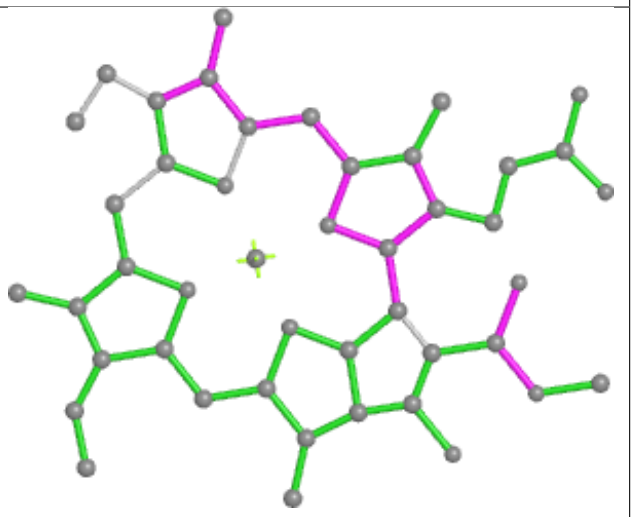
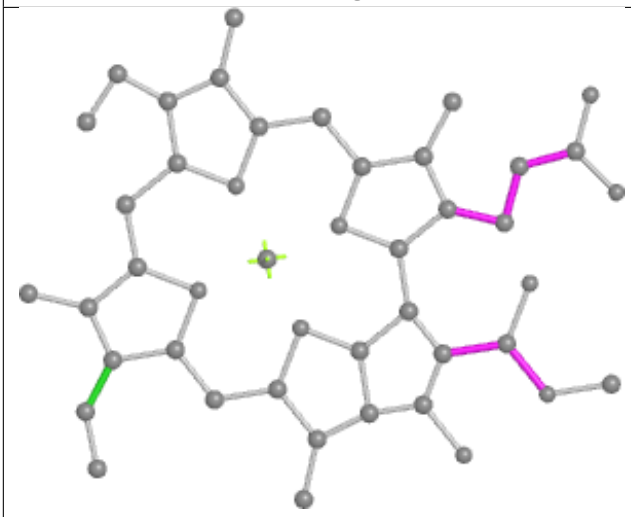


Bond angles



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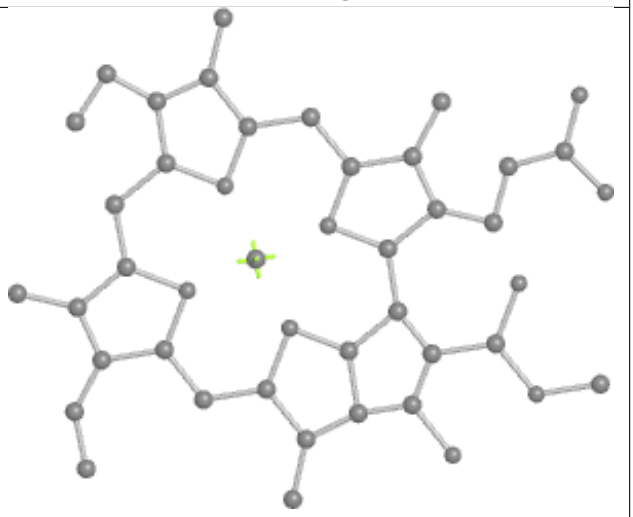
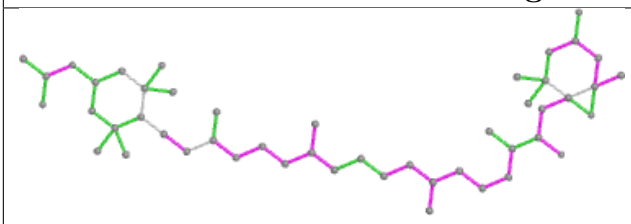


Rings

Ligand A86 32 316



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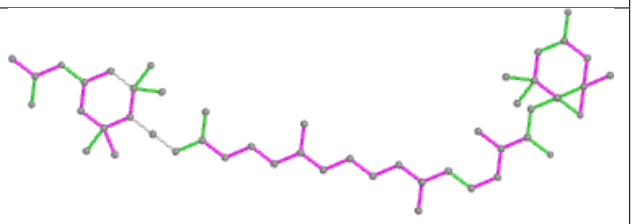
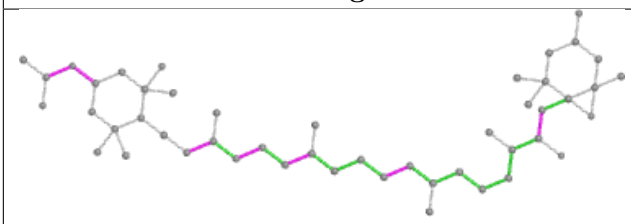


Bond angles



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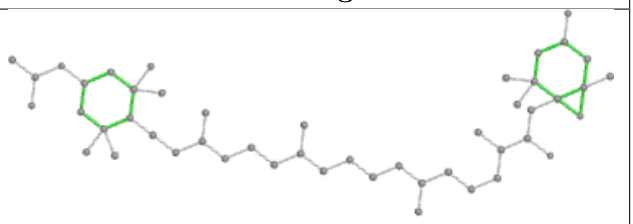
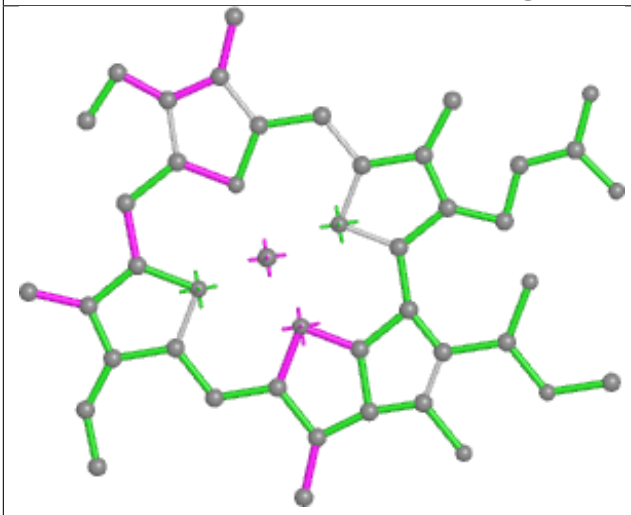


Rings

Ligand CLA 36 309



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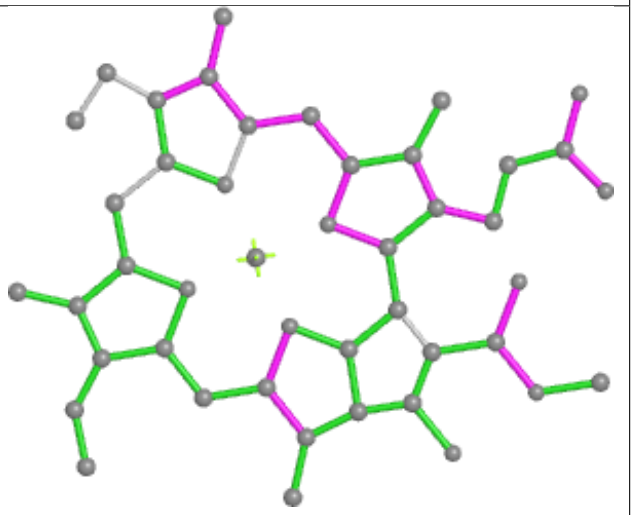
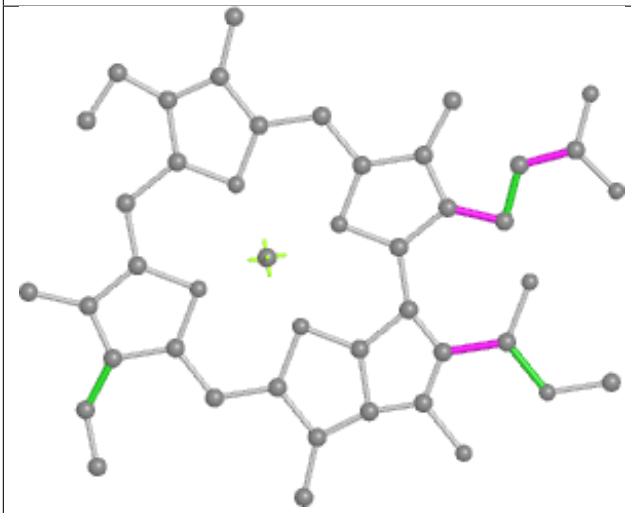


Bond angles



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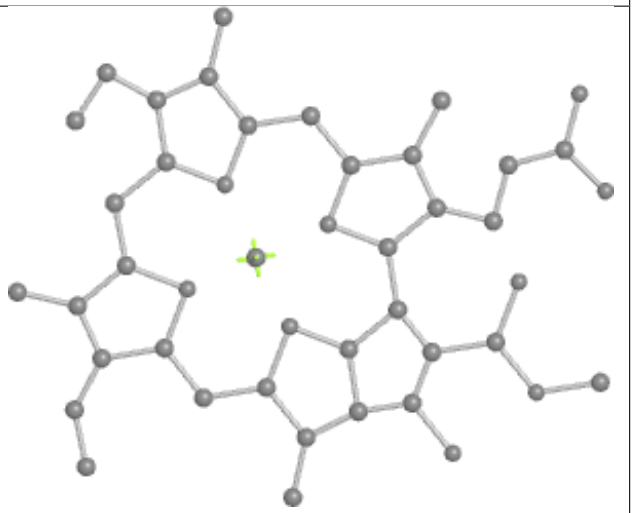
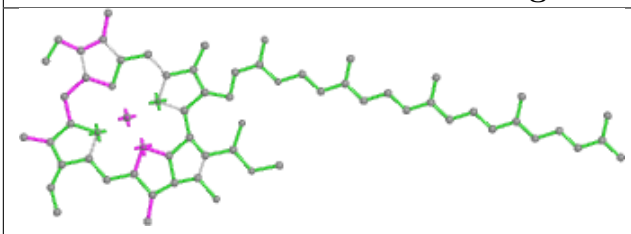


Rings

Ligand CLA c 509



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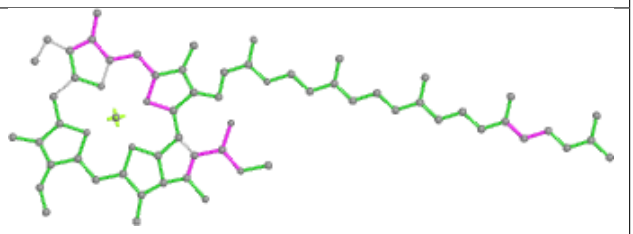
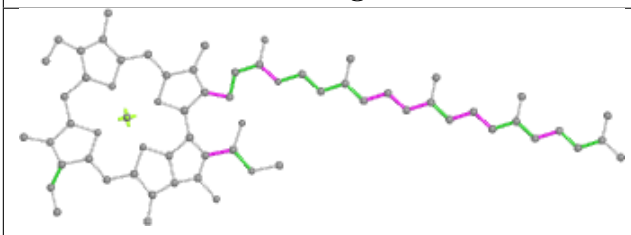
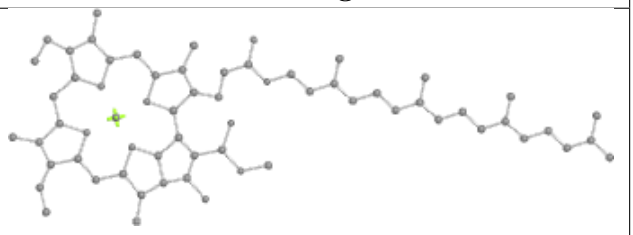


Bond angles

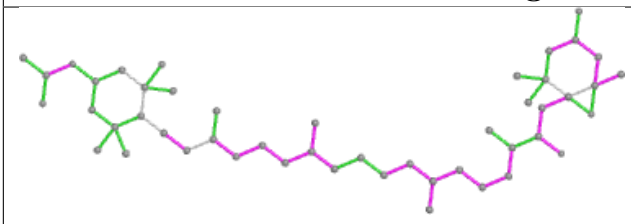


Torsions



Rings

Ligand A86 16 312



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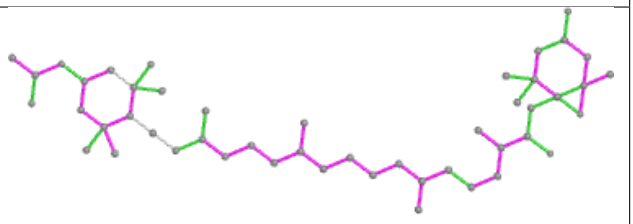

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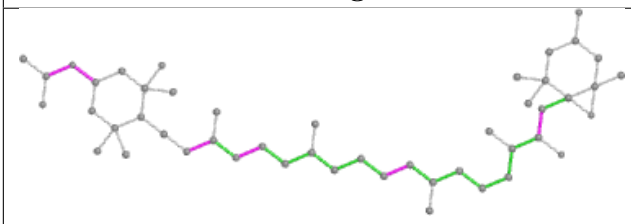

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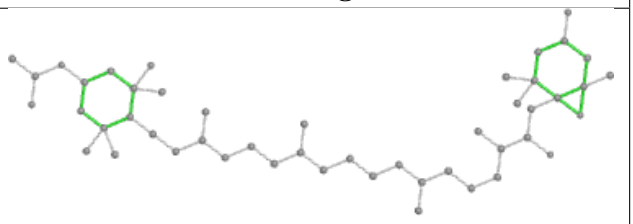
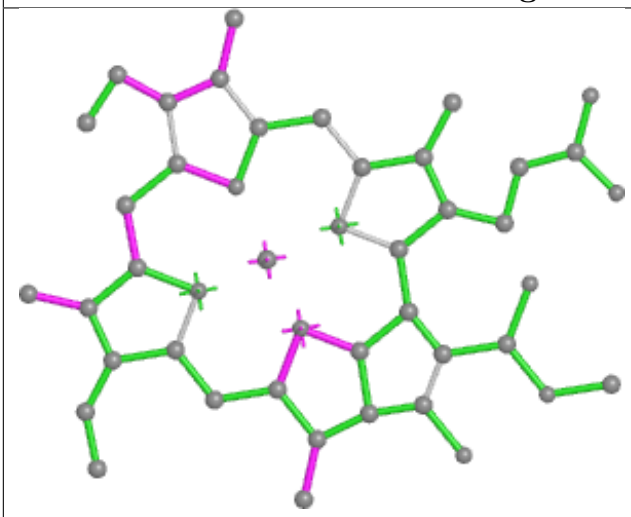


Rings

Ligand CLA 16 309



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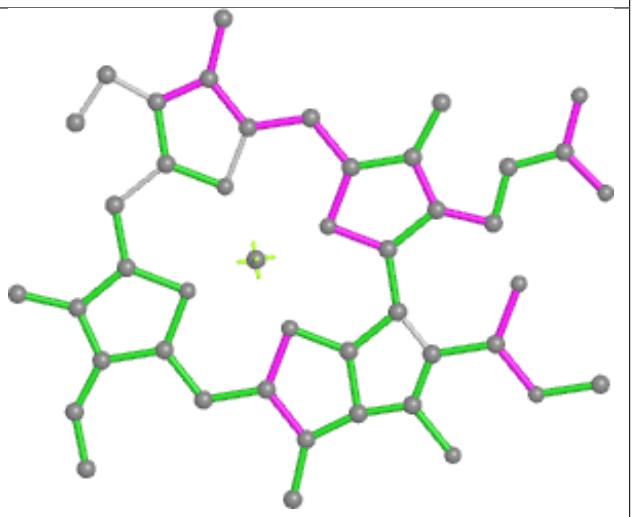

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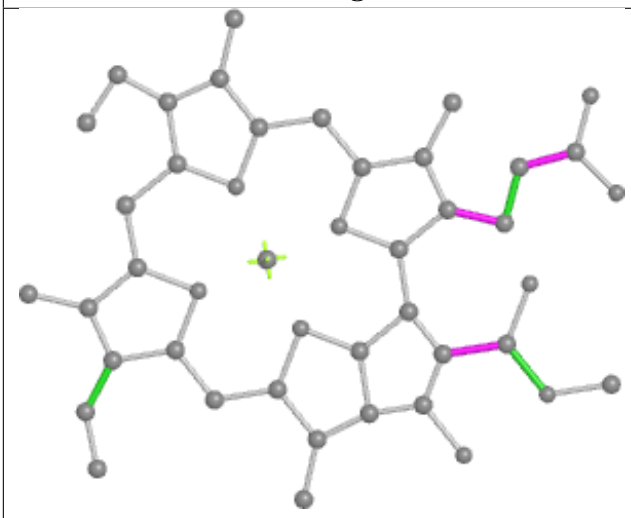

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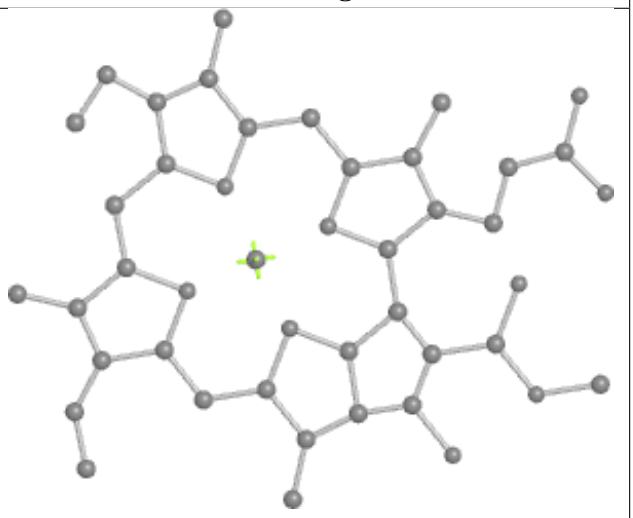
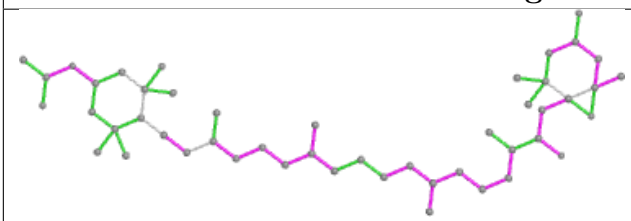


Rings

Ligand A86 36 310



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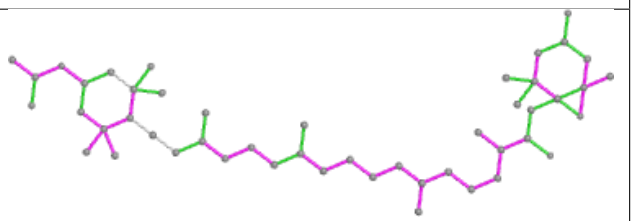

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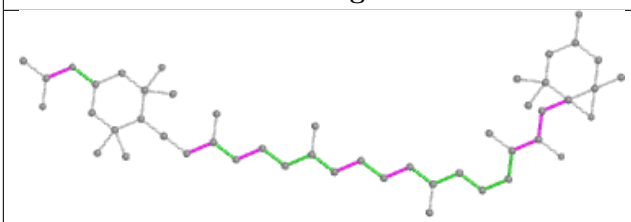

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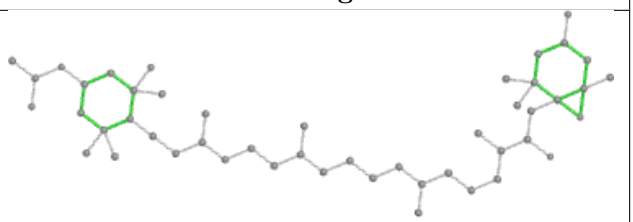
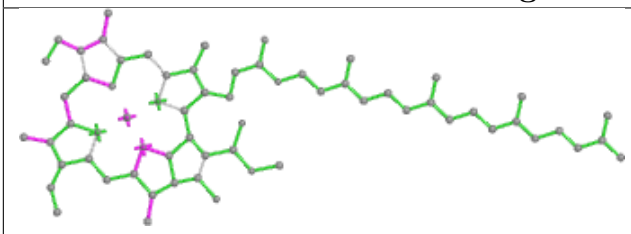


Rings

Ligand CLA 32 305



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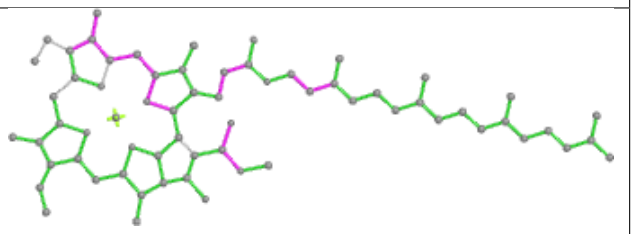

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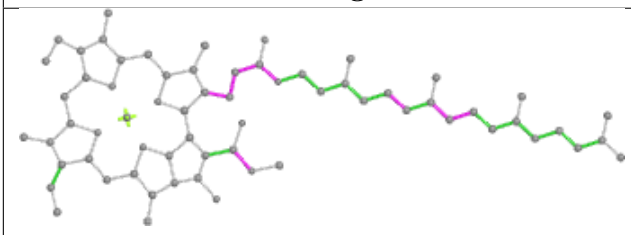

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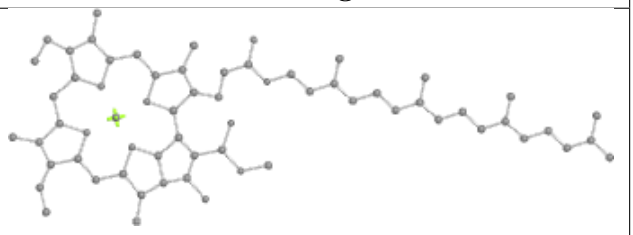
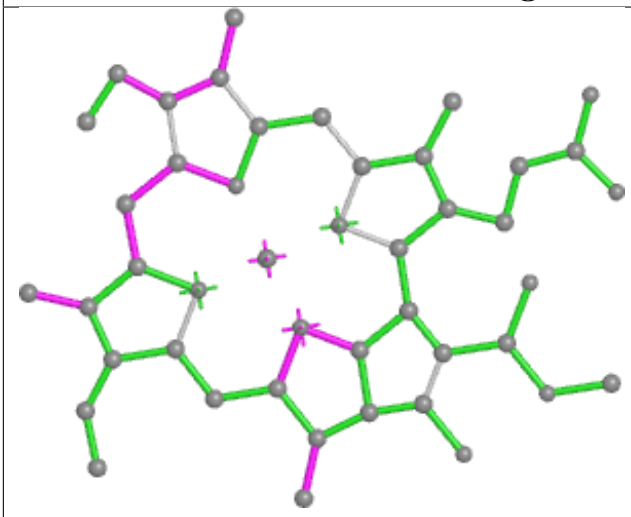


Rings

Ligand CLA 12 306



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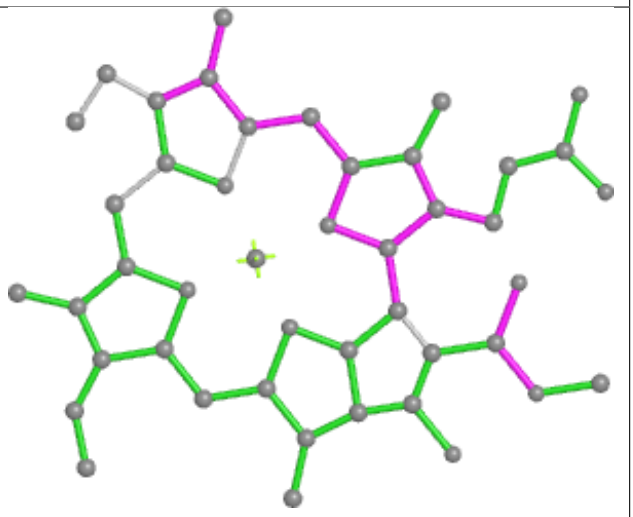

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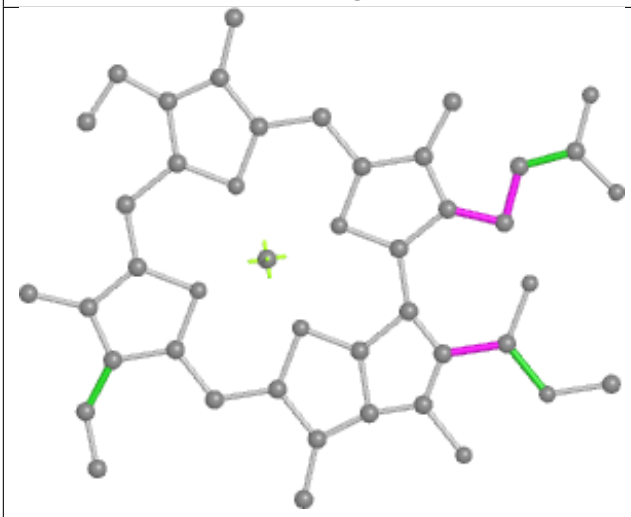

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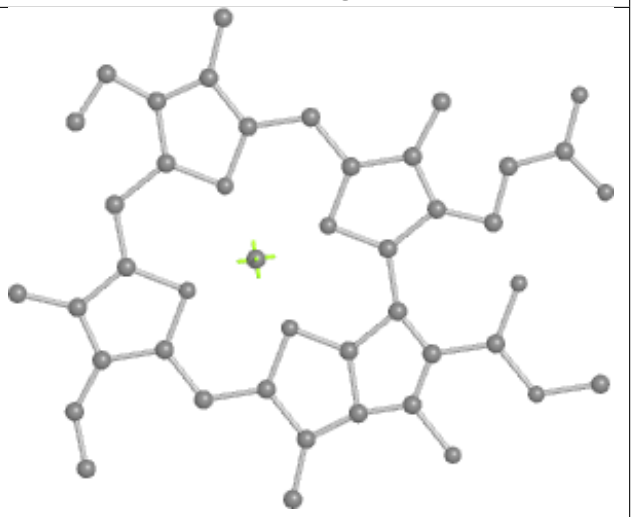
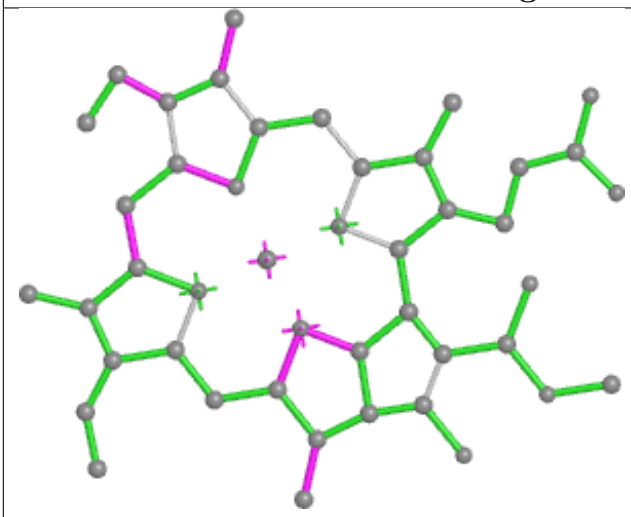


Rings

Ligand CLA 18 312



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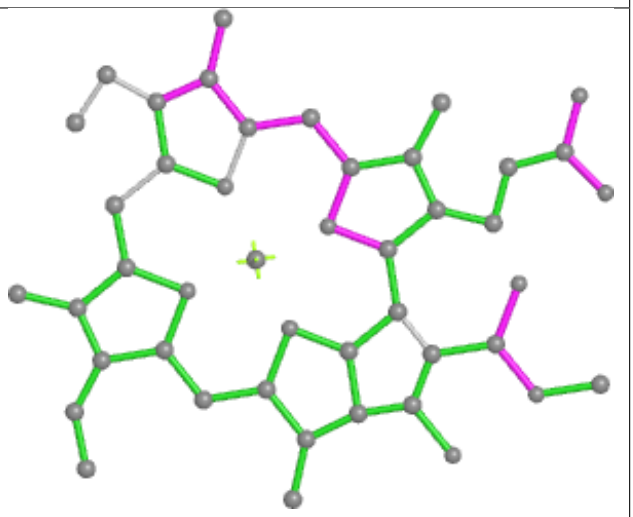

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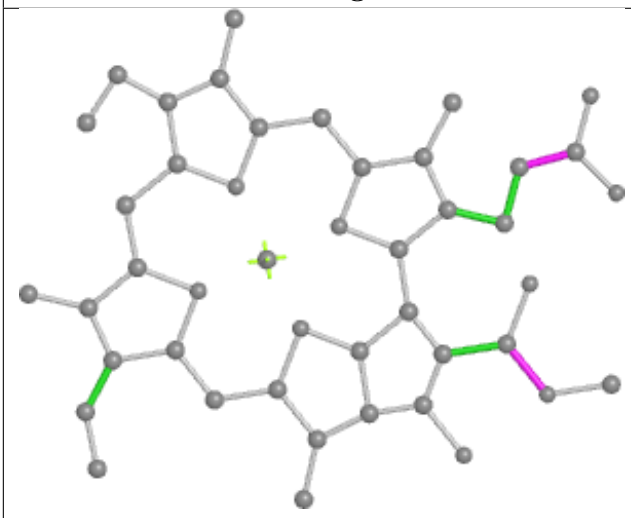

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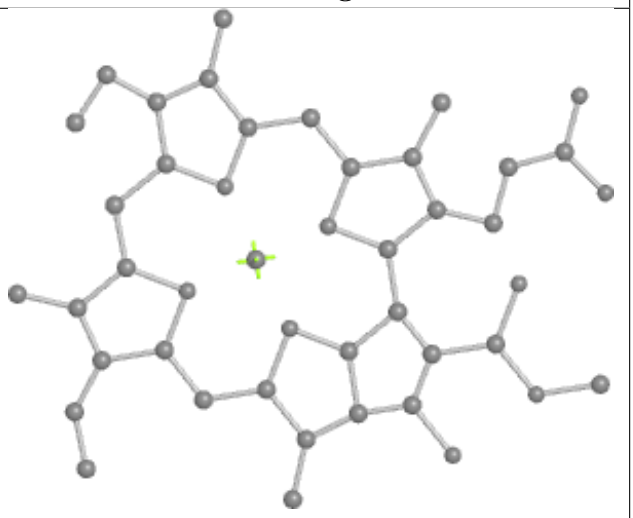
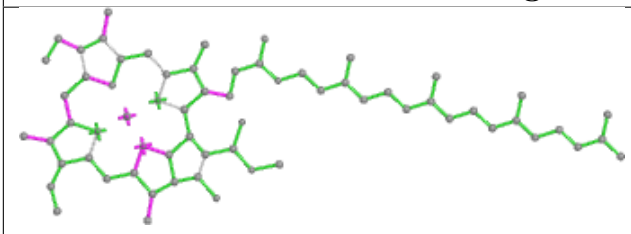


Rings

Ligand CLA D 405



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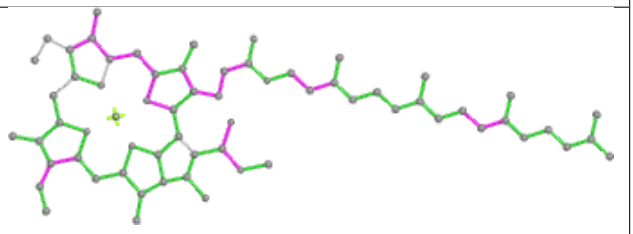

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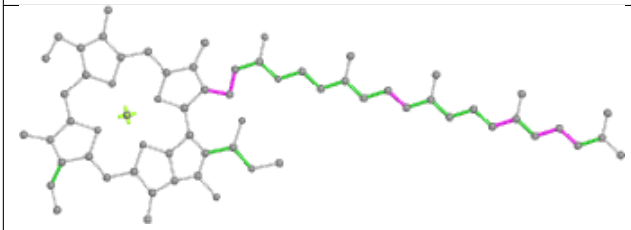

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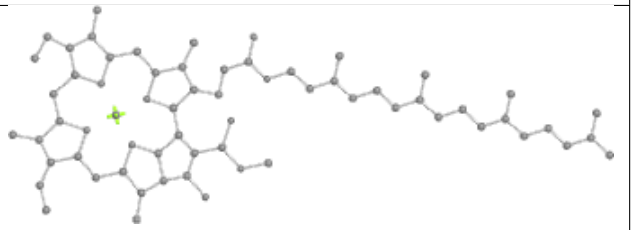
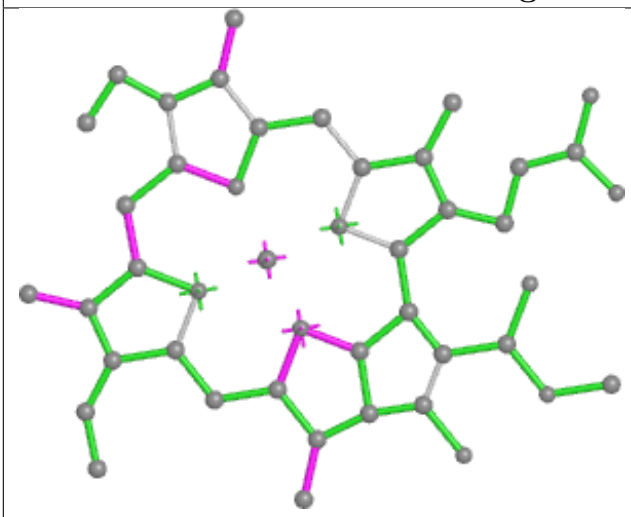


Rings

Ligand CLA 34 310



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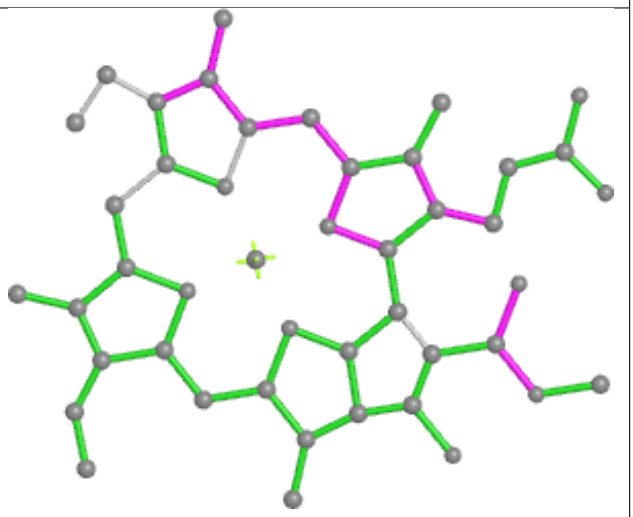

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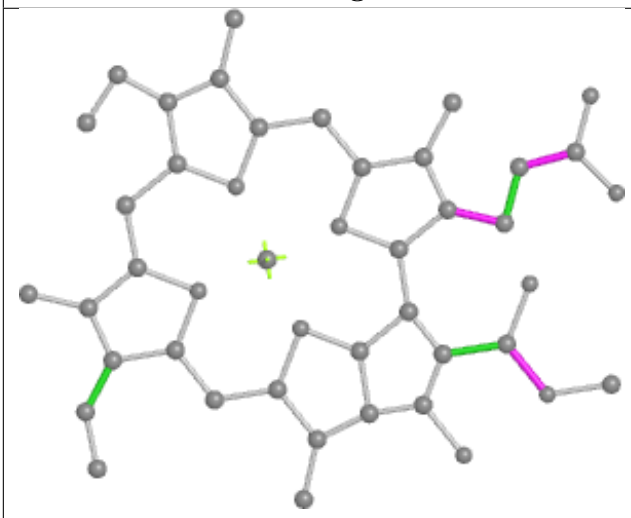

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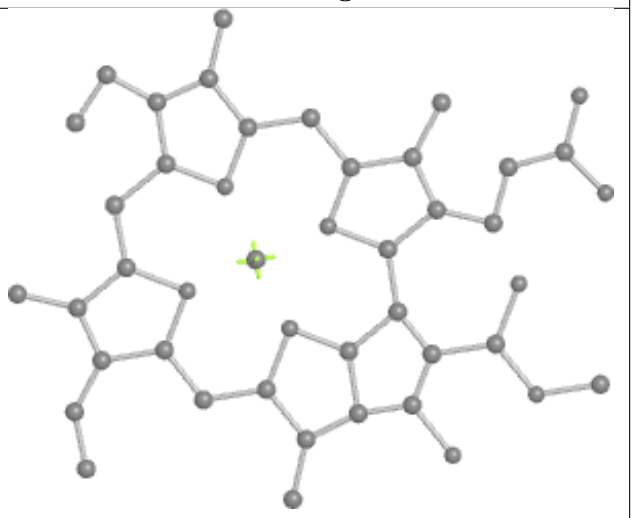
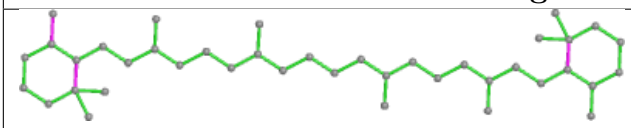


Rings

Ligand BCR f 101



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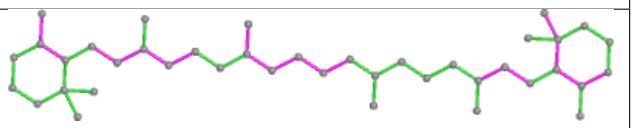

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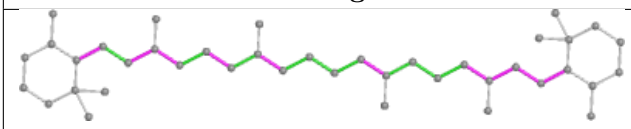

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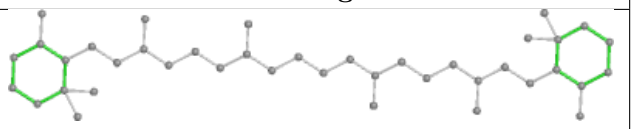
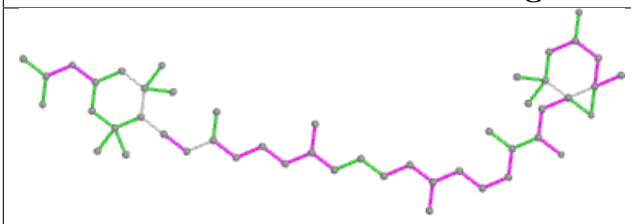


Rings

Ligand A86 35 315



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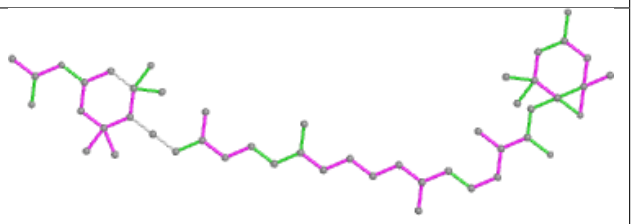

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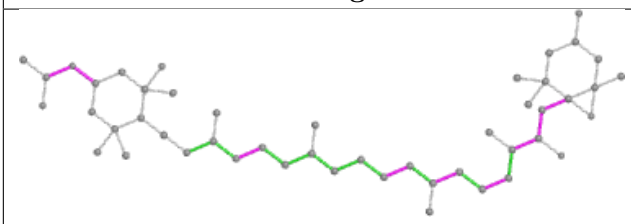

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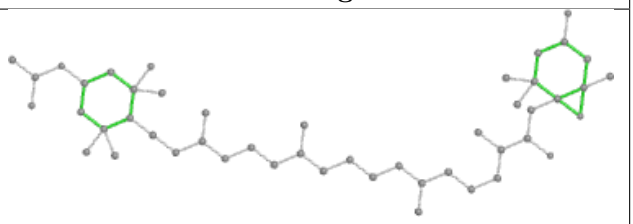
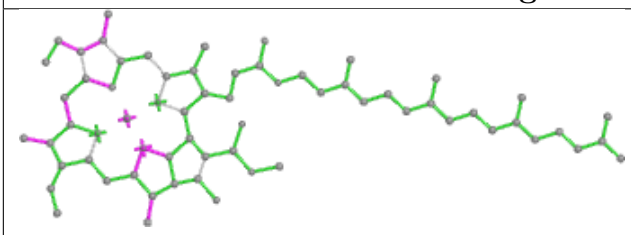


Rings

Ligand CLA 17 303



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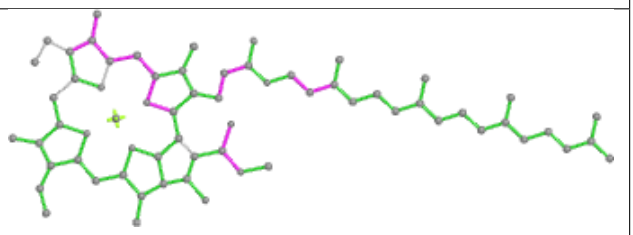

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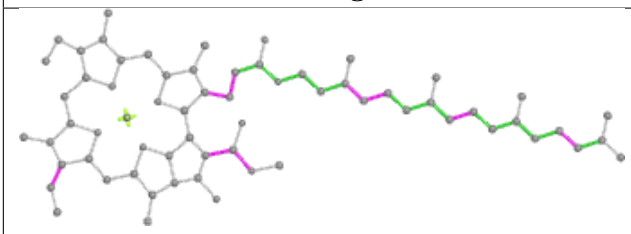

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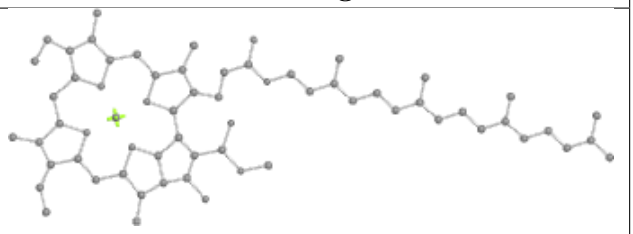
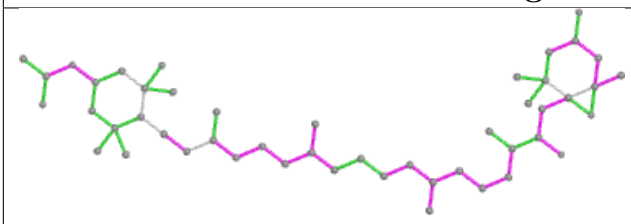


Rings

Ligand A86 20 210



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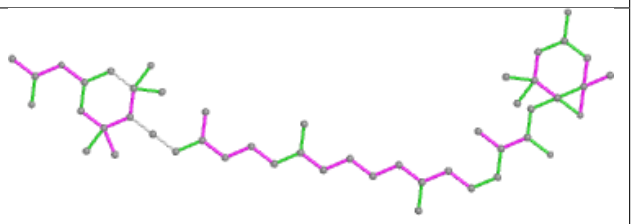

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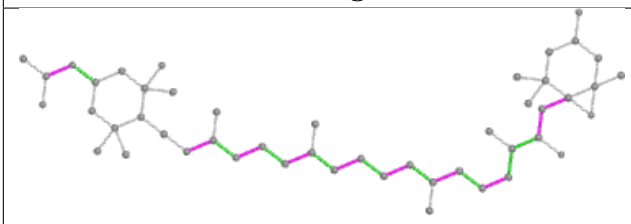

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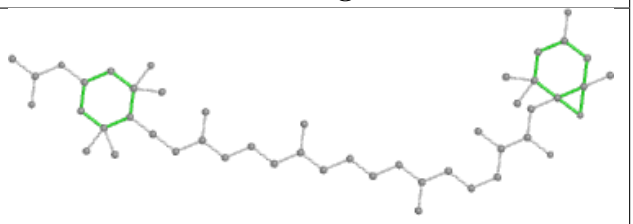
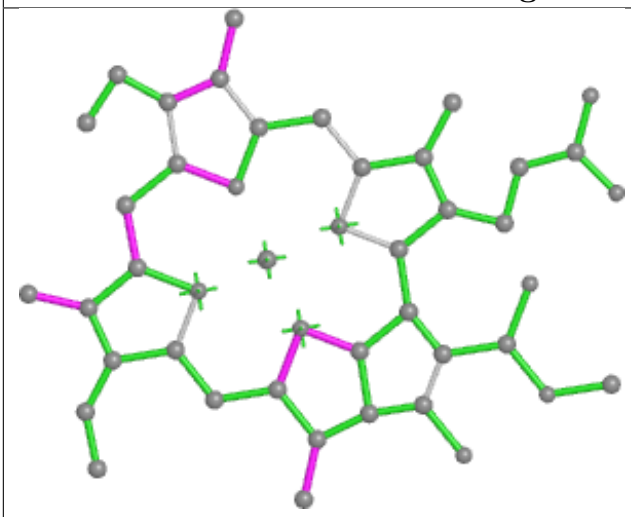


Rings

Ligand CLA 31 305



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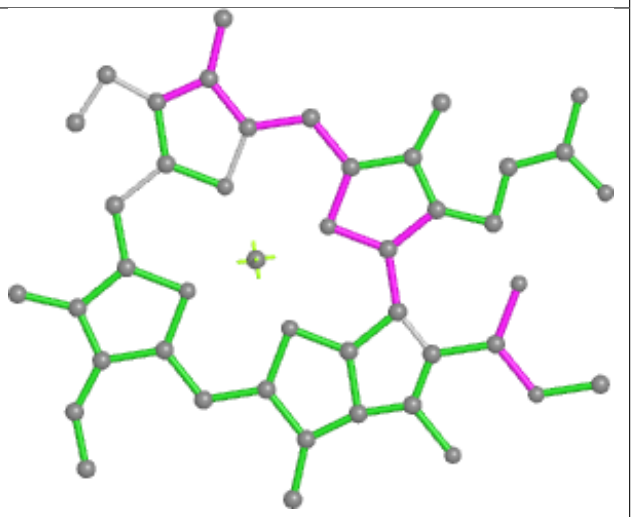

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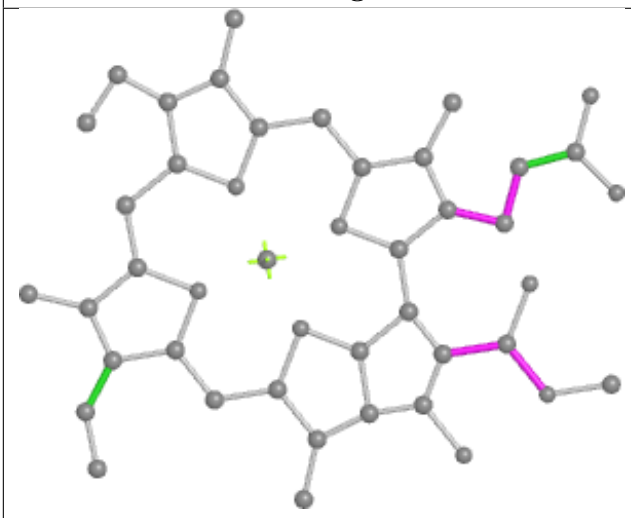

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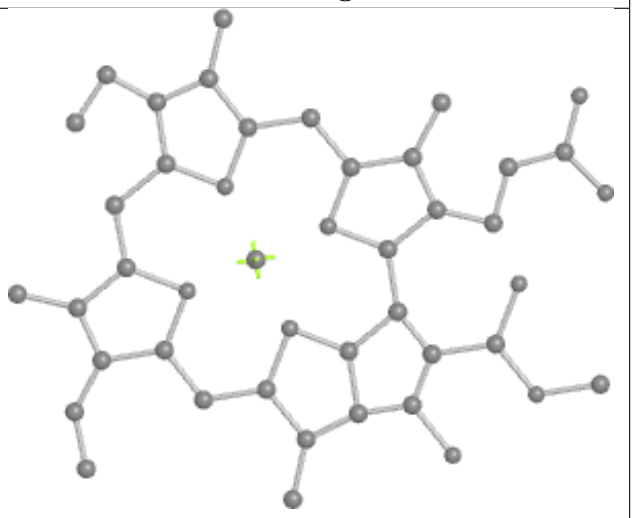
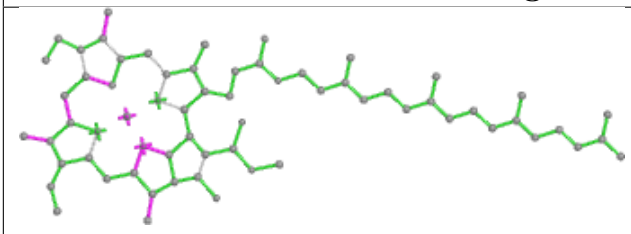


Rings

Ligand CLA A 402



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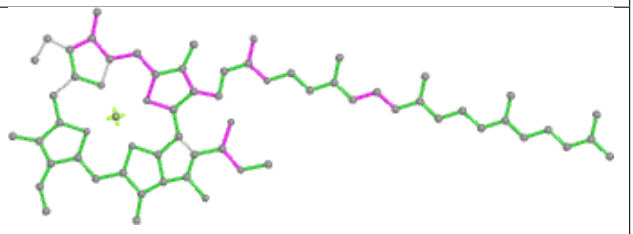

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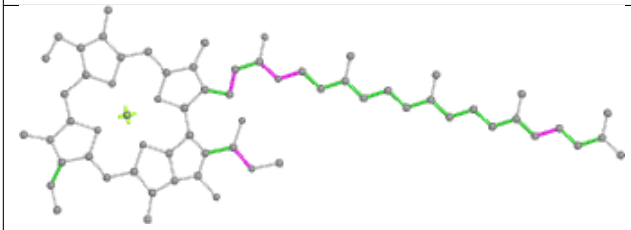
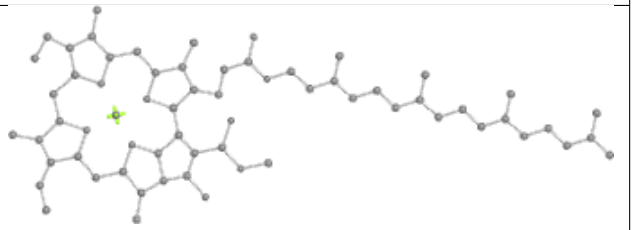
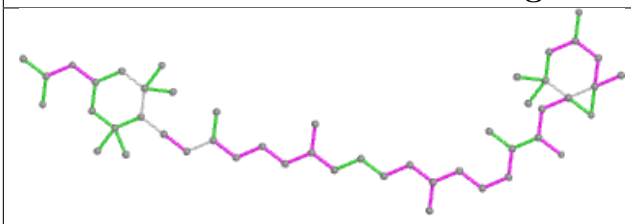


Torsions



Rings

Ligand A86 36 313



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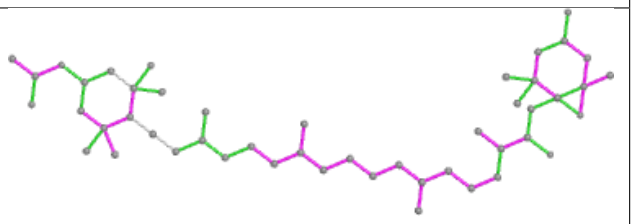

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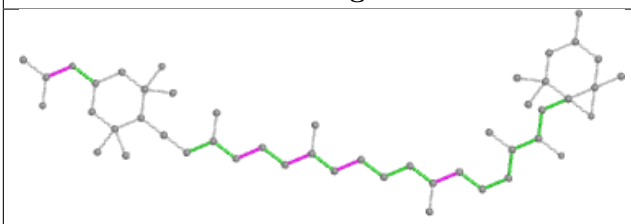

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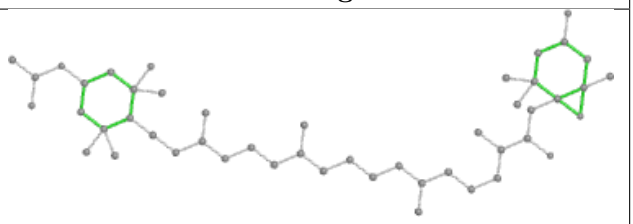
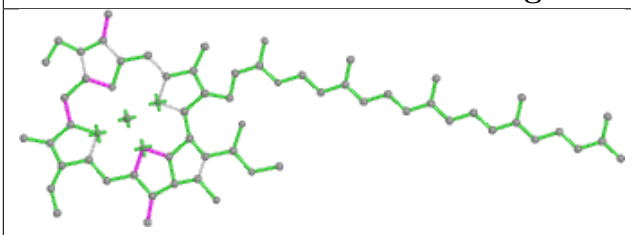


Rings

Ligand CLA w 103



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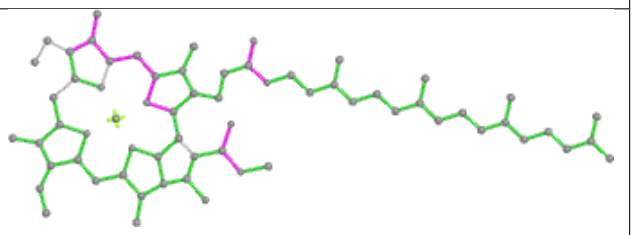

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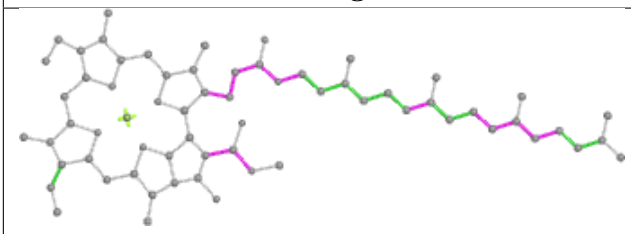

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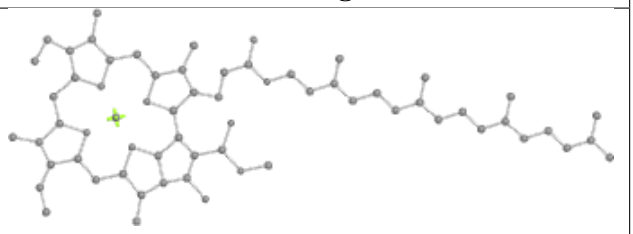
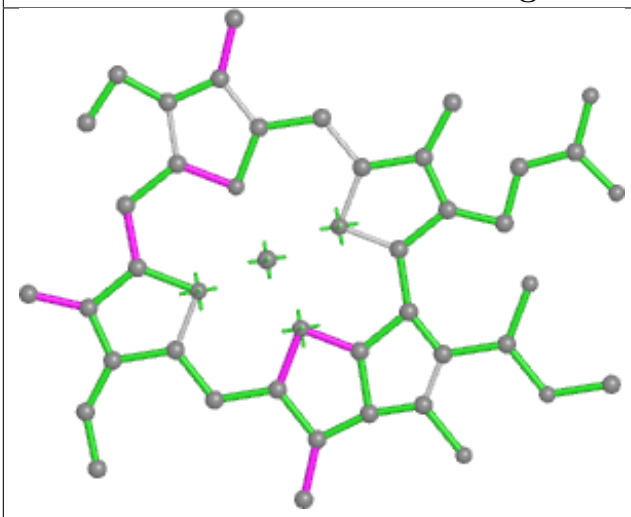


Rings

Ligand CLA 38 307



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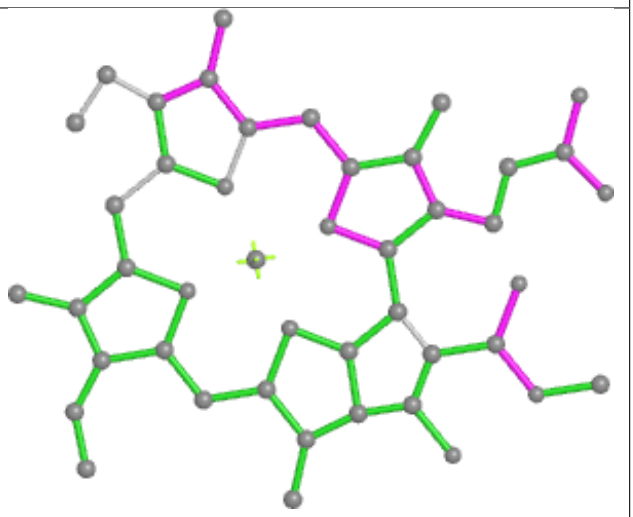

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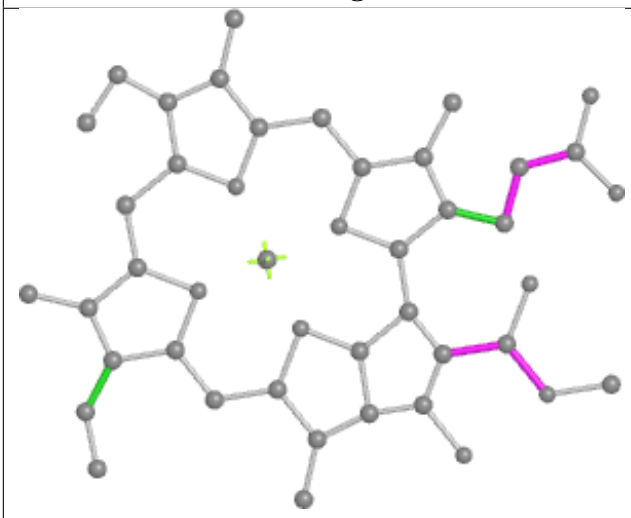

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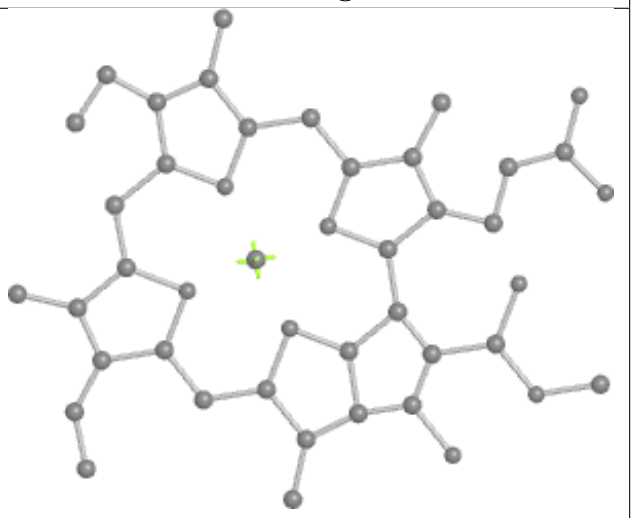

Rings

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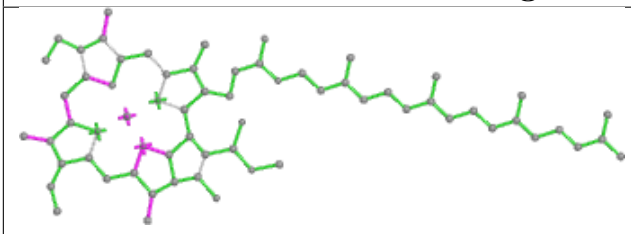

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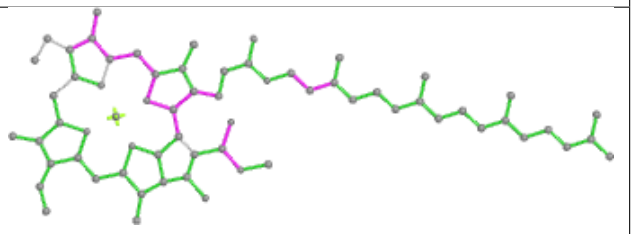

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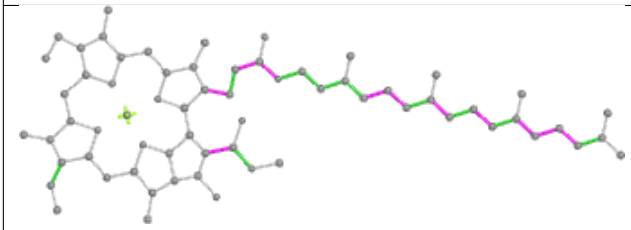

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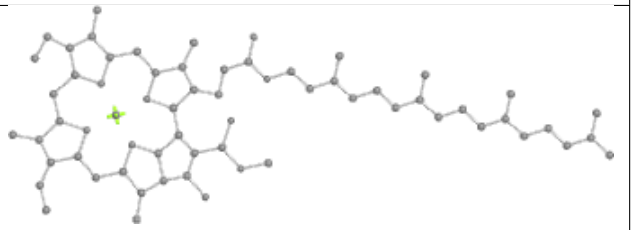
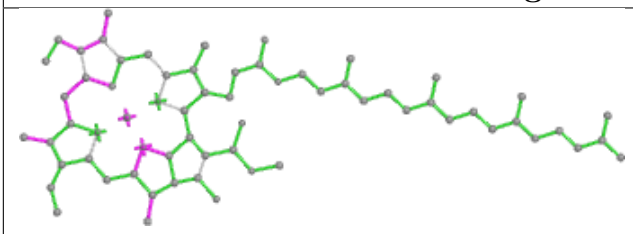


Rings

Ligand CLA C 507



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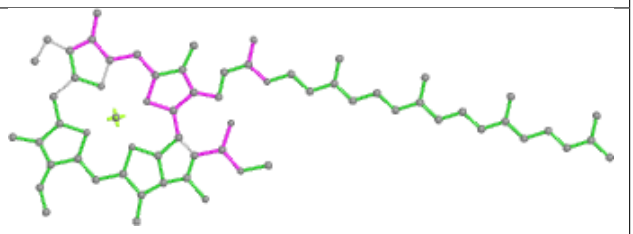

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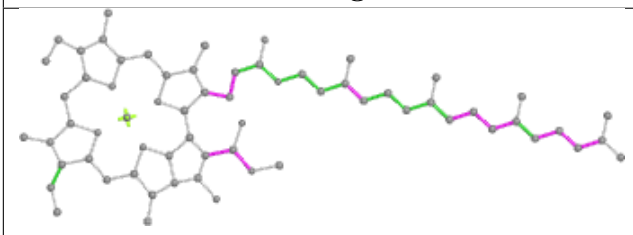

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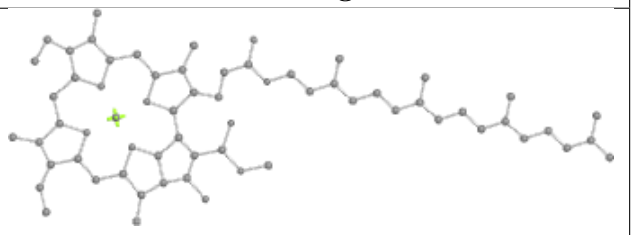
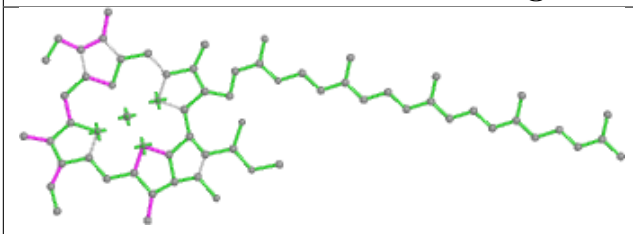


Rings

Ligand CLA b 602



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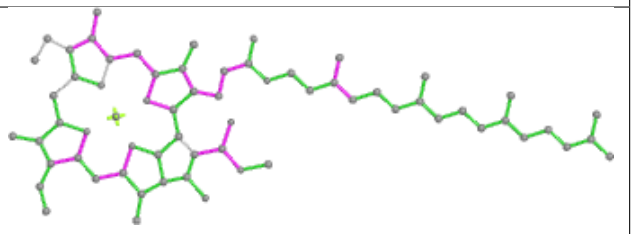

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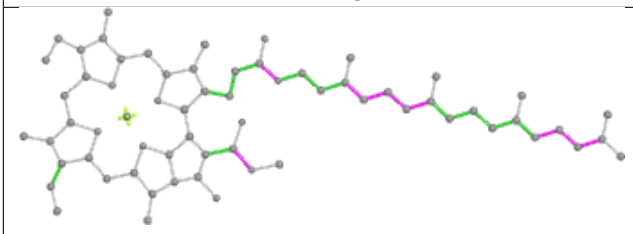

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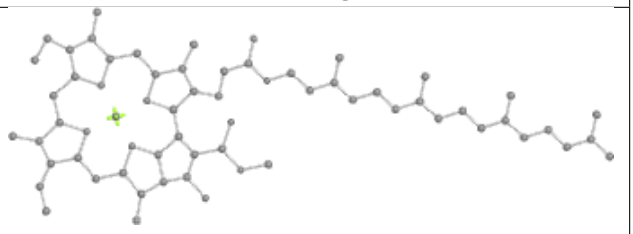
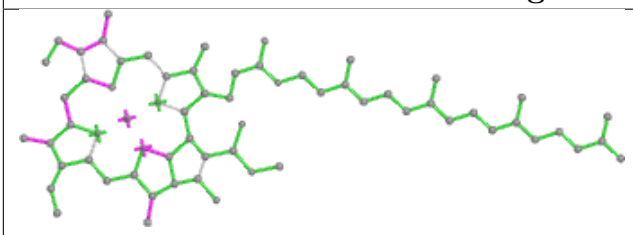


Rings

Ligand CLA b 622



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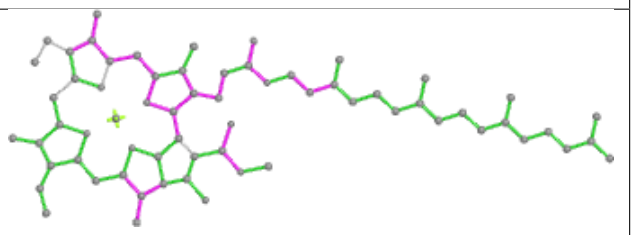

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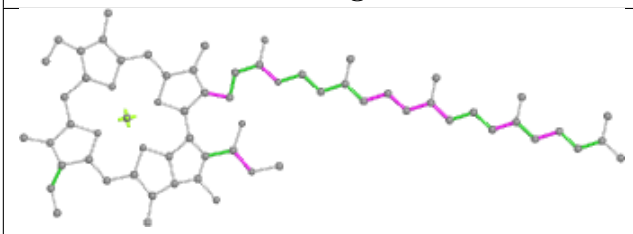

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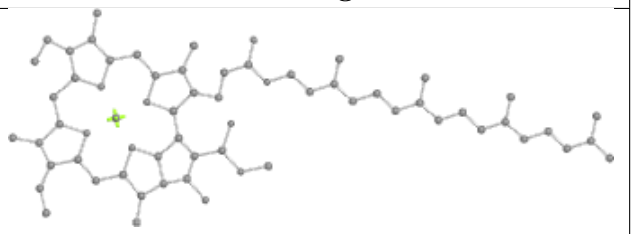
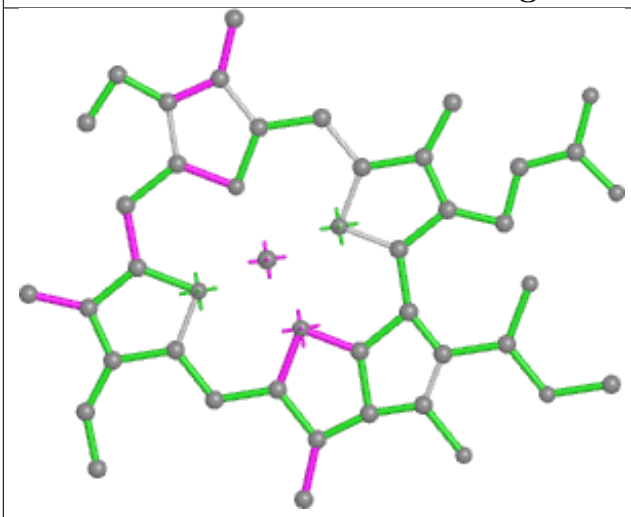


Rings

Ligand CLA 20 207



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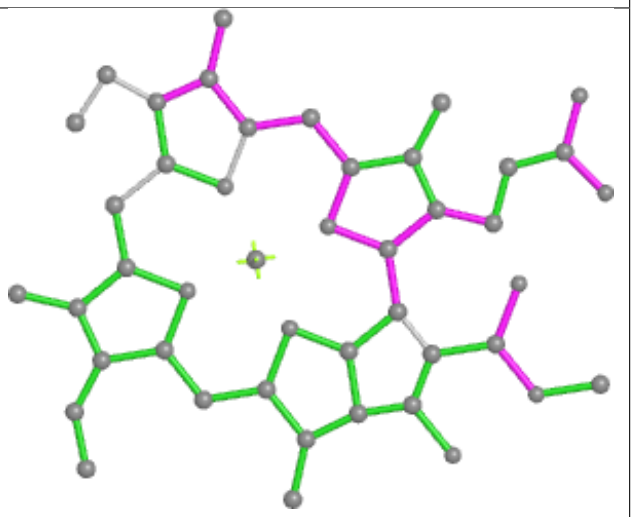

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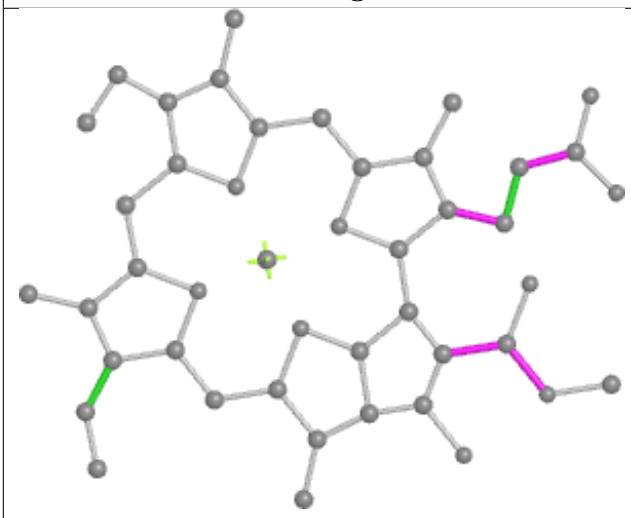

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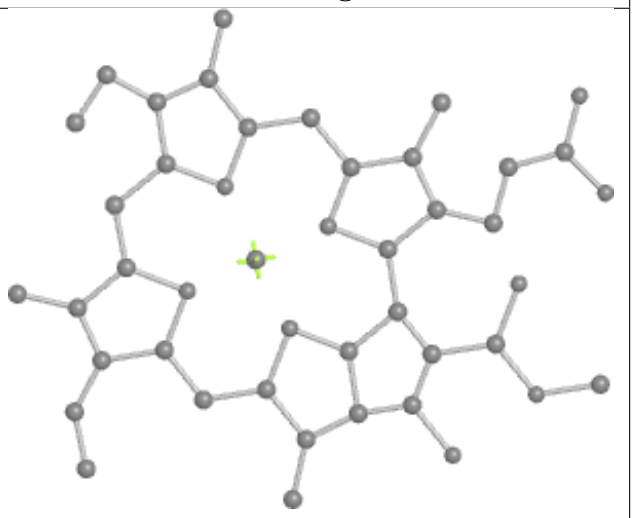

Rings

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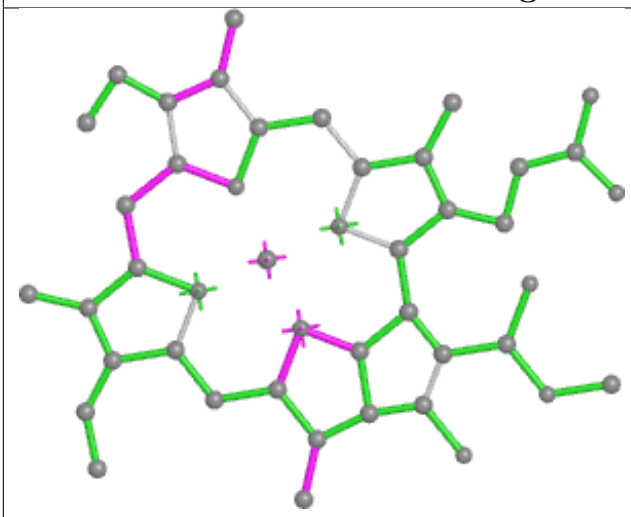

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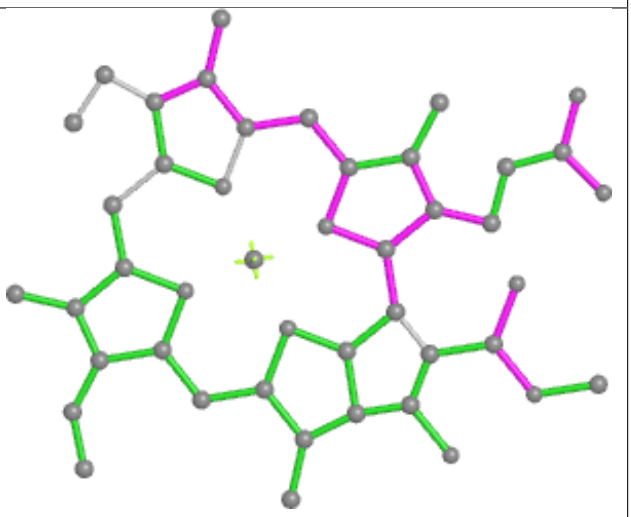

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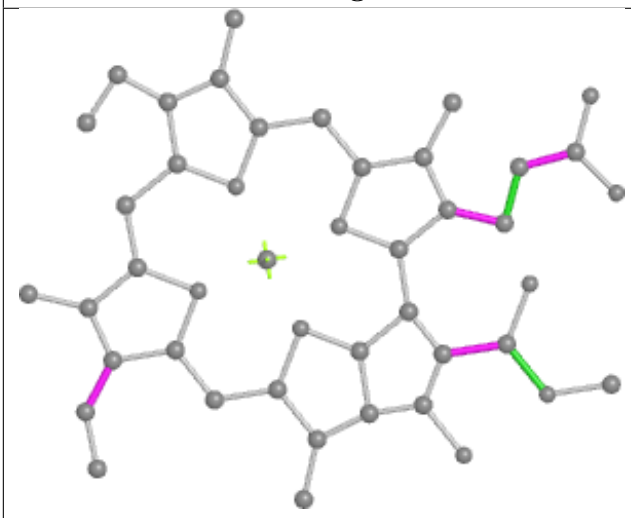

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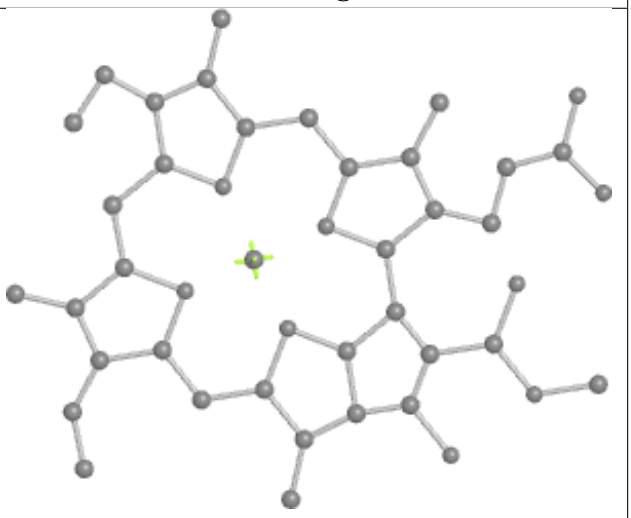
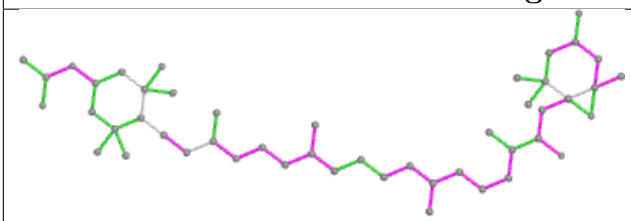


Rings

Ligand A86 12 319



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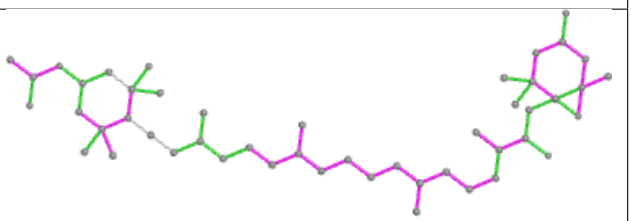

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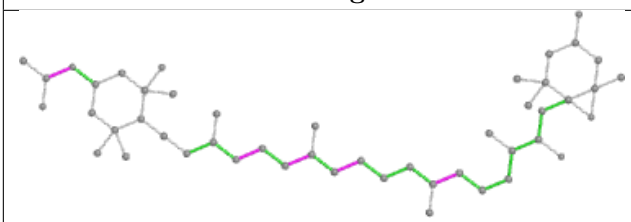

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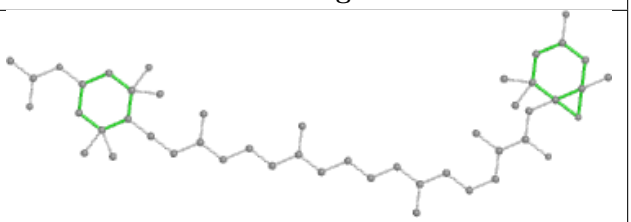
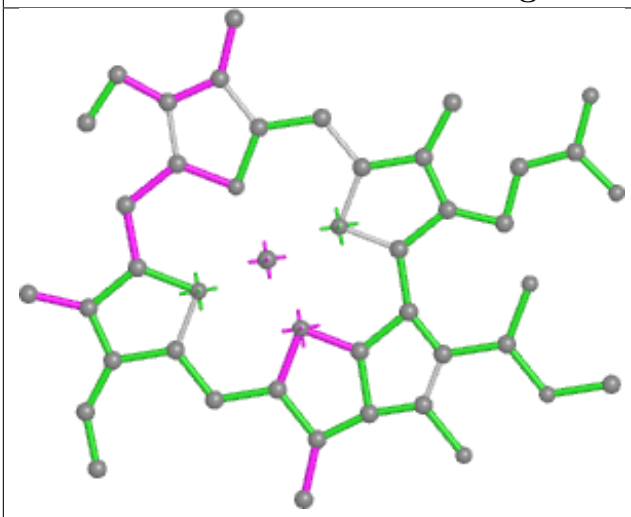


Rings

Ligand CLA 11 302



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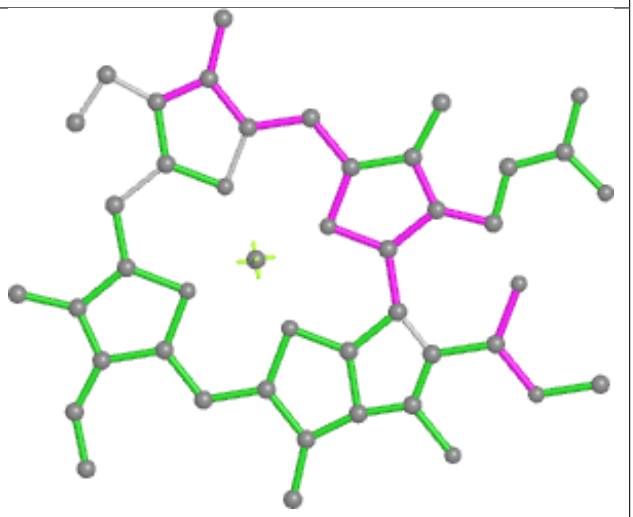

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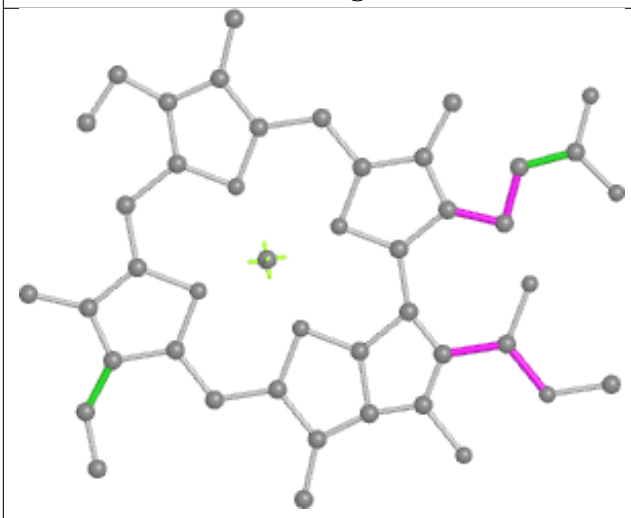

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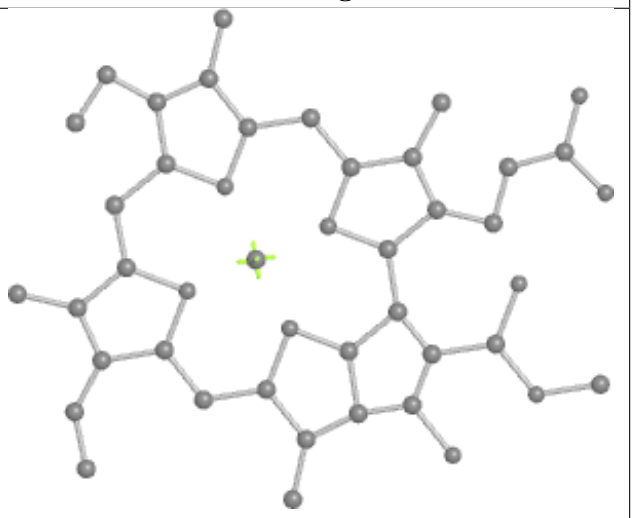

Rings

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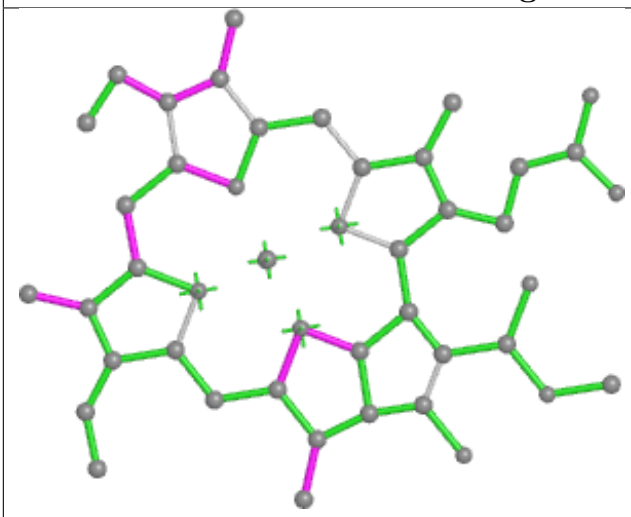

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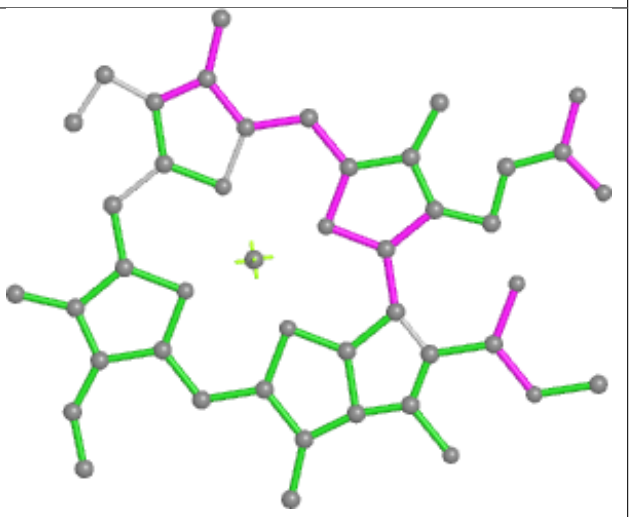

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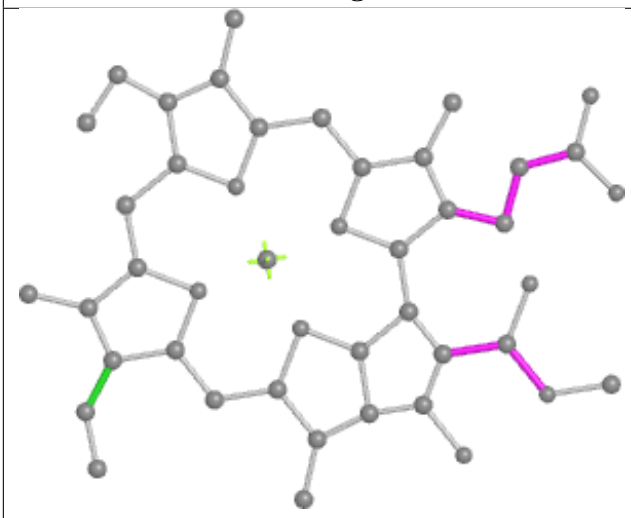

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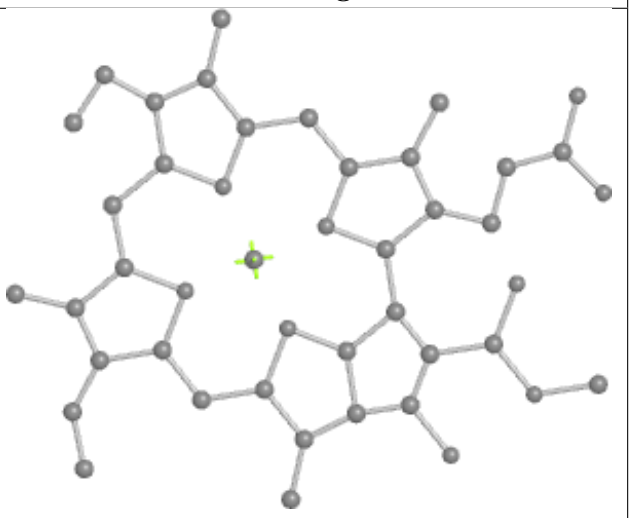

Rings

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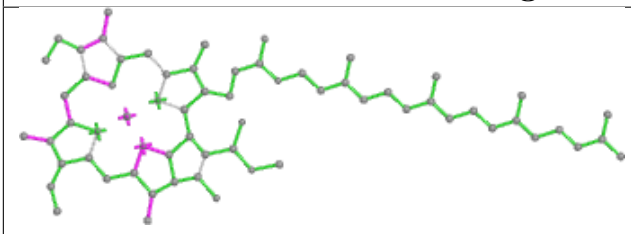

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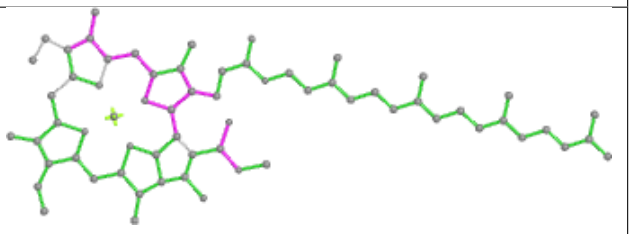
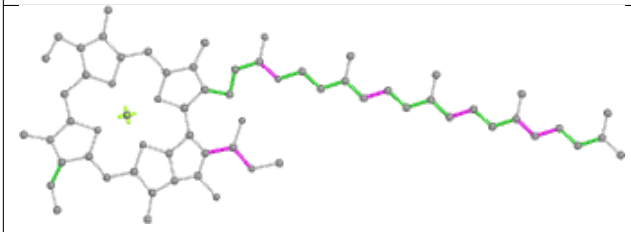


Bond angles



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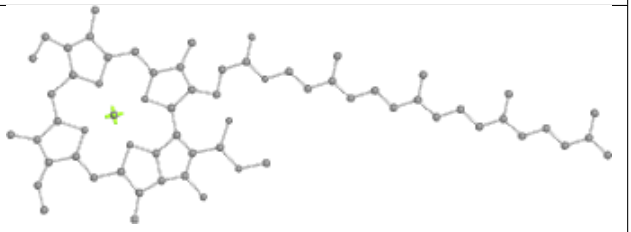
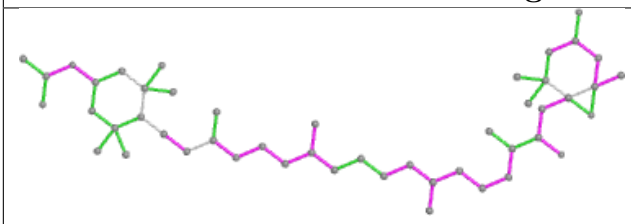


Rings

Ligand A86 19 309



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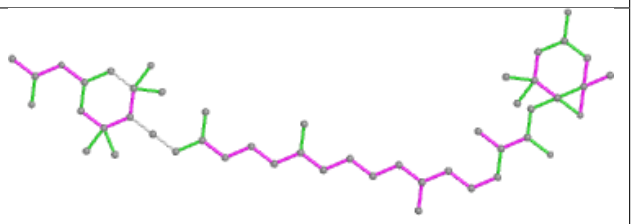

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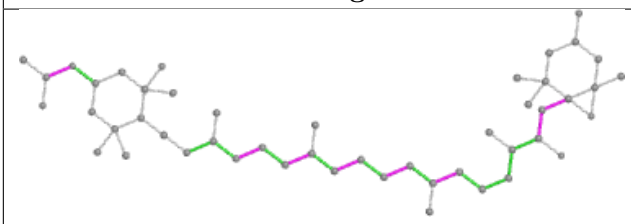
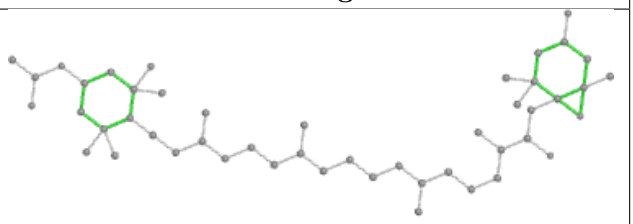
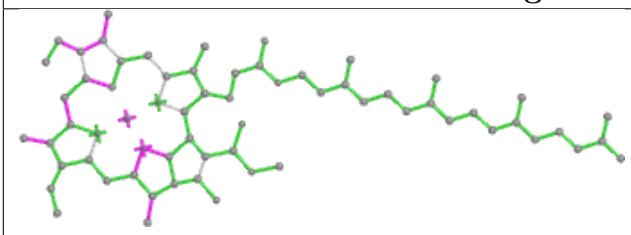


Torsions

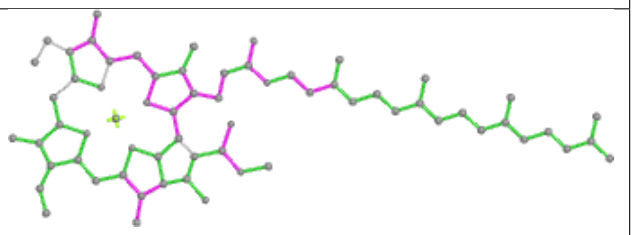


Rings

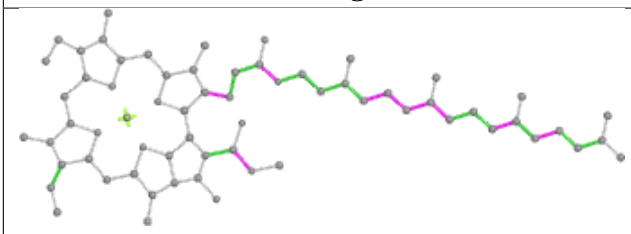
Ligand CLA B 623



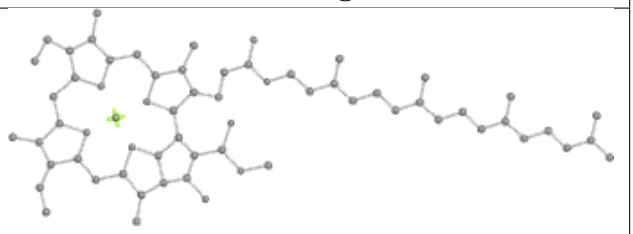
Bond lengths



Bond angles

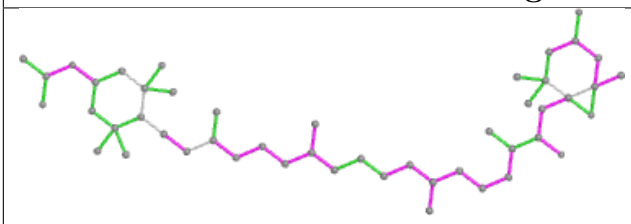


Torsions

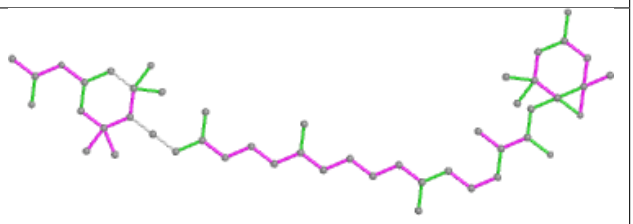


Rings

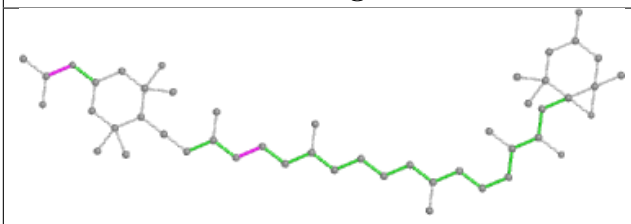
Ligand A86 31 311



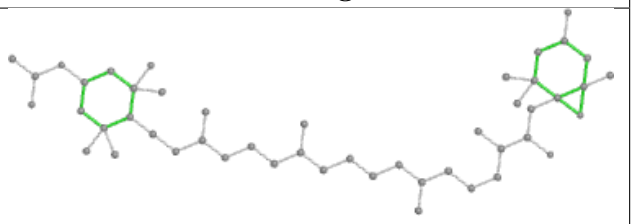
Bond lengths



Bond angles

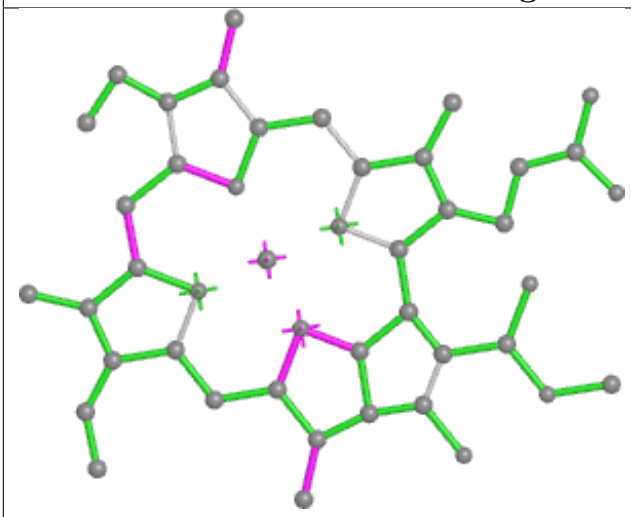


Torsions

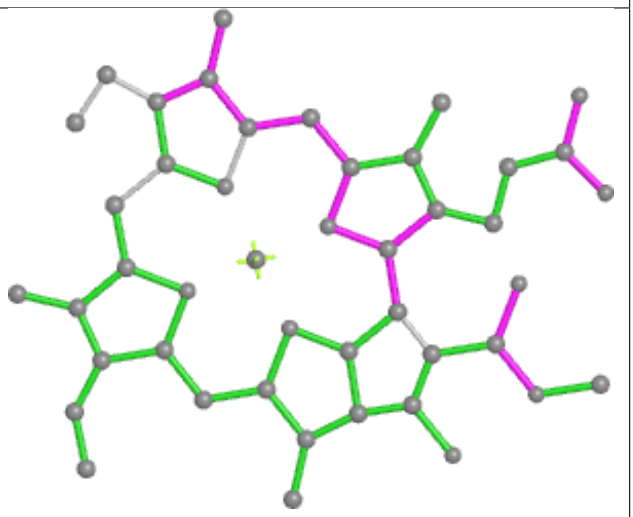


Rings

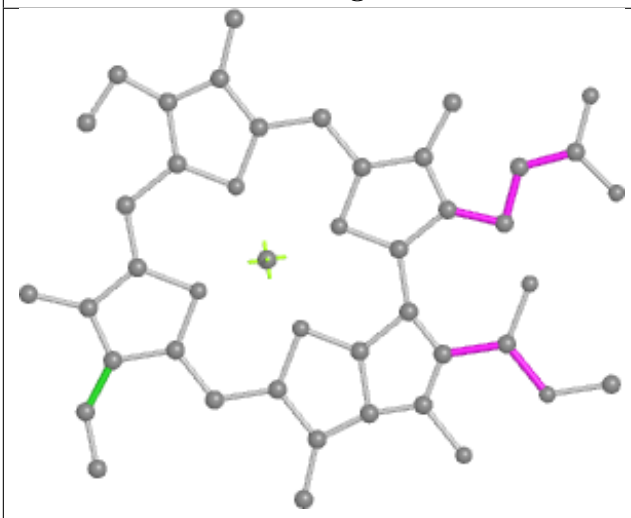
Ligand CLA 18 308



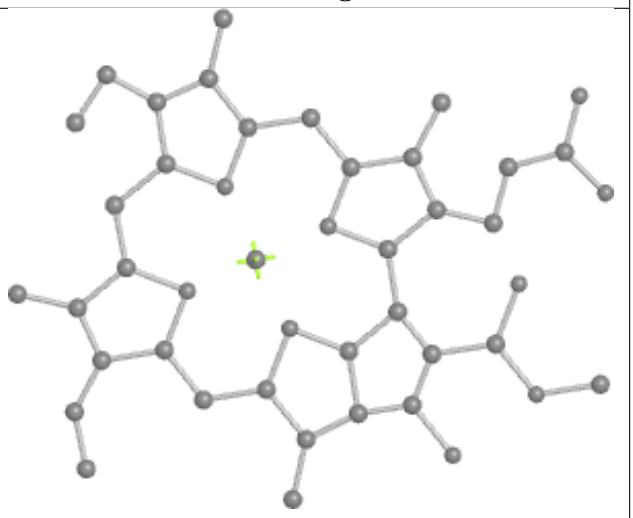
Bond lengths



Bond angles

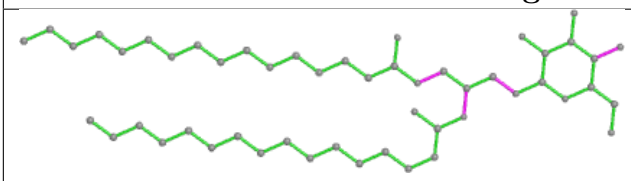


Torsions

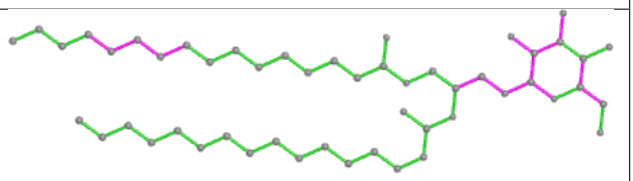


Rings

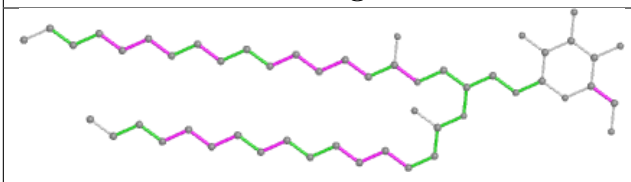
Ligand LMG b 618



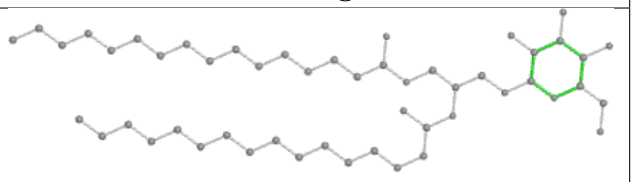
Bond lengths



Bond angles

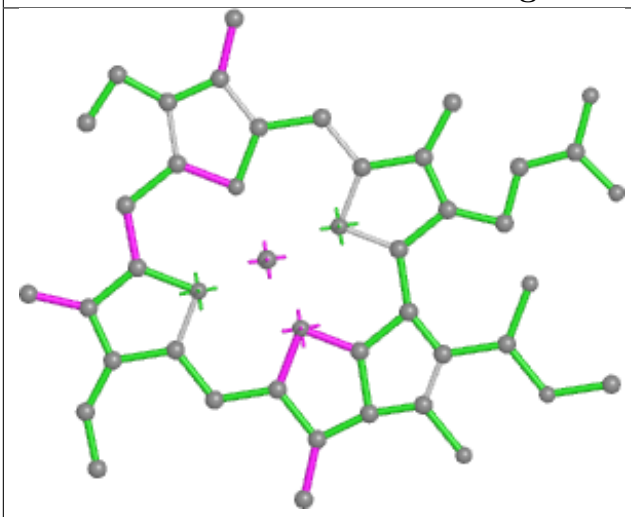


Torsions

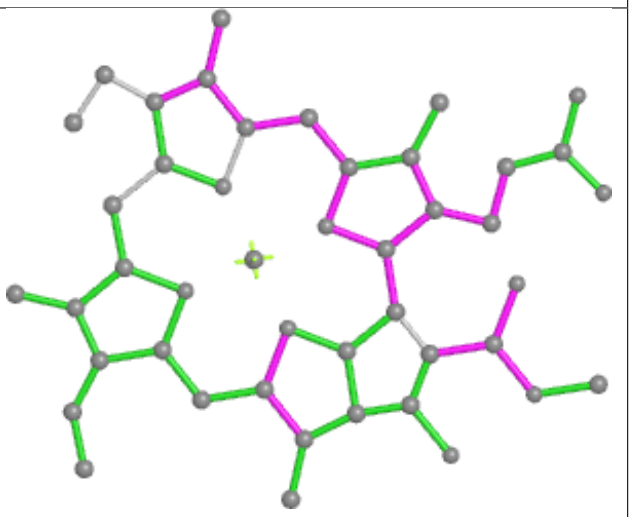


Rings

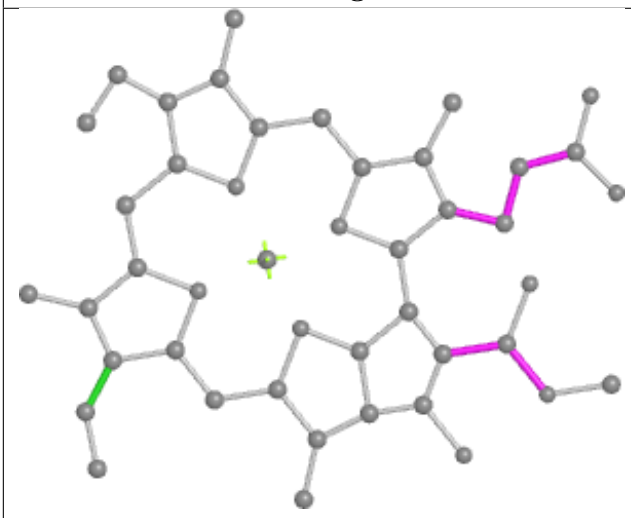
Ligand CLA 13 305



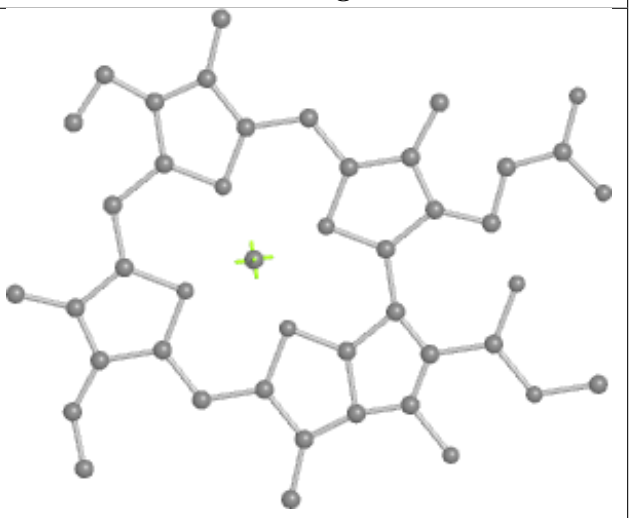
Bond lengths



Bond angles

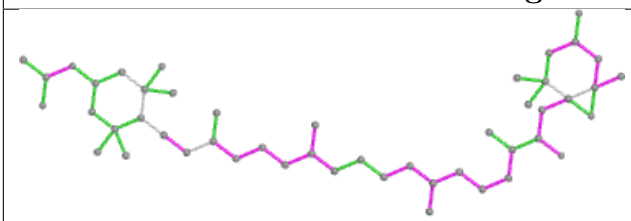


Torsions

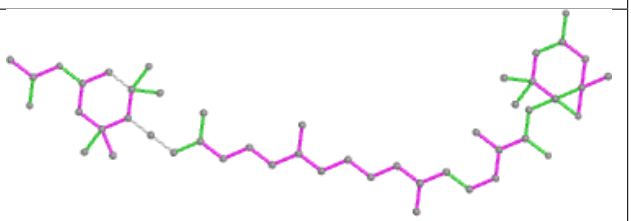


Rings

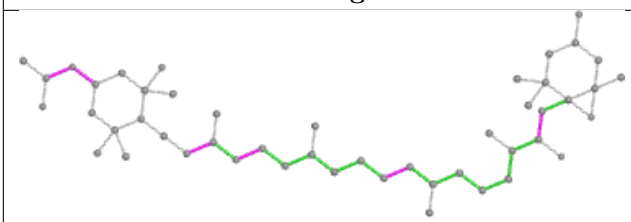
Ligand A86 36 312



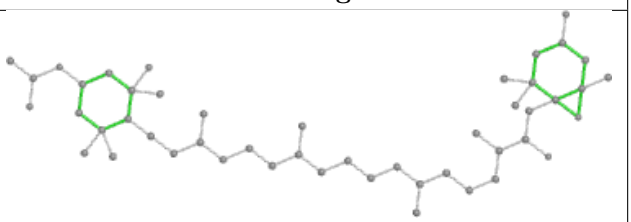
Bond lengths



Bond angles

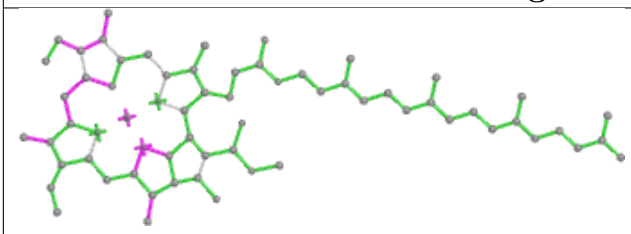


Torsions

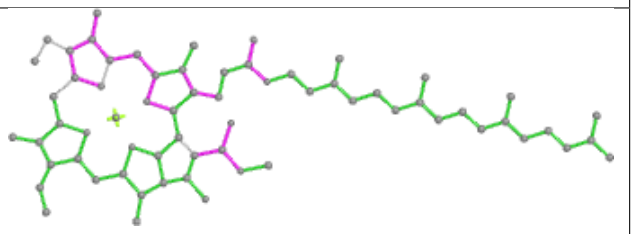


Rings

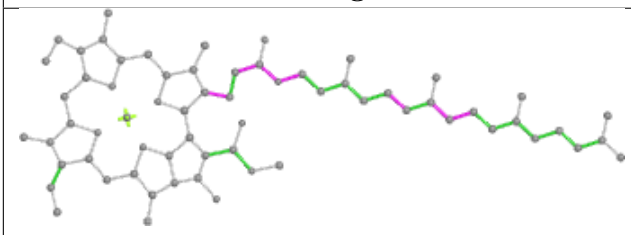
Ligand CLA a 403



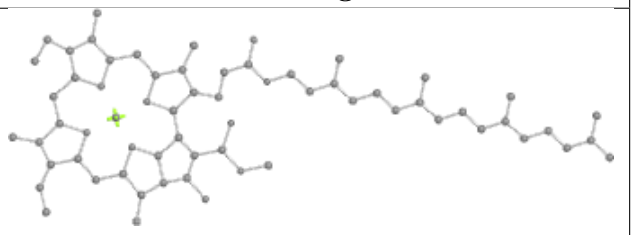
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

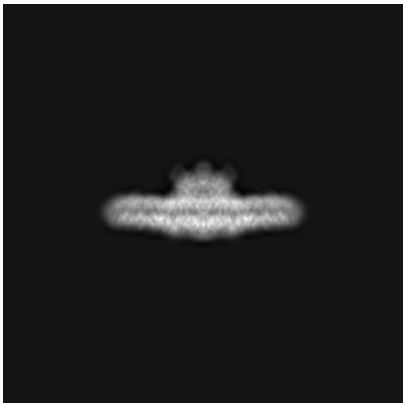
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9777. These allow visual inspection of the internal detail of the map and identification of artifacts.

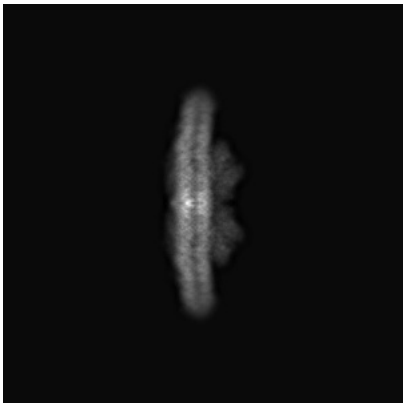
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

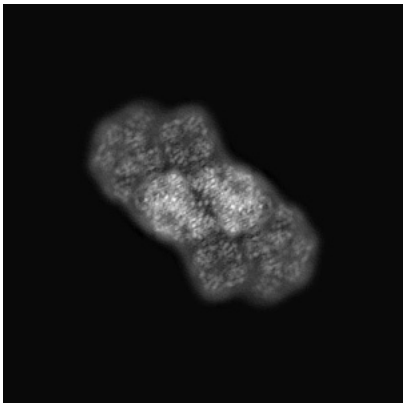
6.1.1 Primary map



X



Y



Z

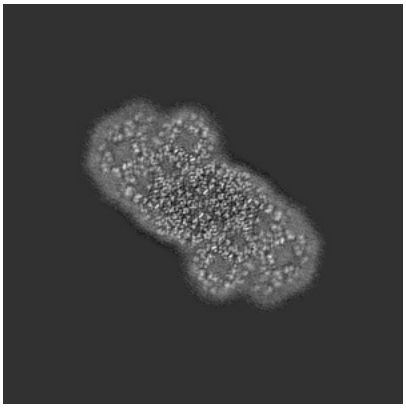
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 256

Y Index: 256

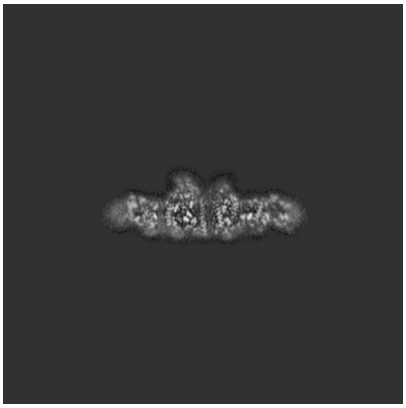


Z Index: 256

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

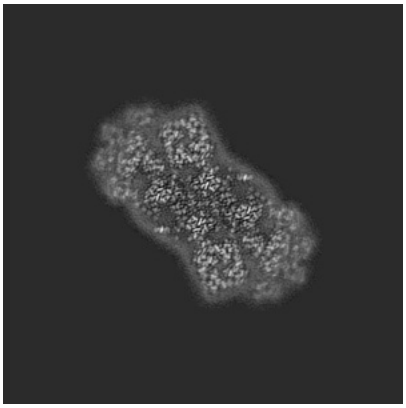
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 253

Y Index: 256



Z Index: 235

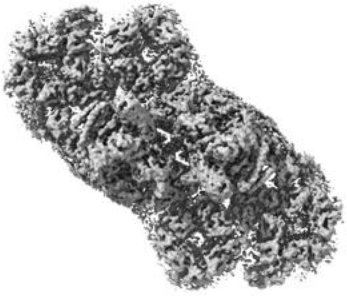
The images above show the largest variance slices of the map in three orthogonal directions.

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

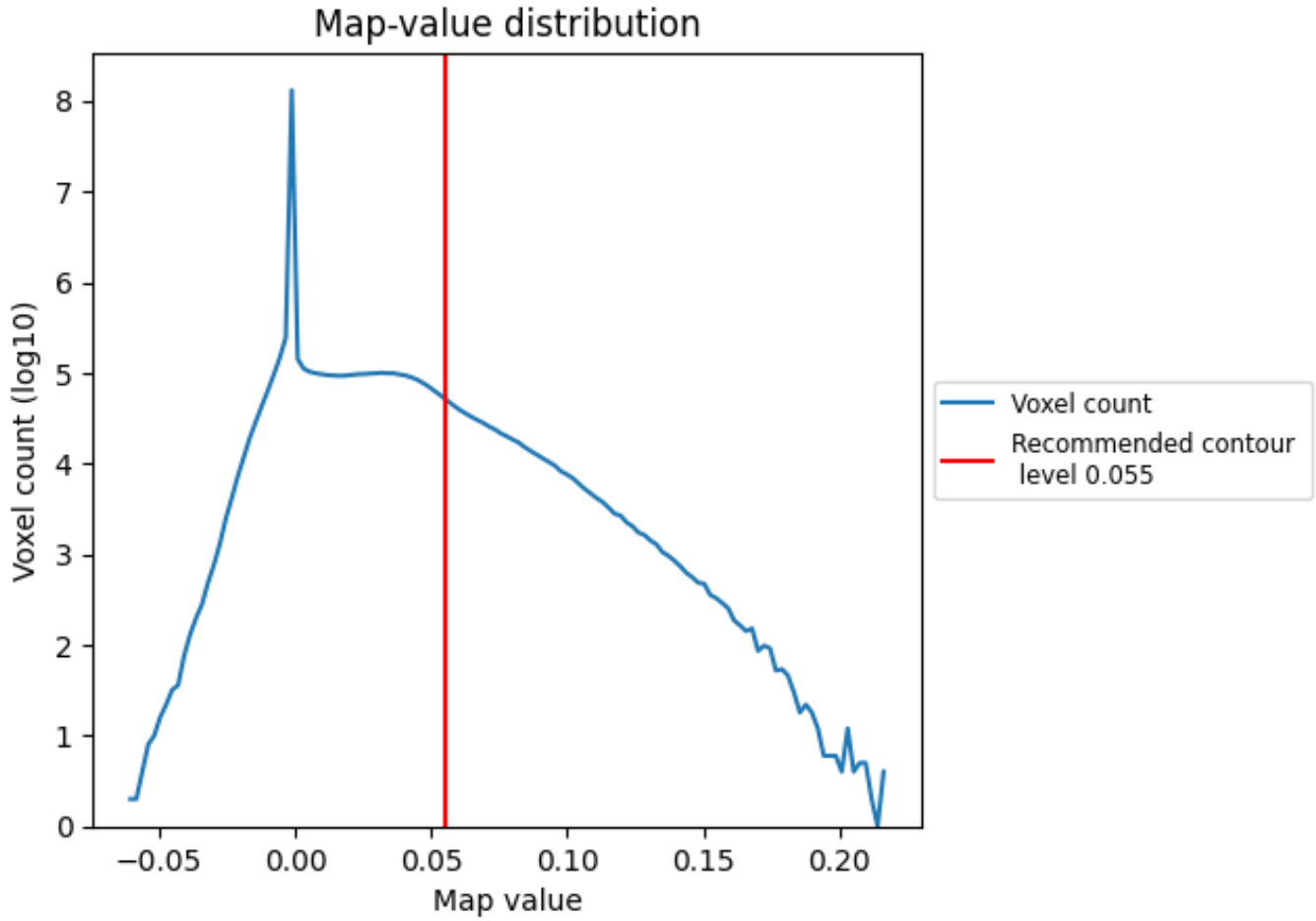
6.5 Mask visualisation (i)

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

7 Map analysis

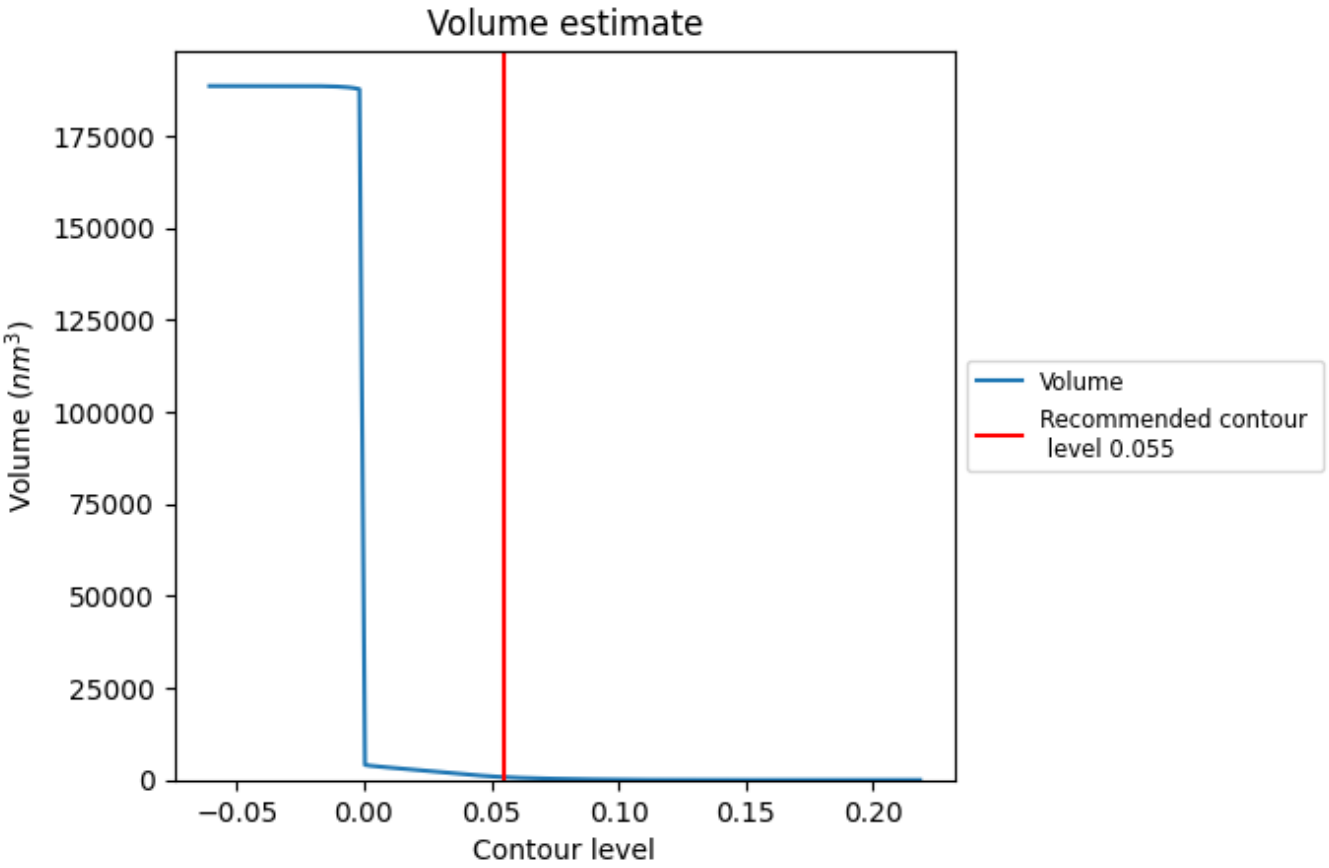
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

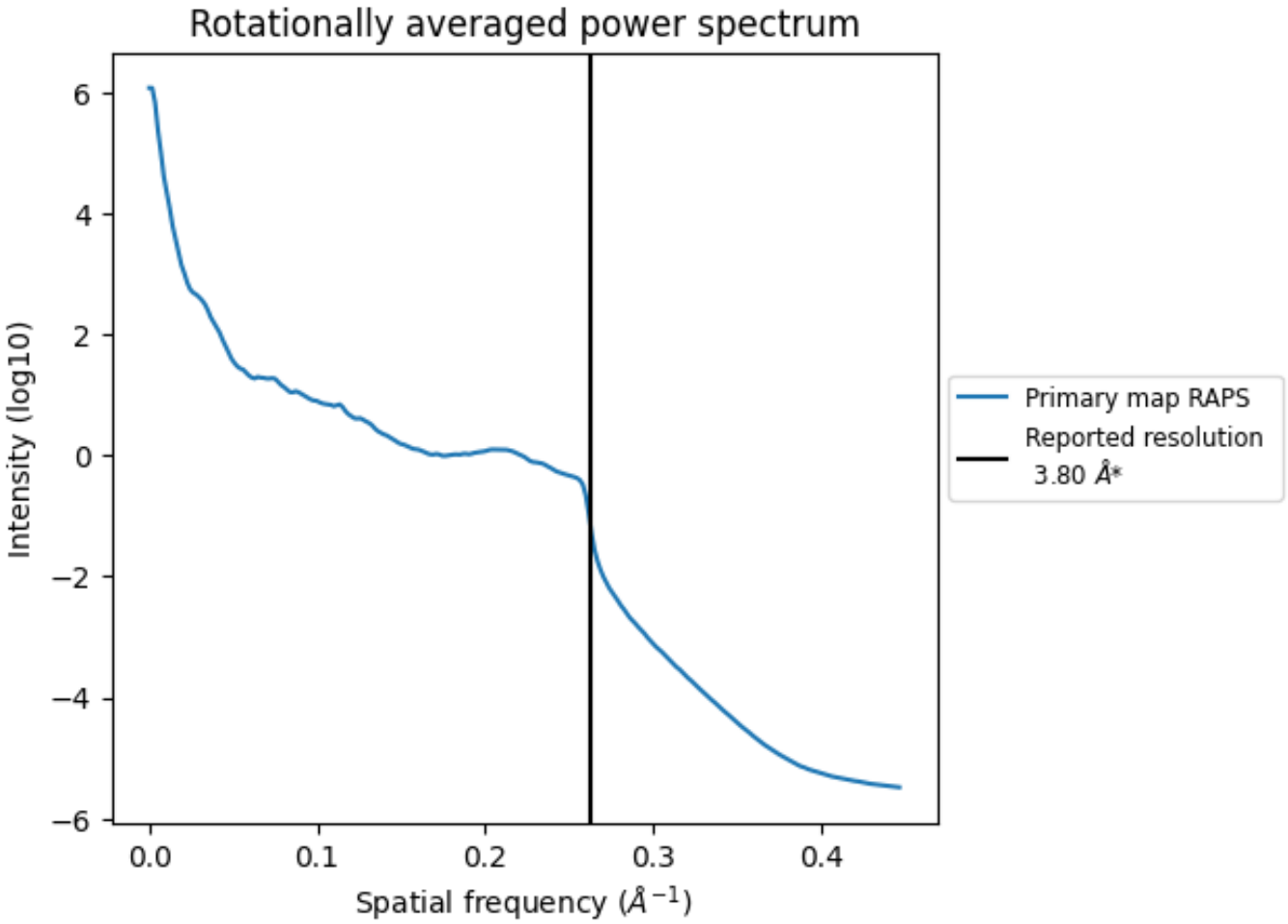
7.2 Volume estimate



The volume at the recommended contour level is 777 nm^3; this corresponds to an approximate mass of 701 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)

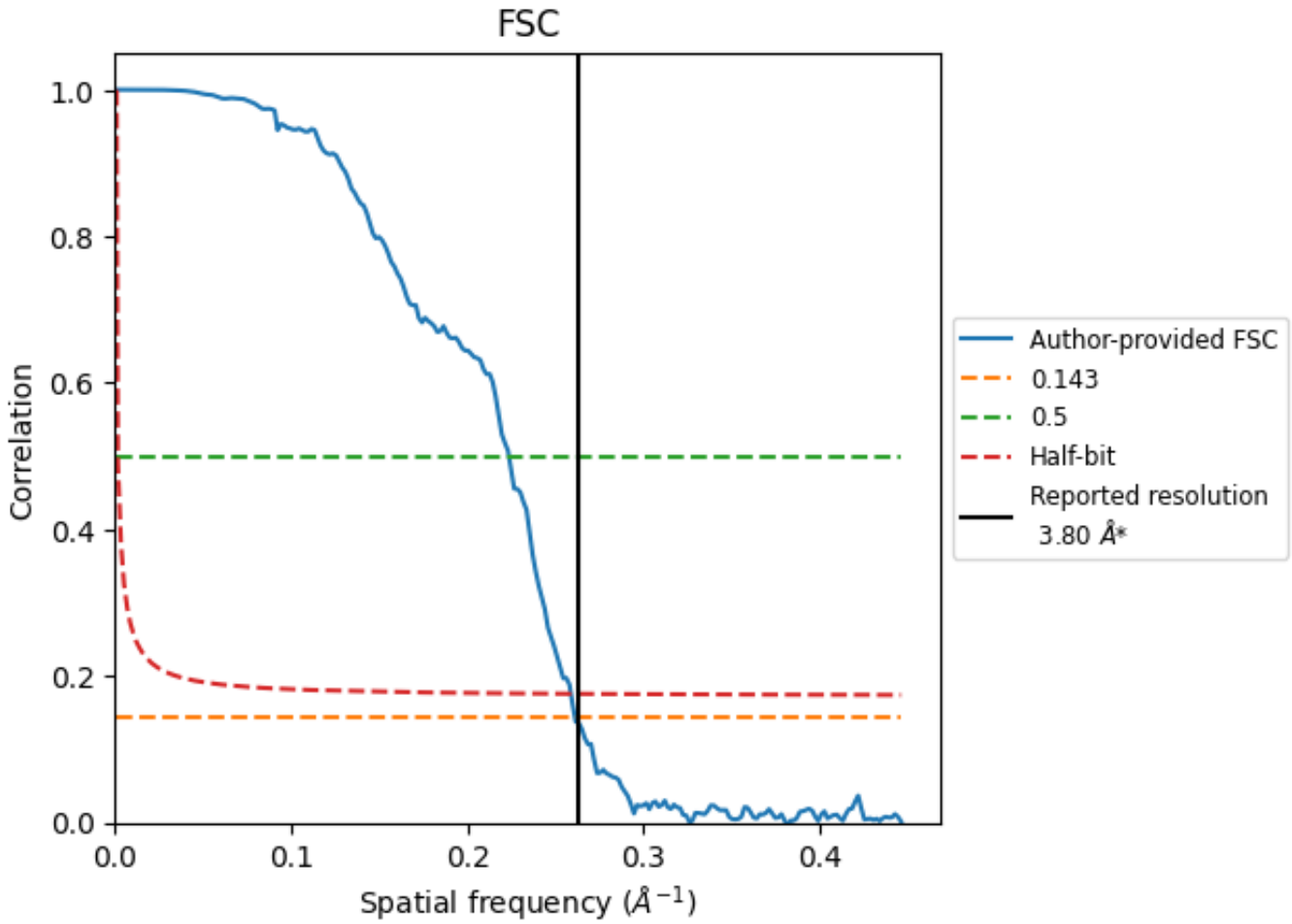


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

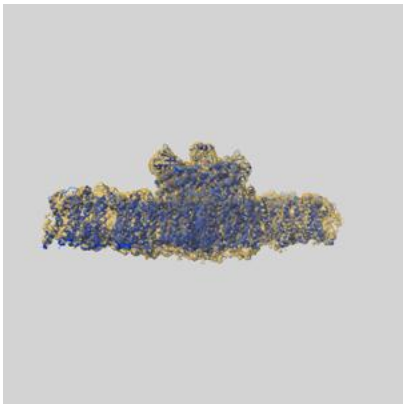
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.47	3.86
Unmasked-calculated*	-	-	-

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

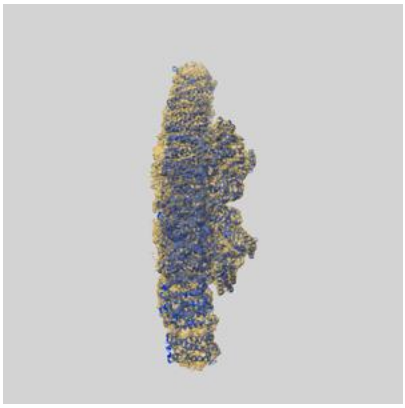
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9777 and PDB model 6J40. Per-residue inclusion information can be found in section 3 on page 49.

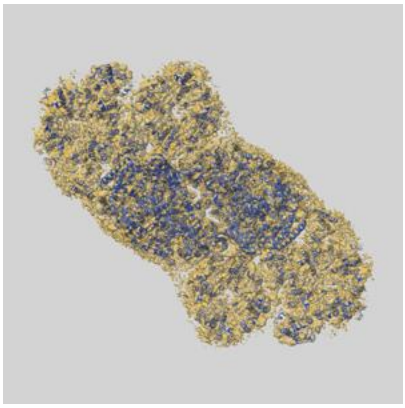
9.1 Map-model overlay



X



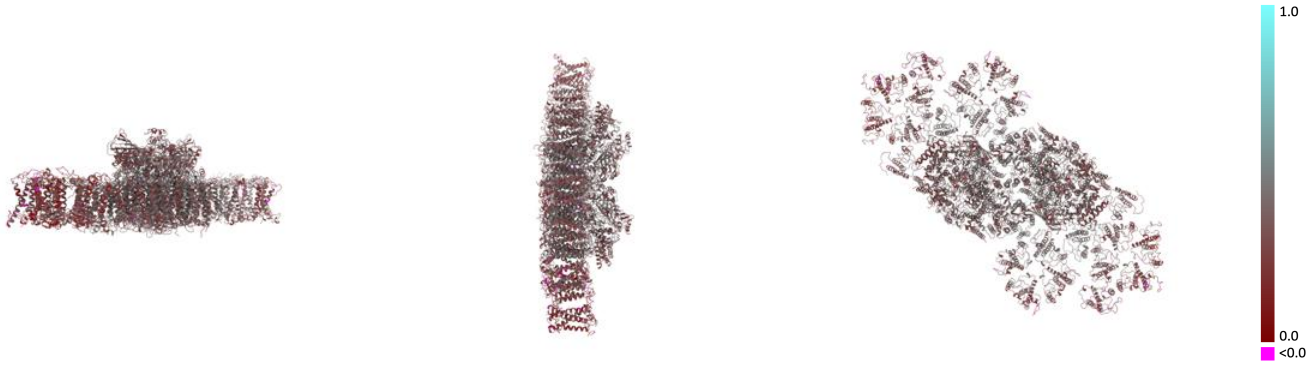
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

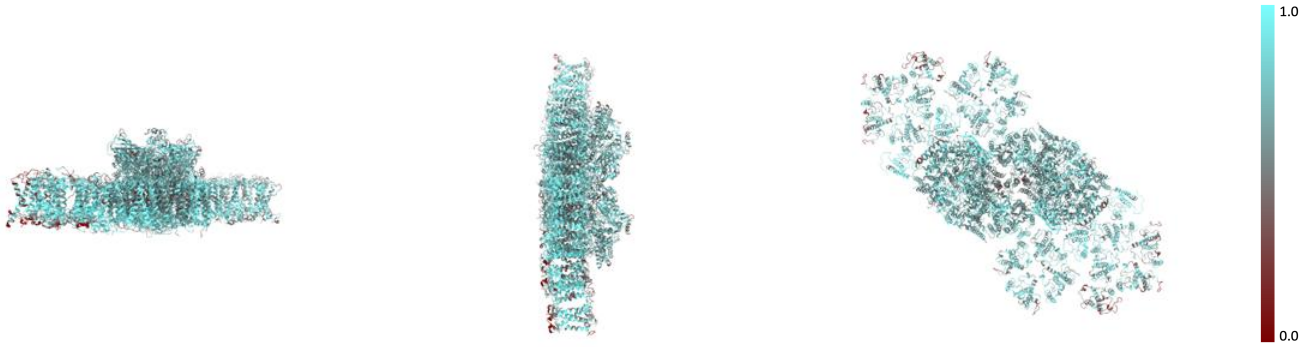
9.2 Q-score mapped to coordinate model



X Y Z

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

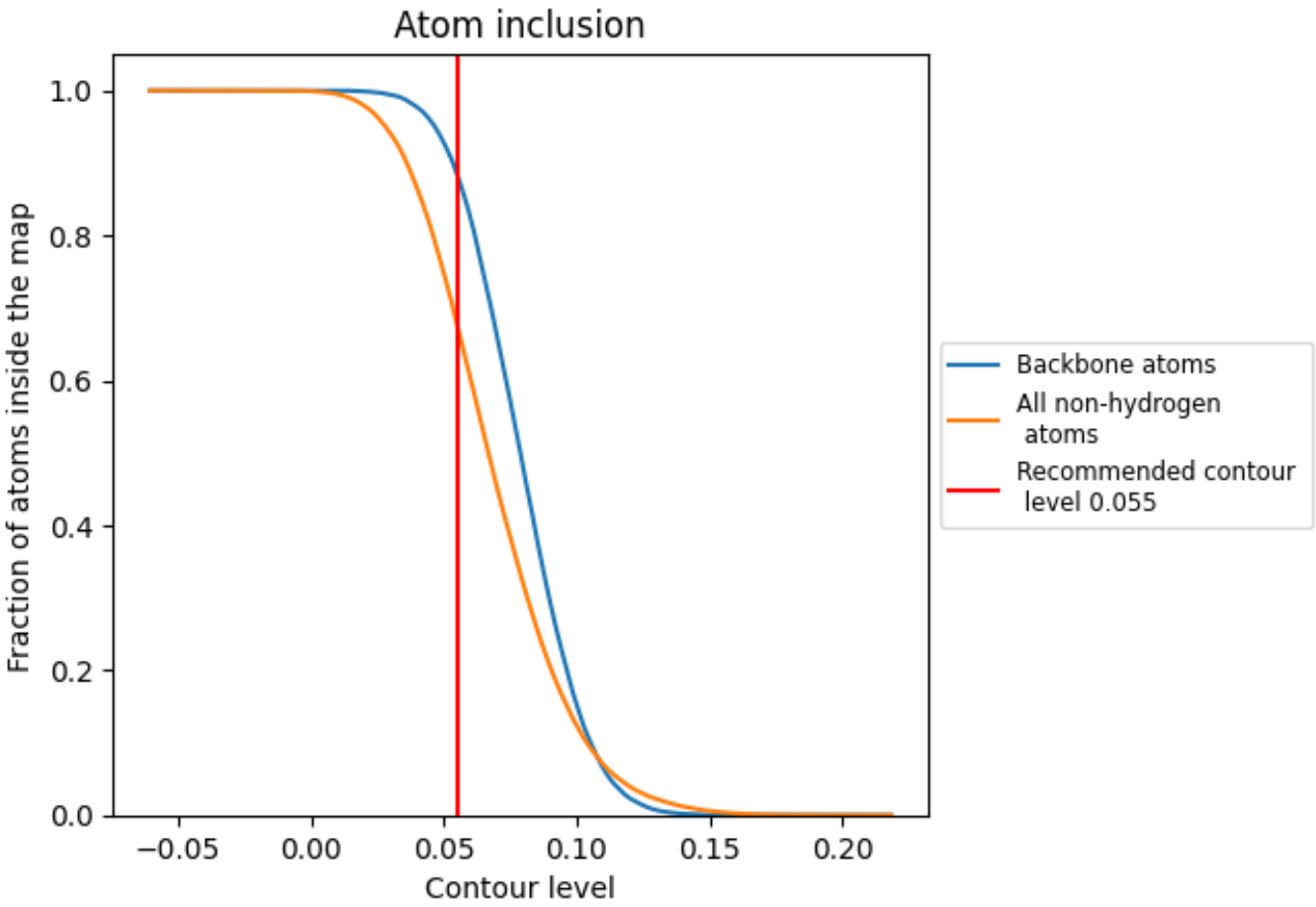
9.3 Atom inclusion mapped to coordinate model



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 68% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6759	0.3490
0	0.7871	0.4230
1	0.8733	0.4170
11	0.7109	0.3840
12	0.6961	0.3490
13	0.6424	0.2830
14	0.6830	0.3150
15	0.5516	0.2140
16	0.7169	0.3000
17	0.6857	0.3060
18	0.5885	0.2310
19	0.8292	0.4090
2	0.9400	0.3970
20	0.7424	0.2860
21	0.4228	0.2190
31	0.7118	0.3840
32	0.7011	0.3430
33	0.6544	0.2860
34	0.6855	0.3140
35	0.5516	0.2140
36	0.7153	0.3040
37	0.6947	0.3120
38	0.5866	0.2260
39	0.8305	0.4100
40	0.7386	0.2890
41	0.4262	0.2260
5	0.8194	0.4340
6	0.8600	0.4310
7	0.8800	0.3920
A	0.6984	0.4220
B	0.7032	0.4120
C	0.7127	0.3990
D	0.6752	0.4070
E	0.7578	0.3350
F	0.6692	0.3530

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Chain	Atom inclusion	Q-score
H	0.7008	0.3950
I	0.6950	0.3930
J	0.6045	0.3660
K	0.7095	0.3670
L	0.5274	0.4190
M	0.5242	0.3750
O	0.6933	0.3620
Q	0.6239	0.3190
T	0.5633	0.3730
U	0.7083	0.3380
V	0.7640	0.3530
W	0.5375	0.3630
X	0.6255	0.2750
Y	0.5640	0.3240
Z	0.6746	0.3140
a	0.7015	0.4220
b	0.7096	0.4180
c	0.6992	0.3950
d	0.6633	0.4120
e	0.7703	0.3360
f	0.6692	0.3530
h	0.7041	0.3980
i	0.7092	0.3880
j	0.6141	0.3590
k	0.7061	0.3710
l	0.5417	0.4100
m	0.5044	0.3780
o	0.6939	0.3620
q	0.6398	0.3130
t	0.5551	0.3790
u	0.6968	0.3390
v	0.7592	0.3510
w	0.5444	0.3590
x	0.6293	0.2800
y	0.5944	0.3020
z	0.6925	0.3120